

InterPore2022

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Book of Abstracts

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Contents

Image-based Petrophysical Characterization of Porous Media: A Comparative Study of Common Deep-learning-based Denoising Algorithms 1	1
Characterization of Fluid-Fluid Interactions in Heterogeneous Porous Media 6	2
Adjoint-based topology optimization of porous structures 8	3
The numerical solution of the micro-scale phase-field equation and its role in a two-scale two-phase flow model. 9	4
Superhydrophilic porous transport layer enhances efficiency of polymer electrolyte membrane electrolyzers 12	5
Experimental study on silylated polyacrylamide based relative permeability modifiers in porous carbonate gas cores 13	6
Experimental study of drying in the presence of fluorescent particles in model porous media 14	7
GeoChemFoam: an open-source toolbox for pore-scale simulation of complex processes 16	8
Experimental study on production law of fault-controlled type fractured-cavity reservoir 17	9
Dispersion and Retention of Colloids in Saturated Sandstone from the Microscale to the Macroscale 18	10
Characterization of water transport in building porous materials based on an analytical spontaneous imbibition model 20	11
Digital Rock Characterization of Glacial Deposits to Refine Pore Systems 21	11
Multiscale characterisation of gas diffusion in coal 22	12
Impact of hydro-chemical conditions on structural and hydro-mechanical properties of chalk samples during dissolution experiments 25	13
Two-equation macroscopic continuum model for drying capillary porous media: Benchmarking against pore network model simulations 26	14
Second order deviation of permeability due to unresolved morphological features at the pore scale 27	15

Pore-Scale Insights into In-Situ Mixing Control By Polymer-Enhanced Low-Salinity Water-flooding (PELS) 28	17
On the effects of the lithostatic, hydrostatic pressures, and the temperature on Plasma Pulse Geo Drilling (PPGD) 31	18
Numerical simulation of desiccation crack nucleation and propagation by a variational phase-field model 33	19
Chromatographic Effects in Inkjet Printing 34	20
Inkjet printing of surfactant solutions onto thin moving porous media 35	21
Shrinkage-induced cracking in Opalinus Clay: investigation of crack modeling parameters and response in the CD-A experiment 36	22
Two-step diffusion in cellular hygroscopic (vascular plant-like) materials 37	23
Foam plugging performance and flow characteristics in fracture system 38	24
Dynamic Mode Decomposition (DMD) for Analyzing Dynamics in Multiphase Flow in Porous Media 39	25
Extension of the SAFT equation of state to capture the effect of the solid wall into the confined fluid properties: using molecular dynamic simulation 40	26
The swelling and shrinking of a thermo-responsive hydrogel 41	27
Analysis of evaporation and transport of stable water isotopologues in a coupled soil-atmosphere model 42	28
Insights into Upscaling of Modeling of Thermal Dispersion in Geothermal Doublets 43	29
Capillary-number Insights into Mobilization of Oil in Porous Media by Foam Injection 44	30
How simplifying capillary effects can affect the traveling wave solution profiles of the foam flow in porous media 46	31
Upscaling of phase-field models for two-phase flow based on fluid morphology 47	32
Estimating permeability of real-rock micro-CT images by physics-informed neural networks 48	33
Nanoscale visualization of dissolution and precipitation at calcite-oil-brine interfaces upon aging at variable salinity 49	33
Mechanisms driving intermittency in preferential flow paths in porous media biofilms 51	35
Water transfers (imbibition, drying) in cementitious materials followed by MRI (Magnetic Resonance Imaging) 52	35
Challenges for Microfluidic Devices in Representing Flow in Geological Formations 53	37
Three-dimensional Rayleigh-Darcy convection at high Rayleigh numbers 54	38
Predicting and measuring pore-scale capillary pressures associated with meniscus movements during slow imbibition 55	39

Steady State Two-Phase Flow Relative Permeabilities in Microfluidic Devices 56	40
Molecules diffusing and relaxing in macro, meso and microporous materials: An NMR approach for studying the behaviour of fluids confined in nanoporous media 57	41
Agrochemical Transport in Heterogeneous Agricultural Soils 58	42
Use of advanced imaging techniques as a valuable tool to analyze the freeze-drying process in more detail in situ 59	43
Micro-macro models for reactive two-mineral systems 60	44
Elasticity of Liquid Nitrogen in Nanoporous Vycor Glass 61	46
Microfluidics-based analysis of dynamic contact angles relevant for underground hydrogen storage 62	46
Time evolution of biofilm permeability field in porous media and control on fluid flow velocities 63	48
The influence of gas bubble interfaces on the acoustic properties of partially saturated poroelastic media 64	49
An efficient preconditioning framework for the coupled simulation of contact mechanics with hydraulically active fractures 65	51
A micro-scale analysis for wettability characteristics of H ₂ in heterogeneous geological media 66	52
Dynamic Pore-Network Modeling of Solvent Vapour Extraction 68	53
Matrix-fracture flow transfer in fractured porous media: experiments and simulations 70	54
NMR characterization of critical boundary of pore fluid in shale 72	55
Simulation of reactive transport in heterogeneous porous media with a Newton-Krylov method 73	56
Low-field NMR studies to investigate the effects of salinity in the behaviour of brines within porous media. 74	57
Reduced-order model to investigate cell-scale hemodynamics through disordered porous networks of the human placenta 75	58
Three-Dimensional Imaging of Density-Driven Convection in Unconsolidated Glass Packings and Consolidated Rock Samples Using X-Ray CT Scanning 76	60
3D X-ray velocimetry for pore-scale flows in geological and industrial porous media 77	61
From Darcy flow to fingering instabilities in a fluid-driven silo 78	62
Microfluidic model of micro-haemodynamics in porous media 80	62
Particle migration and deposition at the pore scale: Eulerian-Lagrangian approach 81	63
Direct prediction of fluid-fluid displacement efficiency in ordered porous media using the pore structure 82	65

Temperature Dependency of Steady-State Relative Permeability Curves: Aquistore CO2 Storage Site, Canada 84	68
How to design a 3D ordered microstructure for redox flow batteries: A pore network modeling study 85	69
Effects of charring temperature on physicochemical properties of wheat straw biochar 87	70
A phase-field approach to model evaporation in porous media: Upscaling from pore to Darcy scale 88	73
Sol-gel transition in porous media by drying 89	74
Digital Rock Techniques to Study Physical Properties of Hydrate-Bearing Sediments: Considering Hydrate Distribution Patterns 90	75
Cr(III)-entrapped Nanocapsules Obtained via W/O/W Double Miniemulsion Nanoprecipitations of Hydrophobic Polymers for Delaying HPAM Gelation 91	76
Gas Flow Simulation in Multiscale and Multimineral Digital Rocks of Shale Samples 93 .	77
A quantitative study of oil mobilization induced by water diffusion in n-alkane phases: from pore-scale experiments to molecular dynamic simulation 94	78
Impact of Aqueous-phase Ions on Asphaltenic Crude Oil-Water Interfaces 95	79
Molecular Dynamics Study of Carbonated Water Confined in Nano Slit Illite Pore: Effect of the Layer Charge 96	80
A multi-dimensional parametric study of variability in multi-phase flow dynamics during geologic CO2 sequestration accelerated with machine learning 97	81
Simulation of CO2 mineral trapping and permeability alteration in fractured basalt: Implications for geologic carbon sequestration in mafic reservoirs 98	82
Multi-scale reconstruction of porous media from low-resolution core images using conditional generative adversarial networks 99	83
Geometric criteria for the snap-off of a non-wetting droplet in pore-throat channels with rectangular cross-sections 100	84
Data-driven production optimization utilizing multi-objective particle swarm algorithm based on ensemble-learning proxy model 101	85
A novel microfluidic PEM water electrolyzer cell for the study of counter-current two-phase flow at the anode side 102	86
The influence mechanism of pore structural properties on gas hydrate saturation and permeability via micro-CT technology 105	87
Visualizing biofilms within porous media using contrast-enhancing staining agents 106 .	88
Experimental evaluation of percolation in evolution of flow 107	90
Experimental Studies on Permeabilities of Thin Fibrous Materials 108	91

Optimisation and characterisation of a dual porosity medical grade porous medium for personalised inkjet printed dosages applications 110	92
Influence of solute transport and capillarity on bubble evolution in porous networks 111	93
A shrinking pore network model for drying porous media 112	94
Extraction of pore networks from X-ray images of single wood particles subjected to drying 113	95
Pore-scale modelling of non-isothermal reactive transport based on the micro-continuum approach: application to coke combustion in a matrix-fracture system 115	96
Quantitative determination of the threshold pressure for a discontinuous phase to pass through a constriction using microscale simulation 116	97
Lattice Boltzmann modeling of the interfacial mass transport and heterogeneous chemical reaction in the multiphase system: numerical models and applications 117	98
Three-dimensional imaging of pore-fracture propagation in Triassic tight sandstones of the Ordos Basin, Northern China 119	99
Modelling pharmaceutical tablet swelling using discrete element modelling and a single particle swelling model 120	99
Comparison between secondary and tertiary low salinity waterflooding in carbonates: pore-scale processes, wettability changes and recovery 121	101
Open-FOAM simulation and analysis of non-Fickian transport in truncated pluri-Gaussian permeability fields. 123	102
Stochastic inverse modeling of transient core-scale three-dimensional two-phase flows 124	103
Study on laboratory measurement method of anisotropic permeability based on passive differential pressure ratio 127	104
Simulation of interface-coupled porous-medium applications using partitioned coupling methods 128	106
Climate change and primary soil salinization: A global scale perspective for the 21st century 129	107
Upscaling and Automation: Pushing the Boundaries of Multiscale Modeling through Symbolic Computing 130	108
INFLUENCE OF SIO ₂ NANOFUID ON ENHANCED OIL RECOVERY INSIDE A TRANSPARENT MICROPOROUS MEDIA 131	109
Minimal surfaces in gas diffusion layers 132	110
Flow heterogeneity impact on dissolution reaction behavior in geologic porous media 133	111
Initial Yield Surface of Cellular Sheet TPMS Lattices 134	112
Surface-Active Compounds Induced Time-Dependency and Non-Monotonicity in Fluid-Fluid Displacement in Porous Media 135	113

Pore-scale two-phase flow simulation of volcanic gas reservoir based on Volume of Fluid method 136	114
Toward integration of NMR and traditional centrifuge capillary pressure curves: A comparison study 137	115
Enhanced Super Resolution Generative Adversarial Network (ESRGAN) for improving the resolution of micro-CT images 138	116
Relative permeability computations using large Digital Rock Physics simulations 139	118
Characterizing Ice Melting Dynamics in Porous Media with NMR-MRI 141	119
Flower-like Porous Structure for Solar Thermal Distillation and Brine Treatment 142	119
Bubble Dynamics on Hierarchical Porous Nickel Phosphide Electrode for Electrocatalytic Water Splitting 143	120
Direct Solar Membrane Distillation Device with Micro-3D Printed Spacer and Titanium Mesh 144	121
Transport of <i>Sporosarcina Pasteurii</i> in porous saturated sands and applications on soil improvement 145	122
Surface-washing of contaminated porous substrates 147	123
An enhanced branch and bound algorithm for phase stability testing of multicomponent mixtures 148	124
Towards Pore Super Segmentation on Artificially Enhanced SEM Images of Opalinus Clay by Voting Classification 149	125
Investigating the pore scale mechanism of miscible phases mixing in porous medium 2D 150	127
A mathematical model of oil-water spontaneous imbibition with dynamic contact angle in the fractal porous media of tight reservoirs 151	127
Particle-Strength-Exchange methods for Lagrangian 3D DNS of rheological and reactive fluids with evolving interfaces at the pore-scale 152	128
Modeling of Multicomponent Flow in Porous Media using Higher-Order Methods 153	130
Experimental measurement of the heat transfer coefficients for gas flow through granular porous media 154	130
Modeling of spontaneous imbibition in porous media from modified Lucas-Washburn equation 155	131
Wave-induced fluid flow in fractal porous media 156	132
Pore structure characterization and seepage law analysis of tight reservoir 157	133
Effect of grain size and distribution on the two-phase flow at pore scale 158	134
Data-Driven Physics-informed Interpolation Evolution Combining Historical-Predicted Knowledge for Remaining Oil Distribution Prediction 159	135

Multiscale pore structure evolution of shale induced by dilute acid 160	136
Study on the dominant factors of rock permeability 161	137
Hydrate growth and electrical properties modeling based on digital rock techniques 162 .	137
Fractal characterization of time-dependent shape factor for counter-current imbibition in fractured reservoirs 163	138
The degree and law of the influence of microscopic pore structure on permeability in digital rocks 164	139
Microstructural and mineral phase changes of reinforced concrete caused by high concentration CO2 165	140
A fast hybrid method of reconstructing 3D digital rock 166	141
Molecular investigation on sorption-induced kerogen deformation and its impact on gas transport 167	142
3D Microscale Flow Simulation of Newtonian and Shear Thinning Fluids in Sandstone and Carbonate Samples 170	143
The Effect of Power Law Index on Shift Factor for Shear Thinning Fluids by 3D Microscale Flow Simulation 171	144
Characterisation and Comparison of Algal Biochar at Different Pyrolysis Temperatures 172	145
The effect of surface tension and contact angle dynamics in averaged models for two-phase flow at the pore scale 173	146
A Geometry-based Throat Shape Correction of Pore Network Models 174	147
3D Visualization of hydrogen storage in sandstones at reservoir conditions 175	148
A directed network feature for thermal anisotropy of granular materials 176	149
Can we trust computers to analyse pore-scale images? 177	150
Transport and retention of nanoparticles in natural porous media-Effect of pore structure and geometry. 178	151
Performance evaluation on temporary plugging of magnetic responsive hydrogel in hydraulic fracturing of hydrocarbon reservoirs 179	152
Improved micro-continuum approach for pore scale simulation of capillary dominated flow with lower spurious velocities 180	153
A porous media flow model for simulating flow of non-Newtonian bone cement inside a deformable vertebra in the context of vertebroplasty 181	154
Multidirectional gel swelling and drying: a linear-elastic-nonlinear-swelling theory for hydrogels 182	155
Optimization of operational parameters for geological hydrogen storage in a saline aquifer - Sothorn North Sea Case Study 184	156

Micro experimental study on residual oil of marine carbonate rocks during water flooding based on CT scanning 186	157
Study on Flow Mechanism and oil Displacement Mechanism of Microcapsule Polymer in Porous Media 187	158
Evidence of anomalous transport controls on long-term variability in stream water chemistry 188	159
on the deformation of porous medium by pressurized flow 189	160
Pore-Scale Modelling of Hydrogen Transport in Porous Media 190	160
Effect of nanoparticles on the water-soluble polymers flow in porous media 191	161
Trapping dynamics during geological carbon storage: Synchrotron time-lapse imaging of pore-scale capillary trapping events over the centimetre-scale in a heterogenous sandstone. 192	162
Experimental Investigation of Relative Permeability Curves in Oil/water Transition Zone of Tight Sandstone Reservoir 193	164
Novel Fabrication of Microfluidic Devices with Mixed Wettability 195	165
Extraction of three-dimensional pore network and corner network with pores of high aspect ratios 197	166
Potential geological sequestration of CO ₂ in Kazakhstan 198	167
Impact of compression on the properties of the fuel cell diffusion layer 199	168
Film-to-pore filling transition during water adsorption in nanoporous media 200	169
Numerical modelling the hydromechanical behavior of undrained triaxial tests on saturated concrete 201	170
Assessing uncertainties and identifiability of foam displacement models employing different objective functions for parameter estimation 202	171
Experiment and model of multi-scale dynamic diffusivity and permeability for gas(CH ₄ /He) flow in micro-nano pores in series connection of coal 204	172
Image-based physics-constraint workflow for multi-phase flow simulation in heterogeneous media 205	173
μCT investigation of liquefaction mechanisms at the pore scale 206	174
Impact of nano-porous coatings on rates of coupled dissolution-precipitation reactions 207	175
Pollutant dispersion in heterogeneous porous media: On the impact of the heterogeneity of the exchange rate and permeability field in Mobile-Immobile transport simulations 208	176
Imaging fluid transfers in pores and pore changes through dynamic NMR relaxometry 209	177
Microporosity-permeability relationship for complex South East Asia carbonate reservoir 211	178

Efficient Solvers based on Hybrid High Order (HHO) methods for flow simulations in fractured rocks. 212	179
Effect of pore structure characteristics on imbibition recovery of shale with different fabric facies 213	180
Upscaling investigations of dissolution using machine learning and GeoChemFoam 214	181
Bifurcating-Paths: the relation between preferential flow bifurcations, void, and tortuosity on the Darcy scale. 216	182
Feedback mechanisms between precipitation and dissolution reactions across randomly heterogeneous conductivity fields 217	183
Pore scale modelling of stress-dependent permeability and tortuosity of hydrate bearing sediment based on high resolution synchrotron x-ray computed tomography imaging 218	184
Development of a salt-impregnated SAPO-34 porous matrix with graphene oxide for water sorption applications 219	185
Fabrication, Characterization, and Testing of Architected 3D Graphene Foams 220	185
Explicit spatial modeling at the pore scale unravels the interplay of soil organic carbon storage and structure dynamics 221	187
Production and characterization of porous sludge-derived biochar as a sustainable solution for the water industry 222	188
Impact of Novel Nano-particle Solutions on Foam Stability, Wettability Reversal and Interfacial Tension Reduction 224	189
Imaging and chemical analysis of ureteral stent encrustation and incrustation 225	190
Evaluation of saturation of tight sandstones using dielectric logs: Ordos Basin, China 226	191
Absolute permeability of glass bead packs: the first principles agreement between experiment and pore-scale simulations 227	192
Dynamic changes in gas concentration in the sap of plants reiterate the enigma of plant water transport under negative pressure 228	193
Effect of osmosis on spontaneous imbibition of fracturing fluid in shale oil formation 229	194
Development and experimental validation of lattice Boltzmann method-based simulator for vapor transport in air over a moist soil layer 230	195
Numerical Analysis of a Mixed Finite Element Approximation a Model of Biofilm Growth in Porous Media 232	196
Comprehensive Study of Fluid-Fluid Displacement in Mixed-Wet Porous Media 233	197
Wettability alteration in thiolene-based polymers: surface characterization and advanced fabrication techniques 234	198
Governing Forces in Fractured Reservoirs: A Data-Driven Sensitivity Analysis 235	199

Study on the distribution characteristics of in-situ stress of Chang 7 reservoir in Ordos Basin 237	200
Understanding induced seismicity for a safe use of porous media to reach carbon neutrality: the case of the Underground Gas Storage of Castor, Spain 238	202
Characterising flow and transport in fractured geological media: 20 years later 240	203
Modelling liquid transport in PEM fuel cells: The effects of compressive stress 241	203
Coupled flow in porous media with thin inclusions: preconditioning based on rational approximations of the fractional interface operators 242	204
Enhancement of in-situ terahertz liquid front tracking technique in porous media using a novel experimental setup and associated analysis tool 243	206
The influence of Wettability and flow rates on two-phase fluid displacement in porous media: Pore scale experimental visualization and numerical simulations 244	207
Efficient permeability prediction of real digital rock based on Darcy’s law 246	209
Modeling evaporation from leaves 247	209
The role of birefringent strands on the stability of viscoelastic flows through porous media 248	210
Complex Fluids –Thin Porous Materials Interactions revealed via Electrical Impedance Spectroscopy (EIS) 249	211
Flow-direction dependence of upscaled capillary pressure-saturation curve 250	212
3D reactive transport modeling of laboratory-scale CO ₂ injection in limestone leading to wormhole formation 251	214
Salt crystallization at a hydrophobic-hydrophilic interface in quasi 2D layered porous material. 252	215
Structure induced vortices control anomalous dispersion in porous media 256	216
Novel Pore Scale Visualization during CO ₂ Injection into CH ₄ Hydrate Saturated Porous Media 257	217
An improved network extraction algorithm by tracking size variation of throats 259	218
Multimodal geo-dynamic flow characterization in heterogeneous carbonate reservoir: An integrated approach linking static and dynamic behavior 260	219
Elastic flow instabilities in 3D porous media 261	220
Confined phase behavior of a CH ₄ -CO ₂ binary system: molecular simulations, equation of state, and lattice Boltzmann method 263	221
A quantitative study of the effect of pore-scale heterogeneity on MICP in meter-long microfluidic porous media analogues 264	222
A Field-Data Based Numerical Investigation of Factors Controlling CO ₂ Plume Migration in Storage Candidate Sites 265	223

Numerical Investigations on the Dissolution Characteristics of CO ₂ in Fractured Porous Media using Density Driven Modelling 266	224
Coupling porous medium-free flow: Formation and evaporation of multiple droplets at the interface 267	225
Capillary imbibition and swelling of thin paper sheets 268	226
Evaluation of zero-valent iron nanoparticles (nZVI) injection tests in porous media using synchrotron X-ray computed microtomography 269	227
Foam Formation and Flow Diversion in Surfactant-Alternating-Gas Injection in Porous Media Micromodels 270	228
THE EFFECT OF POROSITY AND PORE STRUCTURE ON THE ACCUMULATION OF PARTICLES INTO CELLULOSIC FIBROUS FILTERS 271	229
Experimental basis and numerical modeling for a statistical characterization of multimodal spatial heterogeneity of nanoscale calcite dissolution rates 272	230
How does the presence of an oil phase influence the non-Fickian salt transport during low salinity waterflooding EOR? 274	231
Using In-situ Wettability Measurements to Reconstruct the Wetting Conditions of a Natural Rock 275	232
Heterogeneous nucleation and precipitation on solid surfaces: Experimental observation of calcium carbonate formation on primary and secondary substrates 276	233
Impacts of fractures on hydrodynamic trapping for CO ₂ storage in deep saline aquifers 277	234
Impact of nanopores in clay on accessibility and connected porosity in sandstone samples 278	235
The Method Of Solving incompressible Two-phase Seepage Equation In Porous Media By Deep Neural Networks 279	236
Effect of the connectivity of alluvial aquifers on groundwater flow and solute transport 281	237
Ganglia mobilization by purely elastic instability 282	238
Upscaling of Realistic Discrete Fracture Simulations Using Machine Learning 284	239
Optimization of injection strategies for field-scale leakage remediation using microbially induced calcite precipitation 285	240
Unstable invasion during imbibition in regular porous media 286	241
Optimising Micro-CT Imaging Reconstruction Using Iterative Methods 287	242
Copper leaching in low-grade ore: A reactive-transport modelling study revealing controls on local reactions on mineral surfaces 288	243
CO ₂ degassing kinetics in porous media 289	244
A pore-scale level-set approach to Ostwald ripening of gas bubbles in porous media in the presence of residual oil and water 290	246

Wettability effect on Pore-filling events during two-phase flow 291	247
An experimental study of nonlinear flow behavior in fractured porous media by 3D printing technology 292	248
The Transition from Connected to Disconnected Pathway Flow Regime : Understanding the Combined Effects of Wettability and Flowrate 293	249
Quantifying risks of salt contamination of freshwater aquifers during Aquifer Thermal Energy Storage 294	251
Differentiation in biological porous media: a role for diffusiophoresis and surface instabilities 295	251
Pore-scale modelling of polymeric solutions in porous media 296	252
Some analytical results about countercurrent capillary imbibition. 297	253
A probabilistic approach dedicated to the prediction of the reactive mass transport in porous media 298	254
Machine/Deep Learning Methods for Pore-Mineral Characterization and Surface Areas Analysis 299	255
Probing Multiscale Dissolution Dynamics in Natural Rocks through Microfluidics and Compositional Analysis 300	256
Sherwood number correlation for reverse osmosis membrane systems in turbulent regime 301	257
Morphology Decoder: Untangling Heterogeneous Porous Media Texture and Quantifying Permeability and Capillary Pressure by Semantic Segmentation 302	258
Variation of the representative elementary volume (REV) in heterogeneous rocks with changing CT image resolution 303	263
Modeling and Simulation of Long-term Wettability Alteration on CO ₂ Storage Efficiency and Containment 304	264
Pin-fin shape and orientation effects on heat transfer and fluid flow in gas turbine blade 307	265
A multipoint stress-flux mixed finite element method for the Stokes-Biot fluid poroelastic structure interaction model 308	266
10,000-cubed Digital Rock Analysis: Beyond Hardware Super Resolution Imaging and Efficient HPC Modelling 309	266
Pattern formation in carbonate precipitation in confined geometry 310	267
Investigation of coupled processes in fractures and the bordering matrix via a micro-continuum reactive transport model 311	268
CO ₂ dissolution patterns with precipitation reaction under different permeability 312	269
Pore-scale modeling of the dynamics of interface-coupled dissolution-precipitation 314	271

Evaluation of fluid flow behavior and trapped non-wetting phase saturation with modified pore morphological approach in clastic reservoirs 315	272
A One-domain approach for flow near porous media boundaries 316	273
Parameter estimation for unsaturated flow with an efficient encoder-decoder convolutional neural network 318	274
Gravity shapes permafrost melting after saline water invasion 322	275
Pore network simulation of salt subflorescence growth in a porous medium 323	276
Mobilization erases bubbles' hysteresis in porous media 324	277
Pore level vs. continuum level model for solar thermochemical fuel production 325	280
Marangoni Effect Maintains Fast Evaporation in Near-Fracture Porous Media 326	281
Microplastics Effects on Evaporation Dynamics and Cracking Morphology in Drying Porous Media 327	282
Miscible displacement in near-fracture porous media with non-Fickian Diffusion 328	283
Understanding CO ₂ transport and carbonate formation in portland cement-based materials using X-ray micro-CT 329	284
Microfluidic experiments on constrained oil remobilization induced by water transport in the oil phase 330	285
The Role of Gas Composition on Injectivity in Surfactant-Alternating-Gas Foam Processes 331	286
Study on quantitative identification method for lithology of pyroclastic rock 332	287
The First Experimental Design and Application of Large Horizontal Well Spacing Superheated Steam Flooding for Thin Heavy Oil Reservoir in Bohai Bay 333	288
A Novel Analysis Method for Water Breakthrough Mechanism in an Offshore Heavy Oil Reservoir with Bottom Water 334	289
Pore-scale imaging with measurement of relative permeability and capillary pressure in an altered-wettability limestone with bimodal porosity 336	290
Impact of flow rate on chemical gradients and mixing dynamics in porous media 338	291
Pore-scale Assessment of Spontaneous Imbibition from Layer to Layer 339	292
Extended Allen-Chan phase-field equation for ternary fluid flows and phase-change process in binary fluid flows 340	293
Physics-enhanced Convolutional Neural Networks for Predicting Effective Dispersion in Porous Media 341	295
Consistent Treatment of Shear Failure of Embedded Discrete Fracture Networks Using XFVM 343	295
Autocatalytic reaction-diffusion-advection fronts in radial geometry 344	296

Comparison of Pore-network Simulation and Infiltration Experiment Performed on Coarse Sand 345	297
MODELLING OF FREEZING AND THAWING EXPERIMENTS OF SATURATED SAND COLUMN 346	298
Transition from viscous fingers to compact displacement during unstable drainage in porous media 347	299
Two-phase non-Newtonian flow in porous medium 348	300
Stress and Relax: Hydrogel swelling in a confined granular medium and relaxing after extraction 349	301
Estimation of aquifer permeability using aquifer testing with fiber-optic Distributed Strain Sensing 350	302
Physics-driven interface modeling of multiphase flow in different scale of subsurface fractures 351	303
The Effect of Interfacial Elasticity of a Nanofluid/Surfactant system for EOR through a Visual Micromodel Study 352	304
Multiscale modelling of permeability and effective dispersion coefficient in porous media: a deep learning approach 353	305
Semantic segmentation of rock images and ensemble approach for deep learning methods 354	306
Global sensitivity analysis on a groundwater flow model in a regional- scale with uncertain parameters: a case study in the Middle Magdalena Valley- Colombia. 355	307
Coupled poro-elasto-plasticity of geomaterials: Simulation and validation 356	308
Three-dimensional fractal model of hydraulically fractured horizontal wells in anisotropic naturally fractured reservoirs 357	309
Hydrodynamic instabilities of immiscible fluids in a Hele-Shaw cell 358	310
Reduced order modeling with Barlow Twins self-supervised learning: Navigating the space between linear and nonlinear solution manifolds 359	311
U-FNO - an enhanced Fourier neural operator-based deep-learning model for multiphase flow 360	312
Porous ceria foams coated with Ca-doped lanthanum manganite perovskites for solar thermochemical CO ₂ /H ₂ O splitting 361	313
Pore-scale hydrodynamic and biogeochemical controls on manganese biomineralization in granular media 362	313
Preferential Flow of Emulsion through Homogeneous Porous Media 364	315
Physics Informed Neural Networks for Fluid Flow in Porous Media 366	315
On a workflow for efficient computation of the permeability of tight sandstones 367	316

Modeling of Powder Bed Dynamics in Thermochemical Heat Storage 369	317
The anomalous moisture transport in cementitious materials: causes and models 371 . . .	318
Pore-scale study on convective drying of porous media by the lattice Boltzmann method 372	319
Advanced Digital-SCAL measurements of gas trapping in sandstone 373	320
Adaptive Conservative Time Integration with Higher Order Schemes for Transport in Frac- tured Porous Media 374	321
Dynamic pore-network modeling of compositional flow and nanoconfined phase behavior in shale rocks 375	322
Structure and stochastic dynamics of hydrodynamic flow and transport in three-dimensional random fracture networks 376	323
How the Probabilistic Nature of the Nucleation Process Affects and Controls the Distribu- tion of Mineral Precipitates in Porous Media 377	324
Application of Screen Channel Liquid Acquisition Devices for Phase Separation in Micro- gravity 378	325
Analytical analysis of wettability in hydrogen-rock-brine systems 379	326
Imbibition dynamics in cellular, xylem-like nanoporous media 380	327
On the CO ₂ /caprock interaction based on quantitative image analysis from in-situ x-ray tomography 381	328
Operando Determination of Pore-filling Mechanism and Saturation of PEFC Catalyst Layer using Small-Angle X-ray Scattering 384	329
Modelling Transverse Anomalous Solute Transport in Highly Heterogeneous Porous Media 385	330
A Particle-Tracking Scheme with Adaptive Diffusion for Multiphase Flows in Fractured Porous Media 386	331
Understanding the influence of pore-scale structural heterogeneity in CO ₂ geo-sequestration 387	332
Space-time upscaling of reactive transport in porous media 388	334
Twisting the ensemble Kalman filter with random forest 389	335
Pore scale modeling of the moisture transport in cementitious porous media 390	335
Intrinsic Mobility control by Foam-like Emulsion? 391	336
Dynamic mesh optimisation for efficient density-driven flow simulations 392	337
Capillary Wave Tweezers 393	338
High Precision Saline Intrusion Modelling in Heterogeneous Aquifers using Dynamic Mesh Optimisation 394	339

Direct comparing the permeability derivation from Images: Empirical Modeling vs Physics-Based Simulation vs Deep Learning 395	340
An optimization-based method for upscaling carbonate volumetric image data 396	341
Stylolite detection and image classification from whole core images using convolutional neural networks 397	342
Local wettability characterization of porous media under two-phase conditions using lattice-Boltzmann simulations 400	343
Computational and experimental microfluidics for geosciences 401	344
Test of multi task XGBoost model and its application in Maokou-1 Member, east Sichuan Basin 403	345
Machine learning to accelerate nonlinear solvers applied to multiphase porous media flow 404	346
Reliable and efficient error estimates for nonlinear flow processes using linear iterative schemes 405	347
FEATURES OF THE PORE SCALE REACTIVE FLOW WITH COMPLEX CATALYTIC RE-ACTIONS 406	348
Jaynes Statistical Mechanics Applied to Multiphase Flow in Porous Media 407	349
A New Precise Correlation for Permeability Estimation of Tight Carbonate Rocks Using Mercury Intrusion Porosimetry (MIP) Data 408	350
Geochemical studies of CO ₂ -Brine-Rock interaction at surface and subsurface conditions during geological storage of carbon dioxide 409	351
Electrochemical Actuation in Nanoporous Silicon 411	352
Measuring fluid-solid interfacial area during multiphase flow in a porous medium at different wetting and flow conditions 412	353
Effects of porous media morphology on two-phase fluid displacement and distribution 414	354
The Influence of Imaging Contrast Agents on Emulsification under Flow Conditions 415	355
Multiphysics of Fractured Reservoirs in a Unified Modeling Environment 417	355
Wettability Restoration of Reservoir Rocks: A Comparison between Static and Different Dynamic Methods 418	356
Modeling of the Darcy-Brinkman Equation Indicates Possibility of Deterministic Chaotic Behavior for Flow in Fractured-Porous Media 419	357
Evolution of partially miscible ganglia in porous media: A pore-network approach 420	358
A Hybrid Multiscale Pore Network Modeling Method Applied to Complex Carbonate Rocks 421	359
Digital twin of a laboratory-scale porous medium 422	360

Engineering biofilm hydraulic resistance on the microscale 423	361
NEW INSIGHTS IN POROUS MEDIA CHARACTERIZATION: SPECTRAL COMPUTED TOMOGRAPHY 424	362
Modeling digital twins of grain-based reservoir rocks 425	364
Liquid relative permeability through foam-filled porous media 426	365
Hysteresis in Contact Angle and Interfacial Tension: Implications on Multiphase Flow 427	366
Image-based reconstruction of multiscale porous structures and coarsening of microporosity regions 429	367
Impact of salt on sorption isotherms of water in nanoporous media 432	368
Analysis of Stokes-Brinkman modeling for solute/particle transport in a domain with microporous regions 433	369
Use of semi-automatic deep learning algorithms for the segmentation and classification of cavities in carbonate fault rocks 434	370
Design of a model for the prediction of petrophysical properties from microstructural image data 435	371
Additive Manufacturing of open porous structures: correlation of laboratory testing to simulations for application related properties 436	372
Effect of physicochemical properties and structural heterogeneity on reactive transport in saturated porous media 437	373
Hydro-mechanical coupling to uncover stability and permeability of coated biopore on the pore-scale: the way to improve larger-scale modelling 438	374
Transport of Contaminant Slices under Unfavorable Viscosity Ratio in Porous Media with Dead-End Pores 440	375
Regeneration of granular activated carbon by microwave (MW) irradiation and its application in a novel in situ regenerating permeable reactive barrier (PRB) approach (MW-PRB) 441	376
Fungi-enhanced in-situ bioremediation of NAPL: A microfluidics study 444	377
Phase-wise Conservative and Physics Preserving Algorithms for Porous Media Flow 445	378
Comparison of the Generalized Network Model to Direct Numerical Simulation for Two-Phase Flow 446	380
MCMC Convergence Studies for Flow Problems with Multiscale Sampling 447	381
Fitting correlation-based and neural-network-based relative permeability models to a large dataset of forced and spontaneous imbibition experiments 448	381
Investigation of different clay activation techniques to capture and store carbon dioxide (CO ₂) 449	384
A Review on Polymer Adsorption in Carbonate and Sandstone Reservoirs 450	385

Dynamic X-ray micro-CT measurements of tablet disintegration 451	387
Memory, energy dissipation and hysteresis of two-phase flows 453	389
Absorption of surfactants on porous media: Method development and Numerical prediction of surfactant distribution 454	389
Field-scale Modeling of CO ₂ Injection into Highly Reactive Rocks 456	391
An Uncertainty Quantification Workflow for Naturally Fractured Reservoirs using Proxy Modelling based on Poro-mechanically Informed Flow Diagnostics Simulations 457	391
Study on Microscopic Imbibition process in Variable Diameter Capillary Tubes 458	392
From streamlines to discrete fracture modelling of multi-phase flow and deformation in fractured porous media 459	393
Pore-scale imaging of hydrogen in porous media 460	394
Time and spatial resolved X-ray imaging of wicking in interlaced yarns 461	395
Laboratory scale demonstration of cationic organics removal by graphene oxide nanosheets injection in porous media 462	396
Extension and Uncertainty Modeling of Imbibition Processes using the Morphological Method –a Reality Check 463	398
Experimental Research of Spontaneous Water Imbibition in Oil-Saturated Reservoirs with Ultra-low Permeability 464	399
Water confined in salt crusts: insights from molecular simulations 465	400
Decontamination-induced contaminant redistribution in porous media 466	400
Acute observations into multifractal characteristics of bituminous coals by Qualitative analytics 467	401
Simultaneous Uncertainty Analysis for SCAL Data Interpretation 468	402
Montecarlo simulations of gas transportation in multifractal shale reservoirs 469	403
Improving the Performance of Reactive Transport Simulations using Artificial Neural Networks 470	404
Pore-network modeling of the two-phase flow and transport in the MPL-GDL double layer: model validation and exploration of optimal pore structures 471	405
Digital Rock Physics as a Tool for Upscaling Cores Petrophysical Properties from Pore to Continuum Scale 472	406
On the Challenges of Pore Scale Models to Capture Minerals Precipitation and Dissolution in microfluidic setups: A Combined Computational-Lab-on-a-Chip Approach 473	407
Novel maximum entropy algorithm for multiscale pore network reconstruction and extension. 474	408

Investigating compressible gas flow through porous media considering the choked condition and shockwave formation for Pulse-Pressure Decay test: A Computational Fluid Dynamics (CFD) approach 475	410
Supercritical Adsorption of CO ₂ and CH ₄ on Shales and Surrogate Porous Media 476	411
Coupled Geochemical-geomechanical Processes in CO ₂ Storage Reservoirs 478	412
Numerical Simulation of Multi-phase Flow in Porous Media with a Phase-field Method 479	413
Groundwater contamination in the north-east of the UK: Exploring and projecting pollution trends using the Environment Agency data archives 480	414
Long-term retention and leaching of PFAS in the vadose zone: controlling processes, mathematical formulation, and practical modeling approaches 481	415
A novel platform for monitoring and imaging bacterial biofilm growth in complex structures 482	416
Modeling colloid remobilization during temporal variation in ionic strength in porous media 483	417
Thermodynamics-Informed Neural Network for Phase Equilibrium in Subsurface Reservoirs 484	418
Dynamic Behaviours of Foam Flooding assisted by Newtonian and non-Newtonian Viscosifying Agents in Porous Media 485	419
A Full Order, Reduced Order and Machine Learning Model Pipeline for Efficient Prediction of Reactive Flows 486	420
An image-based hybrid pore network-continuum modeling framework for fluid flow and transport in multiscale porous media 487	421
Adsorption of methylene blue from solution using pomegranate and orange peels powder 488	422
PORE-TO-CORE LINKAGES AND UPSCALING FOR GAS INJECTION (CO ₂ STORAGE, EOR) IN CARBONATES 489	422
Investigating the effect of triple-phase boundary in zinc-air cathodes utilizing pore network modeling approach 490	423
A molecular dynamics study on CO ₂ enhanced shale gas recovery in kerogen nanopores 492	425
Quantification of Heterogeneity of Spatially Averaged Generalized sub-Gaussian Random Fields 493	426
2D Particle Tracking Velocimetry in Multiphase Flow in Porous Media 494	427
Parametric study of coolant-injection flow through different pore geometrical patterns for injection flow control in hypersonic flow 495	427
Solvers for Coupled PDE Problems in Porous Media Science 498	429

PIV and Microfluidic Investigation of recirculation induced reaction hot spots in porous media 500	429
Population Balance Equation for Porous Media: Upscaled Dynamics and Evolution 501 .	431
Viscous, gravitational and capillary forces in 3D experiments with a synthetic porous media 502	432
Microfluidic study of biomass-growth induced changes on hydraulic properties. Investigation of growth characteristics under varying nutrient gas environments. 503	433
Multi-scale Confocal Imaging Approach Applied to Study the Complex Pore Systems in Middle-Eastern Carbonates 504	434
Estimating the structure of a spatially layered media from the radial flow experiments with shear-thinning fluids 505	435
Salt precipitation and its impact on rock porosity –An X-ray micro-tomography study 506	436
Effects of compaction on pore structure and soil hydraulic properties 508	437
Investigation of the corner flow development in porous media in the absence of main front movement 509	438
Pore networks meet computational chemistry: a hybrid approach for studying the flow of fluid mixtures under various thermodynamic conditions in nanoporous materials. 510	439
Improving the efficiency of reservoir simulations with the Multiscale Perturbation Method for Two-Phase Flows 511	441
Inertia and 3D Flow Effects on Mixing and Reaction at Channel Intersections 512	441
Micro-scale Laser-induced Fluorescence Thermometry for Multiphase Flow in Porous Media 513	442
Diffusion of methane and carbon dioxide within flexible kerogen from molecular dynamics simulations 514	443
Characterisation of hydrocarbon bio-degradation in porous media 515	444
Molecular dynamics of a fluid confined in kerogen from memory kernels 516	445
Positive DDFV scheme for degenerate parabolic equations arising from infiltration problem 517	446
Nanoparticle-based suspensions and emulsions for enhanced oil recovery 519	447
Ion composition effect on spontaneous imbibition in limestone cores. 520	448
A new Pore Network stochastic generation approach utilising bulk pore characterisation data with application to mudrocks 521	449
Lagrangian modeling and upscaling of pore-scale transport in random media 524	451
A quadrature-based scheme for numerical solutions to linearized unsaturated flow equation 525	452

INVERSE AND FORWARD UNCERTAINTY QUANTIFICATION OF RELATIVE PERMEABILITY AND FOAM MODEL PARAMETERS FOR EOR PROCESSES 526	452
Wetting/drying mechanisms associated with nanoconfined salt solutions: an optical reflectance study on vapour phase imbibition and adsorption 527	453
Simplified simulation of two-phase flow in karst conduits in carbonate rocks 528	455
A numerical approach to incorporating shear thinning effects of polymer in polymer flooding. 529	456
CO2 storage site characterization using variational autoencoders 530	457
Proppant Transport and Coverage in Rock Fractures –A Computational Modeling Approach 531	457
Thermodynamics of continuum scale immiscible and incompressible two-phase flow in porous media: A statistical mechanics approach using the Color Lattice-Boltzmann model 532	458
Modeling contrast perfusion and adsorption in the 3D heart 533	459
Multiscale mixed domain decomposition methods for the simulation of heterogeneous black-oil flows 535	460
Chemotaxis promoted bacterial transport toward residual NAPL in a dual-permeability microfluidic device 536	461
A macro-scale elasto-thermo-viscoplastic constitutive model for saturated frozen soils 537	463
A One-Dimensional Numerical model of Carbon Corrosion in Catalyst Layers of Proton Exchange Membrane Fuel Cells 538	463
Influence of Pore Morphology on Mechanical Properties of Second Gradient Materials 539	464
Monitoring of Brine Leakage form Carbon Storage in Deep Saline Formations: Method Validation Using Intermediate-Scale Testing 541	465
Laboratory-Scale Investigation of Secondary Sulfate Precipitation in Marcellus and Wolfcamp Shales 542	466
Factors influencing shale wettability from nano to macro-scale 545	467
Reactive Transport Modeling of Dissolution/Precipitation in Fractured Porous Media 546	468
Predictive multi-scale network models with micro-porosity 547	469
Linear lignin as a potential consolidant for archaeological wood treatment: a hybrid Monte Carlo and molecular dynamics study 548	470
Effects of Fluid Saturation on Unsaturated Soil Hydraulic and Solute Transport Parameters 549	471
Numerical investigation of the flow and phase transitions of CO2 near its triple-point during a blowout from a plugged well 550	472
Gold Nanocomposite Contact Lenses for Ocular Health Management 551	473

A Novel Mass Transport Model for Direct Contact Membrane Distillation Flux Prediction 552	474
Direct pore-level multiphysical model for solar thermochemical fuel production reactor based on structured porous media 553	475
Machine Learning for Porosity and Absolute Permeability Prediction from Carbonate Rock Images 555	476
Pore-scale imaging of asphaltene deposition with permeability reduction and wettability alteration 556	477
A Novel Technique to Investigate Effects of Thermal Shocks on Cement for CCS Well In- tegrity 557	478
Multiscale Finite element models with Poromechanics for Myocardial Blood Perfusion 559	479
Optimizing laterite soil bed filters via predictive modelling and simulations 560	480
Deep Learning Accelerated History Matching and Forecasting for Geologic CO ₂ Sequestra- tion 561	481
Tightly Coupled Hyperbolic Treatment of Buoyant Two-Phase Flow and Transport in Porous Media 562	481
Molecular Transport in Nanoporous Gold Thin Films for Drug Delivery Applications 563	482
Coupled Thermo-Hydro-Mechanical-Chemical Analysis of CO ₂ Injection in a North Sea Chalk Reservoir 564	483
The yield surface of reservoir chalk from the North Sea: influence of age, mineralogy and water saturation. 565	484
Quantifying the uncertainty associated with reservoir compaction forecasting: Role of the experimental estimation of the hydrostatic yield stress. 566	486
Pore-scale displacement and trapping mechanisms for underground hydrogen storage 567	487
Optimal control analysis of leakage risk in geological CO ₂ sequestration under uncertain- ties 570	488
Design and Fabrication of 4D Fresnel Lenses for Optical and Thermal Sensing Applications 571	489
Life in a Tight Spot: How Bacteria Swim, Disperse, and Grow in Porous Media 572	490
Modelling & Simulation of Multiphase Flow in Highly Heterogeneous Geologic Porous Media 573	490
Impact of Relative Humidity on the Adsorption of Volatile Organic Compounds by Indus- trial Porous Materials 574	491
Experimental Investigation of Conditions Favoring Enhanced Gas Storage in Shales 575 .	492
Surrogate models for aquifer management 578	493

Measurement of capillary pressure and relativity permeability relations for two-phase air-water cross flow in thin sintered metal wicks 579	494
Application of Lattice Boltzmann Method in Pore-scale Characterisation of Flow Dynamics in Three-Dimensional Porous Medium 580	495
Phase-field modeling and simulation of desiccation-induced cracking 581	496
Adsorption and Transport Behaviors of Shale Oil in Kerogen Slit by Molecular Dynamics Simulation 582	497
Development of Carbon membranes and carbon/CNT membranes for wastewater treatment 583	498
Transport and Multiphase Flow in Porous Media for Electrochemical Technologies 584	499
Ex-situ visualization of wetting dynamics in a microporous layer of polymer electrolyte fuel cells by X-ray computed tomography under water vapor supply 585	500
Hysteresis in Multiphase Flow and Application to Hydrogen Storage 586	501
Polymeric Membranes' Morphology and Water Flow Simulation 588	502
Discrete models, continuum models and scale transitions for the drying of porous media 589	503
Modeling Microbial Enhanced Oil Recovery (MEOR) Optimization Augmented with Formation Damage Mitigation Within Sandstone Core Under Adverse Subsurface Oil-Field Conditions 593	504
The Pulse of Plants 597	505
Lessons from flows through porous media for solving nonlinear hyperbolic problems 598	506
Numerical study of single droplet drying in an acoustic levitator 600	508
Fenton Reaction in Porous Media 603	509
A novel technology to remove co-occurring arsenic and atrazine in the groundwater used for drinking 604	510
Fractal Theory of Porous Media 605	512
Print Quality and Particles: pore-scale simulations of particles/liquid interaction with printing substrate 606	512
Simulation of turbulent mixing in channels with reactive boundary conditions 608	513
Numerical modelling of CO ₂ sequestration in coal-seams based on a parallel hybrid discrete fracture –dual porosity model 609	514
Linking structure and catalytic properties of automotive and heterogeneous catalysts for industrial applications through X-ray nanotomography, scanning electron microscopy and cryogenic focused ion beam microscopy in three dimensions 610	515
Novel techniques in X-ray nanotomography, scanning electron microscopy and cryogenic focused ion beam microscopy Linking structure and catalytic properties of heterogeneous and automotive catalysts in three dimensions 611	516

Experimental Research and Application of Fracture Stress Sensitivity 613	517
Dependence of hydraulic conductivity on effective confining pressure in rocks and concretes 614	518
Capillary sealing efficiency of caprock: Implications for hydrogen and carbon-dioxide geo-storage 615	519
Permeability estimation in the low-porous rock sample using the Navier-Stokes equation at slip and no-slip conditions 616	521
A Potential Energy based Lattice Boltzmann Model for Two-Phase Flow in Fractured Porous Media 617	522
The SOPHIE initiative –The first interlaboratory comparison of the wet end of the soil water retention curve 618	523
Advances in pore-scale characterisation of multiphase flow and transport in porous materials 619	525
Predicting thermal potential of a shallow ground to support design of low-temperature district heating and cooling networks 620	526
Digitizing and Exploring 16 Years of the Registry of Contaminated Sites in the state of São Paulo, Brazil 623	527
Experimental study on porosity and permeability characteristics of unconventional reservoir under overburden pressure 624	528
Supercritical CO ₂ flow and heat/mass transfer in micro/nano-porous structures in CO ₂ geological utilization and storage 626	529
Hysteresis of mass transport in porous media 627	530

MS15 / 1

Image-based Petrophysical Characterization of Porous Media: A Comparative Study of Common Deep-learning-based Denoising Algorithms

Author: Miral Tawfik¹

Co-authors: Amogh Adishesha¹; Yuhan Hsi²; Prakash Purswani³; Russell Johns¹; Parisa Shokouhi¹; Sharon Xiaolei Huang¹; Zuleima Karpyn⁴

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Micro-computed tomography (MCT) and Digital rock physics (DRP) have been at the forefront of geoscience research efforts in recent years as a result of huge advancements in imaging techniques and computing power. This advancement renders the visualization, characterization of petrophysical properties, and simulation of flow and solute transport in intricate permeable media possible. Researchers in many domains that make use of MCT made big strides in the development of machine-learning and deep-learning-based image processing protocols including numerous reconstruction, denoising, and segmentation algorithms. Noise is one of the main MCT artefacts that is inevitable in all micro-CT images. As part of the pre-processing workflow of MCT datasets of geomaterials, denoising is a key step to enable accurate quantitative analyses, including characterization of petrophysical properties such as porosity, permeability, interface curvatures, pore topology, fluid occupancy and phase connectivity. However, denoising is a challenging process due to the tradeoff between minimizing unwanted noise while preserving as much fine details and avoiding the blurring of phase boundaries. Selecting a denoising algorithm, or filter, is an optimization exercise that aims to eliminate or minimize noise while avoiding the loss of data by over-smoothing.

Despite its importance, there are no comparative studies in the geoscience domain that quantitatively assess the performance of the most commonly used denoising protocols, and their effect on image-based rock and fluid property estimates. Moreover, there is very little use of rigorous deep-learning-based denoising algorithms in geoscience applications. In this study, ten filters are evaluated, including the commonly used non-local means filter and the deep-learning-based algorithms such as residual dense network (RDN) and noise-to-noise (N2N). The performance of each filter is qualitatively (visually) assessed and quantitatively evaluated using five metrics: peak signal-to-noise ratio (PSNR), structural similarity index (SSIM), blind/referenceless image spatial quality evaluator (BRISQUE), blurring index (BI), contrast-to-noise ratio (CNR) and phase boundary sharpness. Additionally, the effect of each algorithm on image-based petrophysical calculations is also evaluated, including porosity, permeability, saturation, pore size distribution, pore connectivity, saturation and interfacial curvature. This enables a physics-based evaluation of those algorithms in a geotechnical context as opposed to purely assessing image quality while disregarding how those images are used. The results of this study show that the best denoising algorithm as identified by commonly used denoising evaluation metrics doesn't necessarily map with the best algorithm for petrophysical characterization purposes. It also shows that selecting a denoising algorithm will depend on the properties calculated since there is not one algorithm that performs best for all petrophysical properties.

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Poster / 6**Characterization of Fluid-Fluid Interactions in Heterogeneous Porous Media****Author:** Artur Shapoval¹**Co-authors:** Sheik Sheik Rahman ¹; Mohammed Alzahrani ¹¹ *University of New South Wales, Australia, 2033***Corresponding Authors:** a.shapoval@student.unsw.edu.au, mohammed_khaled_a.alzahrani@unsw.edu.au, sheik.rahman@unsw.edu.au

The two-phase flow of water and oil is accompanied by the emulsification process at the interface between the fluids. The compositions and rate of formation of these emulsions can strongly affect the predicted oil recovery. However, it is a scientific challenge to study and characterise the emulsions formed during the flow in porous media since their properties are not reproducible in ex-situ conditions.

In this work, we have conducted a pore-scale investigation on the formation of in-situ emulsions in heterogeneous carbonate rocks. In addition, the effect of injected water chemistry on the composition and volume of formed emulsions was studied. To achieve that, three experimental sets were completed. In each set, a micro-plug sample was first injected with seawater to model the secondary oil recovery. After that, a brine with modified ionic composition was injected in tertiary mode. A high-resolution μ CT image was captured after each recovery step. Next, we have applied a novel methodology for precise identification of the mixed-phase on images by combining images of a sample saturated with pure fluids (100% water and 100% oil) with rock matrix histogram fitting. At last, we applied the compositional gradient technique to analyse the fraction of oil in the identified emulsion clusters.

The results show that the composition of emulsion is dependent on both rock geometry as well as the initial wetting state. Specifically, in an initially oil-wet sample emulsion is mostly of oil content, while for the mixed-wet sample the composition distribution is more evenly spread between water and oil fractions. Emulsion cluster size has shown a log bimodal distribution both before and after modified water injection. Noteworthy, in each case, injection of brine with modified ionic composition caused the growth of emulsion clusters, which led to improved sweep efficiency and oil recovery. The composition of the emulsion generated during tertiary injection was skewed towards the water content in every case. However, the efficiency of oil recovery improvement was observed to be dependent on the type of brine modification. In particular, the brine with depleted Ca^{2+} content was shown to be the most effective, while a brine enriched with SO_4^{2-} has shown to be the least effective.

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MS22 / 8

Adjoint-based topology optimization of porous structures

Author: Natalie Jüngling¹**Co-author:** Jennifer Niessner¹¹ *Heilbronn University of Applied Sciences***Corresponding Authors:** jennifer.niessner@hs-heilbronn.de, natalie.juengling@hs-heilbronn.de

Conventional filters consist of one or more layers of filter material, which are either woven or composed of tangled fibers. The quality of the separation results almost only from the density of the fiber arrangement. Due to the manufacturing process, compromises between separation and pressure loss that are in the opposite relationship to each other are inevitable.

The possibilities of additively manufacturing filters and the use of numerical modeling and simulation in combination with adjoint-based topology optimization extend the conventional parametric filter media development options. The cross section of conventional fibers is always round. During the adjoint process completely new shapes adapted to the flow and the media used, are generated and then realized by 3D printing. This leads to new fiber geometries with both increased separation efficiencies and decreased pressure drops. The aim of this work is to optimize simultaneously two normally opposing variables by using the complex non-linear relationships between the different separation mechanisms. In a gas-particle system, for example, impaction, interception and Brownian diffusion are the main separation mechanisms.

In numerical modeling and simulation, a flow region is generated and divided into volume elements (meshing). The conservation equations are solved for each volume element. An initial geometry is presented to the flow solver, the adjoint solver calculates the sensitivities depending on a change of the design variables (mesh). The mesh deformation adjusts the generated mesh in the direction of the sensitivities.

The adjoint method is used to determine the effect of a change in the design variable of an objective function. A simple algorithm is introduced that combines both sensitivities of the cost functions (pressure drop and separation efficiency). While the optimization of the pressure loss has been state of the art for a long time, we propose a substitute function for the separation efficiency.

A cost function for the adjoint solver has to be continuously differentiable. Depending on the deposition mechanism, different parts of the surface are responsible for the deposition. These are optimized accordingly. For example increasing the surface normal to the flow direction, the separation efficiency by inertia increases. The resistance coefficients for pressure and shear stress are used as functions to influence the separation performance accordingly. Especially the combination of force coefficients for pressure and pressure loss have been identified as effective for the case considered. A pressure loss of 3.9 % combined with an increase in total filtration efficiency of 2 % could be realized in only one deformation step for a gas-particle system.

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MS07 / 9

The numerical solution of the micro-scale phase-field equation and its role in a two-scale two-phase flow model.

Authors: Manuela Bastidas¹; Sohely Sharmin^{None}; Carina Bringedal^{None}; Iuliu Sorin Pop²

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Porous media are complex domains involving hierarchically organized structures, where various processes take place at different scales. An example in this sense is the fluid flow through the pores of a porous medium and, in particular, the two-phase flow. Prominent real-life applications in this sense are geological CO₂ sequestration or oil recovery.

In [1], a two-scale model for two-phase porous-media flow is proposed. This model includes variable surface-tension effects, depending on the concentration of a surfactant dissolved in one of the fluid phases. A phase field is employed to approximate the freely moving interfaces separating the different fluid phases. By formal homogenization techniques, a fully coupled two-scale model is derived, where the macro-scale parameters are determined by solving micro-scale cell problems, which, on their turn, depend on the macro-scale variables.

Our main challenge is to design a robust numerical scheme for the model, accounting for the coupling between the two scales. We study the macro-scale impact of the micro-scale evolution of the phase-field. Here we center the attention on the phase-field cell problems, which are Cahn-Hilliard type equations. To solve it, we propose a mixed formulation and a robustly convergent linear iterative scheme that is combined with a mesh refinement strategy, improving the efficiency of the algorithm.

References

[1] S. Sharmin, M. Bastidas, C. Bringedal, I.S. Pop, Upscaling a Navier-Stokes-Cahn-Hilliard model for two-phase porous-media flow with solute-dependent surface tension effects. (SUBMITTED), 2021. <https://www.uhasselt.be/Documents/CMAT/Preprints/2021/UP2109.pdf>

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[1] S. Sharmin, M. Bastidas, C. Bringedal, I.S. Pop, Upscaling a Navier-Stokes-Cahn-Hilliard model for two-phase porous-media flow with solute-dependent surface tension effects. (SUBMITTED), 2021. <https://www.uhasselt.be/Documents/CMAT/Preprints/2021/UP2109.pdf>

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Participation:

In person

MS19 / 12

Superhydrophilic porous transport layer enhances efficiency of polymer electrolyte membrane electrolyzers

Authors: Benzhong Zhao¹; ChungHyuk Lee²; Jason Lee²; Kieran Fahy²; Jacob LaManna³; Elias Baltic³; David Jacobson³; Daniel Hussey³; Aimy Bazylak²

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A prominent technology for green hydrogen generation is the polymer electrolyte membrane (PEM) electrolyzer. However, the energy efficiency of PEM electrolyzers must improve dramatically to become economically competitive. Here, we engineer the wettability of commercial porous transport layers (PTLs) to make them superhydrophilic. We find the superhydrophilic PTLs increase the efficiency of PEM electrolyzers by >11% at high current operation (up to 20%). We show via electrochemical analyses and in-operando neutron imaging that the improved efficiency stems from reduced gas saturation in the anode PTL, which significantly decreases the mass transport overpotential. We conduct ex-situ microfluidic experiments and demonstrate that capillary-driven corner flow is a key physical mechanism responsible for the reduced oxygen gas saturation and enhanced liquid water transport. Our findings illustrate the importance of PTL wettability on mass transport in PEM electrolyzers and enable design of next generation electrolyzers with much greater efficiency.

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Poster / 13

Experimental study on silylated polyacrylamide based relative permeability modifiers in porous carbonate gas cores

Author: Liming Qin¹

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Relative permeability modifiers (RPMs) have been utilized for controlling excess water in fractured shales¹. The polymers that are employed as RPMs have the capability of dramatically decreasing water relative permeability with a less impact on gas relative permeability^{2, 3}. In the study outlined within we have aimed to control excess water in low permeability carbonate gas reservoirs using a newly developed silylated polyacrylamide based RPM was verified by core flooding tests under gas reservoir conditions. Prior to experiments, the RPM was prepared according to our previous study⁴. As shown in Figure 1, silylated chains in the RPM performs as a part of adsorbing onto rock surfaces via surface functionality and polyacrylamides with long chains act as a role of decreasing excess water in carbonate porous rocks.

Representative carbonate samples were selected for core-flood analysis including an Indiana limestone sample which was achieved through consecutive injection of brine and gas under reservoir conditions (1300psi and 60°C). SEM measurements showed that amorphous polymers were present on the pore surfaces and adhered onto calcite crystals at a high magnification ratio as indicated in Figure 2a. The residual resistance factor to brine (RRF brine) and residual resistance factor to gas (RRF gas) was 10.33 and 2.5 respectively. The disproportional reduction ratio (RRF brine/ RRF gas) was 4.13, showing a higher reduction of water production with a less impact on gas relative permeability. After performing history match of brine production and differential pressure by Sigmund McCaffery correlation⁵, the out profile of simulated brine production and differential pressure was generated and relative permeability correlated with water saturation was calculated as well. As shown in Figure 2b, the results indicate that relative permeability curves after the RPM treatment moved to the right side as a whole and the crossover point dropped as well, implying the higher reduction of relative permeability to brine. In addition, the irreducible water (Sir) increased due to the existence of adsorbed water by the polymer in the porous cores. However, the relative permeability to gas presented a minor change, indicating a less effect on gas production.

This novel silylated polyacrylamide based RPM can provide a potential solution to mitigating excess water in carbonate gas reservoirs and present a significant application in gas fields.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS11 / 14

Experimental study of drying in the presence of fluorescent particles in model porous media

Authors: Elisa Ghiringhelli^{None}; Manuel MARCOUX¹; Marc Prat^{None}¹ *Institut de Mécanique des Fluides de Toulouse***Corresponding Authors:** mprat@imft.fr, manuel.marcoux@imft.fr, elisa.ghiringhelli@imft.fr

The motivation for the present study stems from visualizations of the PTFE distribution in the gas diffusion layer (GDL) of Proton Exchange Membrane Fuel Cell (PEMFC). The GDL is a fibrous carbon layer treated with polytetrafluoroethylene (PTFE), by drying a layer saturated with a solution of PTFE particles, to improve hydrophobicity [1, 2, 3]. During the fabrication, internal surfaces appears to be hardly covered homogenously causing a mixed wettability in the medium, indeed it is showed in [4] that PTFE distribution strongly depends on evaporation conditions. In this context, the objective of the present work is to study the pattern formed by fluorescent particles (1 μ m) in porous media after the evaporation of the water, in different geometries and for different initial conditions, starting from a single pore before moving to a pore network.

The first step was to use a transparent material, the SUEX resin, to make the porous medium, filling it with a solution of fluorescent red particles and let it dry at constant temperature and humidity. With this type of particles, it is possible to follow their position during evaporation, compute the velocity field and relate it to the final deposit. The water flow during evaporation and the pattern of deposited particles are observed under a microscope using a confocal green source. In the picture below, the particles are bright in the image on the left. In the channel on the right, a white light source allows to visualize the pure water case with no particles.

We can notice that the evaporation kinematics is slowed down by the presence of the particles, this is due to their effect on the thickness of the corner films visible in Fig.1. They are thicker with pure water than in the presence of particles, which results in smaller vapour partial pressure gradients in the channel entrance region.

The experiment also indicates that the evaporation of the residual liquid films at the very end of the drying process do have an impact on the final particle deposit. This dynamic can be observed in the double channel experiment as well (Fig.2). In this case, a high concentration of deposited particles

occurs not only at the entrance of the smaller channel where the main meniscus does not recede but also in the entrance region of the larger channel due to the effect of the corner films.

The next step is to study the deposit of particles at a greater scale with a model porous medium as in the Figure 3, where the particles are dark. This experimental set-up will allow us to explain how the liquid moves during drying, thanks to the tracking of particles, how the liquid displacement influences the particle deposition. This will help to establish drying procedures leading to improved GDL's hydrophobicity properties for better fuel cell operation.

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References:

- [1]Tatsumi Kitahara &al. Journal of Power Sources, 2010.
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS09 / 16

GeoChemFoam: an open-source toolbox for pore-scale simulation of complex processes

Author: Julien Maes¹

Co-authors: Hannah Menke²; Sebastian Geiger

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² *Imperial College London*

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Pore-scale modelling is now routinely employed to investigate a wide range of applications such as carbon capture and storage, hydrogen storage, fuel cells, geothermal energy and enhanced oil recovery. Computational Fluid Dynamics (CFD) software such as OpenFOAM, Comsol and Fluent are great tools to investigate these applications by simulating simple processes, such as single-phase flow, multiphase flow or scalar transport, directly in micro-CT images of porous media. However, extending these workflows to more complex processes that include additional coupling relevant to porous media applications such as the link between multiphase flow and geochemistry, requires additional development. Many numerical models and codes have been developed in the literature, but they are often close-source and restricted to one application. The GeoChemFoam project aims at gathering such development into one open-source toolbox that can be used by the wider community. Our objective in presenting the toolbox is to increase our number of users and foster collaborations. GeoChemFoam can be installed and run directly from the source code for the OpenFOAM expert, or using Jupyter notebook on a docker container, so that pore-scale modelling of complex processes

can be accessible to any porous media researcher. The capabilities of the code are aimed to grow but they currently include reactive transport, multiphase reactive transport, phase transfer, heat transfer, mineral dissolution and precipitation, and single-phase flow in multiscale porous media. Our objective is that the next developments are driven by the community and done collaboratively between our institute and new partners.

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Poster / 17

Experimental study on production law of fault-controlled type fractured-cavity reservoir

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Due to multi-stage tectonic movement and dissolution, many fractures and caves are dispersed in the fracture-cavity reservoir. According to reservoir characteristics and formation reasons, fracture-cavity reservoirs can be divided into weathering crust, fault-controlled, and underground river types. The fault-controlled type is the most difficult reservoir to develop, divided into the karst cave and large fracture-cavity system. This paper constructs and manufactures two physical experiment models according to the geological models and sections through CAD design and 3D printing technology. Aiming at low recovery in fault-controlled type fractured-cavity reservoirs, the production law experiments under various production modes were carried out to study the oil displacement effect in different production stages. The results showed that cyclic water injection and gas huff and puff could effectively relieve but not eliminate bottom water coning. In addition, in the karst cave system, the effect of gas huff and puff is better than cyclic water injection. However, in the large fracture-cavity system, the increase in recovery is low if only gas puff and huff were carried out; it must be combined with water flooding. The crude oil close to the production well is the easiest to be displaced, and it is easy to form a dominant flow channel, so it is necessary to control profile plugging and increase well control reserves. This study provides support and guidance for the development of fault-controlled type fractured-cavity reservoirs.

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Online

MS08 / 18

Dispersion and Retention of Colloids in Saturated Sandstone from the Microscale to the Macroscale

Authors: Dian Fan¹; Emily Chapman²; Ronny Pini²; Alberto Striolo³

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Transport of suspended colloids in heterogeneous porous media is a multi-scale process which systematically exhibits preasymptotic behaviors that cannot be captured by the Fickian dispersion theory. Although many studies have documented and quantified mechanisms of colloid transport, they often lack a theoretical basis that links particle- to continuum-scale observations. The experimental observations of preferential deposition of colloids on various pore surfaces, as well as colloids' dispersion in heterogeneous flow fields should be responsible for the preasymptotic behaviors.

To fill this knowledge gap and test our hypothesis, we implement here a multi-scale approach. We compare residence time distributions (RTDs) of solutes and colloidal particles in a heterogeneous media –sandstone sample –and its digital twin, by using core-flooding experiments, core-representative elementary volume-scale numerical simulations, and kinetic theories.

We achieve agreement across the multiple scales of our multidisciplinary investigation. Based on this agreement, we show that the observed preasymptotic transport is particle-type dependent and stems from particles' dispersion in heterogeneous flow fields as well as from their deposition on pore surfaces due to electrostatic interactions. A general RTD formulation is derived that encompasses the full set of observations and enables investigations of a full transition from preasymptotic to asymptotic behaviors.

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Poster / 20

Characterization of water transport in building porous materials based on an analytical spontaneous imbibition model

Author: Mingliang Qu^{None}

Co-authors: Shengyue Lu ; Qingyang Lin ¹; Sajjad Foroughi ²; Zitao Yu ; Martin Blunt ³

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Spontaneous imbibition controls the movement of water into natural and engineered porous such as building and construction materials, including stone, concrete and cement. We measured the sorptivity –the imbibition rate –for a homogeneous Bentheimer sandstone for both initially dry and wet conditions for three replicate experiments and matched the measurements to an analytical model to determine the wetting phase (water) relative permeability. We suggest that using imbibition rate is a robust, quick and accurate way to estimate water relative permeability, for it avoids uncertainties inherent in traditional steady-state measurements. Furthermore, this then allows a complete mathematical treatment of imbibition, to predict the saturation profile as a function of time and the sorptivity for different rock and fluid properties.

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MS09 / 21

Digital Rock Characterization of Glacial Deposits to Refine Pore Systems

Authors: Ivan Deshnenkov¹; Paul Tarabbia ¹; Aqeel Khalifa¹

¹ *Saudi Aramco*

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This paper presents the results of the pore system digital characterization of glacial Upper Paleozoic clastic rocks in Saudi Arabia by employing high-resolution X-ray microscopy (XRM) and digital rock analysis workflows. Glacial sediments in this study are essentially devoid of clays and have undergone a complex burial history that manifests itself as a composite pore system. The objective of this study was to carry out detailed scans of selected plugs to better understand reservoir properties, i.e., porosity, permeability and pore throat sizes distributions.

Careful sample selection of representative facies was based on the screening of associated petrographic thin-section scans and X-ray diffraction mineralogy data of the main geological units. The digital rock physics (DRP) workflow deployed in this study includes high-resolution (10 microns) scanning of the rock samples with XRM, segmentation of the tomograms to identify pores and grain fabrics, building the pore network model and calculation of petrophysical properties. This workflow was used, not only to predict rock properties, but also for the spatial distribution of the rock features and pore network assemblages causing these properties. The end products of the workflow were verified with conventional core analysis data.

XRM revealed that grain dissolution vugs were fairly common in the bulk of the plugs, with very few clues of these features found on visual inspection on the surface of the plug. A feature of the vugs that could only be extracted from the MicroCT images were that they usually appeared flattened or deformed, but display well formed edges of the precursor clasts. This suggests induration of sediment before dissolution of clasts. The DRP demonstrated that the plugs exhibiting vuggy porosity are free of cement and have better porosity and permeability that make vuggy intervals prioritized exploration and development targets as they would contribute to extra storage capacity in zones where they occur. Fine grained sections of the plugs were associated to glacial flour which is an indicative texture and brings with it an influx of heavy minerals. This study was able to supply evidence of how the stratigraphy could be resolved using XRM.

As the glacial flour is made up of fine particles, these particles may be mobile when a well is put on production, which may reduce permeability and cause productivity issues. Identification of the glacial flour helps to refine well testing and production mechanisms. As yielded by DRP, vugs associated with studied rocks may also be a way of distinguishing glacial sediments, and impact storage capacity of the formation.

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Time Block B (14:00-17:00 CET)

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Multiscale characterisation of gas diffusion in coal

Authors: Yu Jing¹; Lkhamsuren Baatar¹; Meng Yuan¹; Peyman Mostaghimi¹

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Coal is not only a combustible sedimentary rock, but also a source rock for coal seam gas (CSG). It is typically a dual porosity medium, consisting of fractures and porous matrix. Gas flow in coal matrix is under concentration gradient, which is characterised by diffusivity. It is a controlling factor for both CSG production and the gas drainage process in coal mining industry. Therefore, experimental and modelling study of gas diffusion in coal is of great significance.

Common experimental methods to measure diffusion coefficient include particle method and courterdiffusion method. In this work, we apply the courterdiffusion method, as it can measure the bulk sample, while particle method requires the sample to be crushed into particles to eliminate fractures and mesopores. During the test, two gas chambers of 100% helium and 100% methane with the same pressures are connected to each side of a coal sample. Courter diffusion process is initiated due to the concentration difference. After different diffusion times, the gas concentrations of two gas chambers are measured. Applying Fick's first law, diffusion coefficient can be calculated. In addition, the test is conducted using krypton gas and helium gas. Since krypton, similar as methane, has high X-ray attenuation values. So, under X-ray micro-CT imaging, the krypton diffusion process can be visualised, where coal matrix with different krypton concentrations will present different greyscale values in the micro-CT images. Gas diffusion in coal is then modelled by a multicomponent gas diffusion model with dual-continuum modelling approach.

In this work, time-dependant diffusion coefficients of bulk coal samples can be studied. The gas diffusion process is modelled and validated with micro-CT images. The obtained true diffusion coefficient can be applied to in a wide range of areas, such as CSG development, gas drainage design and greenhouse gas emission estimation in coal mining.

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MS23 / 25

Impact of hydro-chemical conditions on structural and hydro-mechanical properties of chalk samples during dissolution experiments

Authors: Delphine Roubinet¹; Linda Luquot²; Marie Leger³

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The importance of karst reservoirs for water resources, and their complexity in terms of structural properties and hydraulic responses, require a better understanding of the formation and location of conducts in these systems, in particular for chalk reservoirs. For this purpose, we conduct laboratory experiments of acid solutions injection in chalk core samples using a homemade experimental device. Three different flow rates and two acid concentrations are applied on six samples at atmospheric conditions with Peclet numbers around 1 and low Damköhler numbers. Hydraulic and chemical measurements are carried out during the experiments, while petrophysical characterization is conducted on the samples before and after the reactive percolation experiments. The analysis of these data shows an increase in permeability of the rock samples due to calcite dissolution, which is associated with the creation of preferential conducts. We also observe that the initial structural properties control the dissolution regime with the following main conclusions. For homogeneous systems, the overall dissolution rate and percolation time are directly linked to the considered flow rate and injected acid concentration. For heterogeneous systems, (i) pre-existing large-scale structural heterogeneities control the location of newly created paths while reducing the value of the dissolution rate, and (ii) micro-scale heterogeneities result in highly heterogeneous general structures, which are responsible for channels formation while applying low Damköhler numbers.

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Poster / 26

Two-equation macroscopic continuum model for drying capillary porous media: Benchmarking against pore network model simulations

Authors: Faez Ahmad¹; Marc Prat^{None}; Evangelos Tsotsas^{None}; Abdolreza Kharaghani²

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In this work, a two-equation macroscopic continuum model (CM) is developed that accounts for the local non-equilibrium mass transfer in a drying capillary porous medium. The two-equation CM is based on the volume averaging method and the formulation is formally derived from the upscaling of the pore-scale mass conservation equations of the liquid and vapor phases, where the respective state

variables are the saturation and partial vapor pressure. The vapor transport is driven by diffusion in the gas-side boundary layer and in the gaseous pore space, while liquid flows due to the viscous capillary effects induced by evaporation. The two equations are coupled by a source/sink term that characterizes the local non-equilibrium mass transfer between the respective phases. Within the framework of the volume averaging method, mass transport at the medium surface is also modeled by considering the individual boundary conditions for the two continuum model equations. The results of the two-equation CM are compared with pore network model predictions. The macroscopic parameters of the two-equation CM (i.e. effective liquid diffusivity, effective vapor diffusivity and specific interfacial area) are determined heuristically using pore network simulations as a guide. The results indicate that the newly developed two-equation CM captures the non-local equilibrium effect and it reproduces with a good degree of accuracy the phase distributions and drying kinetics predicted by the benchmark pore network model drying simulations.

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MS14 / 27

Second order deviation of permeability due to unresolved morphological features at the pore scale

Authors: Sarah Perez¹; Francisco J. Valdés-Parada²; Didier Lasseux³; Philippe Poncet¹

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² *División de Ciencias Básicas e Ingeniería, Universidad Autónoma Metropolitana-Iztapalapa, Mexico*

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Pore-scale dynamics of one phase flow commonly involves adherence (no-slip) boundary conditions at the fluid/solid interface. However, improved modeling such as flows at moderate Knudsen numbers (i.e. for values below 0.1), or homogenization of rock matrix roughness, may require slip conditions [1,2]. It turns out that a lack of knowledge on the rock matrix wall, built by X-Ray micro tomography, leads to the same type of slip conditions

$$v = \frac{\beta}{2}(I - nn) \cdot (\nabla v + \nabla v^T) \cdot n$$

where v is the pore-scale velocity, n is the unit normal vector oriented towards the fluid and β is twice the slip-length.

The macroscopic model corresponding to steady one-phase flow in the creeping regime (Stokes equations) at the pore-scale with the slip condition was derived in [1, 2]. The macroscopic momentum equation corresponds to Darcy's law in which the permeability tensor is slip-dependent. This leads to a computation of an apparent permeability that depends on β and that we denote K_β . This apparent permeability can be expanded in a power series of a Knudsen number, the zeroth-order term identifying to the intrinsic permeability with no slip and the higher order terms to slip-correction tensors, the first one generalizing, for an ideal gas, the classical Klinkenberg correction. All the tensors are given by the solution of coupled closure problems at the successive orders [2]. While this expansion has been addressed in [1] and [2] and used in the case of synthetic geometries, it has been used in large three-dimensional real geometries in [3] in the context of isotropic permeability, that is to say $K_\beta = \kappa_\beta I$ where κ_β is a scalar. In this last case, the expansion

$$\kappa_\beta = \kappa_0 + \beta\lambda_1 + \frac{\beta^2}{2}\lambda_2 + \mathcal{O}(\beta^3)$$

is shown to describe the uncertainty on the permeability values that results from the gray scale uncertainty generated by micro-tomography.

The coefficients λ_k , capturing this uncertainty estimation, are given by the solutions of the Stokes-like closure problems reported in [2] by formal expansion (from averaged equations) and re-established in [3] by asymptotic analysis (two-scale homogenization). They satisfy a non-homogeneous Dirichlet boundary condition (prescribed velocity) at the pore walls, whose value involves the immediate lower order slip momentum.

While the first order of this expansion has been detailed in [3], its second order estimation is provided for the first time in this presentation for operational 3D geometries: we apply our results to the high resolution rock sample studied in [4] and show that the second order brings a significant improvement of the uncertainty estimation on the absolute permeability. These results in a real geometry confirm what was anticipated in [2] for simplified 2D geometries and are relevant as they show the importance of slip at the macroscale.

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References:

- [1] D. Lasseux, F.J. Valdés-Parada, J.A.O. Ochoa Tapia and B. Goyeau, A macroscopic model for slightly compressible gas slip flow in homogeneous porous media, *Physics of Fluids* 26(5), 053102, 2014. doi:10.1063/1.4875812.
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Time Block B (14:00-17:00 CET)

Participation:

In person

MS11 / 28

Pore-Scale Insights into In-Situ Mixing Control By Polymer-Enhanced Low-Salinity Waterflooding (PELS)

Author: Hassan Mahani¹

Co-authors: Mohammadreza Poshtpanah¹; Behzad Rostami²

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Physical dispersion and in-situ mixing of brines during low-salinity waterflooding (LSWF) occurs due to the unfavorable mobility ratio between high- and low-salinity brines. Dispersion negatively affects the performance of miscible processes, such as LSWF, and their economic viability. In our previous publication (Darvish Sarvestani et al., *Energy & Fuels*, 2021), we demonstrated that adding a viscosifying agent like polymer to the injected low-salinity brine can be an efficient solution to overcome this challenge and suppress the mixing of brines. Adding polymer alters the mobility ratio (between the injection brine and the resident brine) toward a more favorable state and improves the displacement front integrity throughout the porous media. This study focuses on the pore-scale investigation of physical dispersion during LSWF in absence/presence of HPAM (partially hydrolyzed polyacrylamide) polymer. Using purpose-built micromodels with special design of inlet and outlet sections, a series of single-phase mixing experiments was performed and the impact of polymer concentration, injection rate and degree of heterogeneity of porous medium on salt dispersion were studied. The high-resolution images captured during the tests were analyzed for quantitative determination of the salinity breakthrough curves, the length of mixing zone length, the breakthrough time and the effective dispersion coefficient (using advection-dispersion theory). The results show that adding only 250 ppm of HPAM reduces the salt dispersion by up to 62%. A higher dispersivity reduction can be obtained by adding a further amount of polymer. In absence of polymer, non-uniform salinity transport and fingers of low-salinity brine into the high-salinity brine were clearly visible. By adding polymer, the mobility ratio became favorable, thus fingering was suppressed, the displacement front became sharper, and the breakthrough time of the injected low-salinity brine was delayed. It was also found that higher injection rates negatively affects the mixing control. Increasing the injection rate from 0.5 ml/hr to 1.0 ml/hr reduced the Peclet number by up to 28%. Increasing heterogeneity of porous medium increased the salt dispersivity by up to 41% depending on the polymer concentration. This can be compensated for by increasing the polymer concentration. The results of this study provides novel pore-scale insights into the mixing control by polymer-enhanced low-salinity brine (PELS) and supports the our previously published results at the core-scale. The results imply that the performance of LSWF can be improved and a lower pore-volume of low-saline brine would be required to establish low-salinity condition in the porous medium.

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References:

1- Darvish Sarvestani, A., Rostami, B. and Mahani, H., 2021. Polymer-Enhanced Low-Salinity Brine to Control In Situ Mixing and Salt Dispersion in Low-Salinity Waterflooding. *Energy & Fuels*, 35, 13, 10540-10550. <https://doi.org/10.1021/acs.energyfuels.1c00871>

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS17 / 31

On the effects of the lithostatic, hydrostatic pressures, and the temperature on Plasma Pulse Geo Drilling (PPGD)

Author: Mohamed Ezzat¹

Co-authors: Jascha Börner²; Daniel Vogler³; Wittig Volker⁴; Martin O. Saar³

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Geothermal energy is, in principle, a limitless energy resource that exists everywhere. Geothermal energy can be used as a baseload power source (i.e., it is available at all hours of the day throughout the year) or as a dispatch power source (i.e., it can support other intermittently available energy sources, such as wind and solar, by providing power when there is no wind or sunshine). However, producing heat or generating electricity from geothermal reservoirs, employing so-called “advanced”[1] or “enhanced”[2] geothermal systems, requires deep drilling into rock layers (i.e., crystalline basement) that exhibit temperatures $\geq 150^{\circ}\text{C}$ [3]. For example, drilling to depths of 5 km is required in Europe to reach the required temperatures ($\geq 150^{\circ}\text{C}$), given that the geothermal temperature gradient is typically $\approx 30^{\circ}\text{C}/\text{km}$.

Drilling costs, particularly into crystalline basement rock, can contribute up to 80% of the total investment required for a geothermal power plant when using mechanical rotary drilling, which can render such power plants uneconomical. High drilling costs can be attributed to long tripping times, which is the time spent replacing worn or damaged drill bits once the often short lifetime of a drill bit has been exceeded. Contactless drilling methods, however, do not rely on mechanical abrasion, thereby eliminating mechanical abrasion and extending the lifetime of the drill bit[4–7]. Plasma Pulse Geo Drilling (PPGD) in particular uses high voltage pulses that last for a few microseconds to fracture the rock[8–12]. During PPGD, two electrodes transmit these pulses to the rock surface, inducing plasma formation inside the rock pores, increasing the pore pressure, exceeding the rock tensile strength, and causing rock fracturing. Under ambient conditions, PPGD has proven to be cheaper than mechanical rotary drilling, and further research and development could reduce the cost by 90%, compared to rotary drilling costs[3,13]. Nonetheless, no experimental work on PPGD drilling investigates deep well pore conditions, i.e., high lithostatic pressures, hydrostatic pressures, and temperatures.

This study aims at understanding the effect of the aforementioned conditions on the following five parameters: (1) PPGD performance (i.e., excavated rock volume per electric pulse); (2) Specific excavation energy (i.e., required energy to excavate a unit volume of the rock); (3) Cutting size (i.e., rock fragment size resulting from PPGD drilling); (4) Relative penetration depth (i.e., the penetration depth per unit inter-electrode gap distance); and (5) Pre-damage phase of the PPGD process.

The experimental design uses a bi-axial cell that can apply lithostatic pressure of up to 150MPa (i.e., simulating 5 km deep conditions) on a granite specimen (Figure 1a). Deionized water immerses the entire experiment setup, i.e., simulating the drilling fluid. Next, a few dozen electric pulses of 200kV, with rise-times shorter than 0.5 microseconds, are applied to the specimen. To investigate the effect of hydrostatic pressure and of temperature, rock specimens are placed in the so-called i.BOGS autoclave (Figure-1b). Pressures up to 50 MPa and temperatures up to 80°C can be reached in the

i.BOGS. The results of these experiments shed light on the viability of the PPGD process as a deep drilling technology and highlight the key factors driving PPGD drilling success.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

Numerical simulation of desiccation crack nucleation and propagation by a variational phase-field model

Author: Keita Yoshioka¹

Co-authors: Tuanny Cajuhi²; Thomas Nagel³; Olaf Kolditz⁴; Wenqing Wang⁴

¹ *Helmholtz Centre for Environmental Research*

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³ *TUBAF*

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Clay formation is a prominent candidate for barrier rock in radioactive waste management. Thus we must assess its integrity (or lack thereof) under varying conditions such as drying around excavations or heat sources. As the porous rocks dry, the moisture gradient alters the effective stress and may initiate cracks at the exposed surface. Unlike cracks driven purely by mechanical loading, desiccation cracks can form in a geometrically complex pattern. When one of the drying material's dimensions is much larger than the other, cracks tend to develop parallel to each other. Otherwise, a more complex, polygonal crack distribution may develop. Although material heterogeneity contributes to crack nucleation and complexity, we also observe complex cracks in a dried homogeneous plaster.

When stress concentration is not clearly present such as for cooling or drying cracks, the classical fracture mechanics framework struggles to determine the crack initiation and propagation path. To overcome these challenges, a variational approach, also known as a phase-field model, for fracture has been proposed and successfully applied to simulate complex fracturing including desiccation cracks without prescribing heterogeneities in the domain. However, as phase-field modeling of desiccation crack is still at its infant stage, there are various and ambiguous ways to treat crack nucleation or define the effective stress.

In this study, we compare several available phase-field models implemented in an open-source code, OpenGeoSys, in terms of crack nucleation and propagation. We investigate the model in two- and three-dimensional settings and the influence of the material properties. We find that, unlike some reported studies, crack nucleation induced by drying does not need to be instigated by material heterogeneity or mesh irregularity, but shows a dependency on the chosen phase-field model. We also show that the onset of crack is largely dependent on the definition of the effective stress, which couples the hydraulic, mechanical crack fields, and on the choice of the phase-field model. Furthermore, we discuss the application of the phase-field model in experiments at larger spatial and temporal scales.

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Poster / 34

Chromatographic Effects in Inkjet Printing

Authors: Gianmarco Venditti¹; Vignesh Murali¹; Anton Darhuber¹¹ *Eindhoven University of Technology***Corresponding Authors:** a.a.darhuber@tue.nl, g.venditti@tue.nl, v.murali@tue.nl

We have studied the chromatographic separation of solvents and dyes after deposition of a dye solution on a paper substrate. Due to their larger molecular size, dyes typically exhibit a stronger interaction with the paper constituents. Consequently, the imbibition process of the dye is usually delayed compared to that of the solvent. This impacts the achievable resolution and color homogeneity in inkjet printing. We present experiments and a comprehensive numerical model to illustrate and quantify these effects. The model accounts for the solvent evaporation, heat transfer, multi-component unsaturated flow, and dye adsorption, as well as the presence of permeable fibers in the paper substrate. We identify the key parameters that can be tuned to optimize the pattern fidelity of the printing process.

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Langmuir 37, 11726–11736 (2021)
<https://doi.org/10.1021/acs.langmuir.1c01624>

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS16 / 35

Inkjet printing of surfactant solutions onto thin moving porous media

Authors: Gianmarco Venditti¹; Vignesh Murali¹; Anton Darhuber²¹ *TU/e*² *Eindhoven University of Technology***Corresponding Authors:** v.murali@tue.nl, a.a.darhuber@tue.nl, g.venditti@tue.nl

We have studied the combined imbibition and evaporation of surfactant solutions into thin porous media by means of experiments and numerical simulations. Solutions of anionic and non-ionic surfactants were deposited onto moving sheets of paper by a droplet-on-demand inkjet system. Optical transmission imaging and infrared thermography were used to monitor their lateral transport and

evaporation. Moreover, we propose a theoretical model based on a dual-porosity approach that accounts for moisture and surfactant transport in both the pores and the fibers of the paper sheets as well as for surfactant adsorption. The numerical simulations reproduce the experimental data qualitatively well.

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Colloids and Surfaces A: Physicochemical and Engineering Aspects, Volume 634, 5 February 2022, 127832
<https://doi.org/10.1016/j.colsurfa.2021.127832>

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS03 / 36

Shrinkage-induced cracking in Opalinus Clay: investigation of crack modeling parameters and response in the CD-A experiment

Author: Tuanny Cajuhi¹

Co-authors: Keita Yoshioka ; Gesa Ziefle ¹; Jobst Maßmann ¹; Thomas Nagel ²; Wenqing Wang ³

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The long-term storage of heat-generating radioactive waste requires enhanced material and process understanding of potential host rocks such as clay. Opalinus Clay formations are intensely researched in the laboratory- and field-scale experiments. In the Mont Terri Rock Laboratory in Switzerland, the strongly coupled hydro-mechanical behavior of Opalinus Clay is investigated in the field-scale Cyclic Deformation (CD-A) experiment whose measurements started in October 2019. The experiment consists of two twin niches, which are compared with the help of (i) long-term direct and indirect measurements e.g., resistivity, water content, suction and crack development and (ii) numerical simulations. The niches have identical dimensions but differ in their environmental conditions. While one niche is closed to retain high humidity conditions, the so-called “open niche” is exposed to the influence of the neighboring gallery and subjected to the effects of seasonal air humidity changes. One of these effects is shrinkage-induced cracking, which we observe in periods when the relative air humidity decreases.

We model the cyclic deformation behavior of Opalinus Clay with a macroscopic poromechanic approach by considering partial saturation under the Richards assumption. The formulation consists

of the balance equations of the solid and liquid phases with displacements and pore pressure as independent variables. Hydromechanical coupling is achieved via the effective stress concept. The deformation behavior, e.g. swelling, shrinkage, is mainly driven by the pressure gradients. These exert a strong influence on the effective stress field, which may lead to cracking. To account for such shrinkage-induced cracking, we couple the hydro-mechanical model with the phase-field fracture model. The coupled equations are numerically implemented within the open-source finite element software OpenGeoSys (OGS-6).

Using a set of material parameters obtained from field measurements and literature, we compare the hydro-mechanical response of a laboratory scale and of a local in-situ scale model, which represents the open niche. The size and setup of the local in-situ model are determined accordingly to the desaturated and/or damage zone interpreted from field observations. We investigate the sensitivity of certain fracture mechanical parameters and attempt to reproduce in-situ observations of crack opening variations in response to humidity fluctuations in the open niche. Finally, we propose a preliminary methodology for applying the phase-field modeling approach at the spatial and temporal scales of the CD-A experiment.

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MS20 / 37

Two-step diffusion in cellular hygroscopic (vascular plant-like) materials

Author: Philippe Coussot¹

Co-authors: Benjamin Maillet²; Rahima Sidi-Boulenouar²; Sabine Caré²

¹ *Univ. Paris-Est*

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Vascular plants, a vast group including conifers, flowering plants, etc, are made of a cellular hygroscopic structure containing water in the form of either free (i.e. in a standard liquid state) or bound (i.e. absorbed in the cell-walls) water, which makes water transport processes in such materials rather complex [1-2]. From NMR (Nuclear Magnetic Resonance) relaxometry and MRI (Magnetic Resonance Imaging) we are able to distinguish the details of bound water and free water transport in a typical material with such a structure (softwood) under convective drying. Thus, we show that

water extraction relies on two mechanisms of diffusion depending on whether the material still contains free water or only contains bound water [3]. For a sufficiently weak (dry) air flux the free water is extracted homogeneously from the sample by absorption in the cell walls; then it is transported as bound water towards the free surface, which results in a constant drying rate. For a sufficiently strong air flux a region without free water grows from the sample free surface while water diffuses through both regions, and the drying rate continuously decreases. Remarkably, as a result of this process, in this case the drying rate is limited by the diffusion of bound water so that further increasing the air flux intensity does not change it. Thus, we demonstrate that when subjected to dry air flux, such natural systems control and limit the rate of extraction of free water. This constitutes a general reversible self-protective system which makes it possible to prolong free water storage despite dry external conditions, but can be fed back by diffusion under humid conditions. This full description and characterization of the internal processes opens the way to a simple physical description of drying, and provides key elements for a general understanding of water transport in various hygroscopic porous systems.

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Poster / 38

Foam plugging performance and flow characteristics in fracture system

Authors: Zhengxiao Xu¹; Zhaomin Li²; Binfei Li²

Co-authors: Qifeng Zhang²; Lei Zheng²; Yongjin Song²; Tong Yu³

¹ China University of Petroleum(East China)

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Fractured-vuggy carbonate reservoirs are characterized by strong heterogeneity. In a multi-fracture system, compared with secondary fractures and matrix, the main fracture has stronger conductivity, and it is of great significance to investigate the fluid flow characteristics in the main fracture.

Based on this, combined with actual reservoir conditions, a fracture core model and a visualized slab fracture model were prepared. The plugging performance of the ordinary foam and the enhanced foam system in the fractured core model was compared. The flow characteristics of ordinary foam and enhanced foam system in the visualized slab fracture model was explored. The research results show that in the single fracture core model, as the fracture depth decreases, the plugging capability of the foam gradually increases, and the plugging capability of the enhanced foam is higher than that of the ordinary foam. In the parallel fracture core model, the flow regulation effect of ordinary foam flooding under the same fracture level difference is better, and the flow regulation effect of enhanced foam flooding under different fracture level difference is relatively stable. Under the condition of the same fracture depth, the lower the surface roughness, the smaller the shear and resistance effects of the corresponding foam flooding. Under the condition of the same surface roughness, the greater the fracture depth, the smaller the flow resistance of the foam. After the same foam system flows in the slab fracture model for the same time, the burst of foam is the lowest under the condition of high depth and low roughness, and the shear collapse of ordinary foam is larger than that of enhanced foam during the flow process. Combined with various factors, the migration and distribution characteristics of foam in the fracture system are summarized, in order to provide guidance for the application of foam in plugging performance and flow regulation in fractured carbonate reservoirs, so as to better realize the development of deep fractured-vuggy carbonate reservoirs.

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MS06-A / 39

Dynamic Mode Decomposition (DMD) for Analyzing Dynamics in Multiphase Flow in Porous Media

Authors: Steffen Berg¹; James McClure²; Ryan Armstrong^{None}; Catherine Spurin³

¹ Shell Global Solutions International B.V.

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The advances in imaging technology over the past decade provide us with a much richer set of capability both in terms of quality and resolution to visualize the structure and processes in porous media. In particular the improvement in time resolution brings us into the position of gaining insight into dynamic process both at pore and Darcy scale at an unprecedented level. While we are finally able

to resolve the dynamic processes at their natural time and length scale at flowing conditions, it also poses a challenge to analyze large data in time-resolved data sets. While we traditionally analyze time series of 1D or even 3D imaging data sets by visual inspection, there are relatively few tools that help us to quantitatively characterize the dynamics. We do have methods such as Fourier analysis to extract characteristic signatures of the dynamics e.g. periodic aspects of the dynamics, that then occurs largely de-coupled from spatial structure –and the other way around. Also, in Fourier analysis, we often struggle to identify the dominant modes because long time series would be required, and the signal is not separated from the noise very well.

Dynamic Mode Decomposition (DMD) provides an approach to analyze spatio-temporal experimental data in a quick and largely automated manner and allows for simultaneous analysis of both spatial modes and their dynamics, in a consistent manner. Here we provide an application case where DMD is used to analyze spatio-temporal behavior of an instability in 2-phase “steady-state” flow in a Darcy scale fractional flow experiment. The (1D) space-time data which exhibits periodic “traveling wave” features is analyzed by DMD by decomposing it into the underlying modes and respective Eigenvalues. We observe that the system is well approximated by 4-5 modes and their respective dynamics. For the analysis of dynamics in porous media flows this is a paradigm shift compared to the traditional approach which starts either with a traditional scaling-up approach or directly commencing with fitting models to the data. The dynamic mode decomposition is an entirely data-driven approach that allows to extract the relevant dynamics within a few characteristic modes, which can then serve –at much better signal-to-noise ratio, for instance as surrogate models for further analysis.

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[1] J. N. Kutz, S. L. Brunton, B. W. Brunton, and J. L. Proctor. Other Titles in Applied Mathematics: Dynamic Mode Decomposition: Data-Driven Modeling of Complex Systems. Society of Industrial and Applied Mathematics, 2016.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS13 / 40

Extension of the SAFT equation of state to capture the effect of the solid wall into the confined fluid properties: using molecular dynamic simulation

Authors: Sajjad Ahmadigoltapeh¹; Rohaldin Miri²; Per Aagaard¹; Helge Hellevang¹

¹ University of Oslo

² *Iran University of Science and Technology (IUST)*

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The thermodynamic characteristics of water confined inside a nano-mineral pore differs from the bulk properties because of the competition between water-water and wall-water attractions near the solid walls. We used molecular dynamic (MD) simulation, to capture the influence of the solid walls of a slit shape calcite nanopore on the confined water provided in different widths namely 2 nm, 3 nm, 4 nm and 5 nm. The simulations are conducted with NVT ensemble at T = 300 K, 350 K, 400 K, and 450 K while each simulation run is completed within 6 ns. The results shows the density and total energy near the pore wall increases with temperature. To determine the new properties imposed by the nano-calcite pore, an equation of state (EoS) was developed based on the statistical association fluid theory (SAFT) by introducing a new term for Helmholtz free energy. Within a reliable absolute relative error (ARE), the results of the modified SAFT overlap with the outcomes of MD simulation. This approach can be applied in predicting the fluid properties near wall, which is the concern of several fields such as CO₂ storage, hydrogen storage and enhanced oil recovery (EOR) and etc.

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MS04 / 41

The swelling and shrinking of a thermo-responsive hydrogel

Authors: Matthew Butler¹; Tom Montenegro-Johnson¹

¹ *University of Birmingham*

Corresponding Authors: m.butler.3@bham.ac.uk, t.d.johnson@bham.ac.uk

Thermo-responsive hydrogels are a promising material for creating controllable actuators for use on micro-scale devices, because they expand and contract significantly (absorbing or expelling fluid) in response to relatively small temperature changes. Understanding the dynamic behaviour of such systems can be difficult because of the spatially- and temporally-varying properties of the gel, and the complex relationships between the elastic deformation of the polymer structure, the fluid dynamics within the pore spaces and chemical interaction between the polymer and fluid. We investigate such a gel using a poro-elastic model, considering the dynamics of a homogeneous thermo-responsive spherical hydrogel after a sudden change in the temperature that should result in substantial swelling or shrinking. We typically find that swelling and shrinking have qualitatively different behaviour: swelling happens smoothly from the edge, whereas shrinking results in the formation of

an inwards-travelling spherical front that separates a swollen core and shrunken shell. An approximate analytical form for the front dynamics is developed that well-approximates the numerical solutions.

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MS02 / 42

Analysis of evaporation and transport of stable water isotopologues in a coupled soil-atmosphere model

Authors: Stefanie Kiemle¹; Katharina Heck¹; Rainer Helmig¹

¹ *University of Stuttgart*

Corresponding Authors: rainer.helmig@iws.uni-stuttgart.de, katharina.heck@iws.uni-stuttgart.de, stefanie.kiemle@iws.uni-stuttgart.de

Stable water isotopologues can be used as natural tracers to better understand evaporation and mixing processes within soils. Due to their physical characteristics, the isotopic species tend to fractionate from ordinary water during evaporation processes resulting in an enrichment of stable water isotopologues in the soil. The fractionation process can be split into equilibrium fractionation and kinetic fractionation. Especially kinetic fractionation is influenced by processes in the soil as well as in the atmosphere. Due to the complex coupled processes that need to be considered to describe this accurately, modeling and analyzing the kinetic fractionation correctly is still an open issue. We present a two-dimensional multi-phase multi-component transport model that resolves both, the atmosphere and the soil and models the transport and fractionation of the stable water isotopologues using the numerical simulator DuMuX. With that, we can simulate transport and fractionation processes of stable water isotopologues in soils and the atmosphere without relying on existing formulations of the kinetic from literature. The isotopic fractionation simulations are carried out for laminar (Navier-Stokes) and turbulent (RANS) flow problems.

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Poster / 43

Insights into Upscaling of Modeling of Thermal Dispersion in Geothermal Doublets

Author: Jinyu Tang¹**Co-authors:** Pelle van Nieuwkerk²; William Rossen³¹ *Department of Chemical and Petroleum Engineering, United Arab Emirates University*² *Department of Geoscience and Engineering, Delft University of Technology*³ *Delft University of Technology***Corresponding Authors:** j.tang@uaeu.ac.ae, w.r.rossen@tudelft.nl, pellematthijs@hotmail.com

Representing the fine-scale heterogeneities of geological formations is computationally expensive in the modeling of geothermal processes. Upscaling is necessary for efficient modeling, using coarser grids and average rock and fluid properties. In modelling geothermal doublets, the breakthrough time of injected cold water at the production well is critical to project viability. Breakthrough time in turn depends on thermal dispersion in the reservoir, which arises largely from reservoir heterogeneity.

Tang and Rossen (2021) present an improved upscaling method for thermal dispersivity in modeling heterogeneous reservoirs and demonstrate its accuracy in representing thermal dispersion when layers are combined in reservoir modeling. Here we illustrate this approach through application to a geothermal doublet using the reservoir well log and a 2D layer-cake model. We show the relative roles of numerical dispersion, effects of thermal conduction between upscaled layers and effects of overburden and underburden in determining the breakthrough time. We report the grid resolution needed to keep numerical dispersion from dominating physical dispersion, based on the study of Lantz (1971) for 1D flow. The results show that it may be necessary to upscale thermal diffusivity in the transverse direction as well. The importance of overburden and underburden layers is crucial in relatively thin reservoirs where heat conduction from the overburden and underburden is dominant. It is possible that accurate thermo-physical properties are not crucial when reservoir is relatively thin. In that case, heat conduction from the overburden and underburden dominates thermal dispersion in the reservoir and thus cold-water breakthrough time.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS01 / 44

Capillary-number Insights into Mobilization of Oil in Porous Media by Foam Injection

Author: Jinyu Tang¹

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The mobilization of oil in porous media is a function of capillary number (N_{ca}), i.e. the ratio of viscous to capillary forces. With foam injection, N_{ca} increases considerably, a result of the combined effects of an increase in pressure gradient (∇p) due to gas-mobility reduction by foam and reduction in oil/water interfacial tension (IFT) by foaming surfactant. However, the relative importance of ∇p and IFT in published foam coreflood studies remains unclear. Our goal is to understand the dominant driving force for oil mobilization by foam in laboratory corefloods and provide insights into the extrapolation of laboratory results to field applications. We present a critical review of foam-oil displacement data reported in the literature, based on the correlation between remaining oil saturation (S_{or}) and N_{ca} (i.e., the capillary desaturation curve (CDC)) available for various formation types. In this, we update the results of Heins et al. (2014).

Most coreflood studies of foam-oil displacements do not report the IFT. For the purpose of our study, we investigate the correlation between S_{or} and ∇p in their data and place the data on a standard CDC correlation plot (Lake et al., 2014) based on the value of S_{or} . If oil is displaced by high ∇p created by foam in the coreflood, as often reported in laboratory corefloods, such high ∇p cannot be seen in geological formations, considering the difficulty in injectivity and risk of fracturing. Then, upon lower ∇p values feasible in field, we relate the reduced N_{ca} to S_{or} expected in field application using the CDC plot. We also examine the oil relative permeability implied in published studies. The high ∇p reported in foam corefloods often corresponds to very low oil relative permeabilities, meaning very slow oil recovery at the much lower ∇p in oil reservoirs. Thus, oil mobilization by high ∇p in foam corefloods as observed in laboratory cannot be directly extrapolated to field applications. Care is needed in extrapolating laboratory coreflood results directly to field application.

Foam can substantially improve sweep efficiency, and thereby increase oil recovery in field application. That advantage is independent of the question of reduced residual oil saturation with foam.

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References:

Heins, R., Simjoo, M., Zitha, P. L., & Rossen, W. R. (2014, October). Oil relative permeability during enhanced oil recovery by foam flooding. In SPE Annual Technical Conference and Exhibition. Lake, L. W., Johns, R. T., W. R. Rossen and Pope, G. A., Fundamentals of Enhanced Oil Recovery, Society of Petroleum Engineers, Richardson, TX, 2014.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS06-B / 46

How simplifying capillary effects can affect the traveling wave solution profiles of the foam flow in porous media

Authors: Luis Fernando Lozano¹; Jhuan Cedro¹; Rosmery Quispe Zavala¹; Grigori Chapiro²

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Neglecting or simplifying capillary pressure is a common starting point for analyzing the fluid displacement in porous media. From the mathematical perspective, the effect of such simplifications was addressed in the context of conservation laws. In this talk, we address the issue in the context of traveling waves. Mainly, we are interested in the case of one-dimensional incompressible two-phase gas-liquid flow in a porous medium in the presence of foam. We show two physically admissible intuitive simplifications resulting in solutions, which are qualitatively inaccurate in the variable describing foam texture. Besides these examples, we also show one procedure, which produces qualitatively accurate solution approximation. In order to sustain that our conclusions are not connected to any numerical error, we investigate the existence of the traveling wave solutions in all examples. We stress that the profile differences are related to the dynamical system behavior in the phase space. All semi-analytical results were verified through direct numerical simulations, evidencing the applicability of the presented analysis.

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References:

Lozano LF, Cedro JB, Zavala RV, Chapiro G. How simplifying capillary effects can affect the traveling wave solution profiles of the foam flow in porous media. International Journal of Non-Linear Mechanics. 2022: 103867.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS07 / 47

Upscaling of phase-field models for two-phase flow based on fluid morphology

Author: Mathis Kelm¹**Co-authors:** Carina Bringedal ; Bernd Flemisch ²¹ *University Stuttgart*² *University of Stuttgart***Corresponding Authors:** carina.bringedal@iws.uni-stuttgart.de, bernd@iws.uni-stuttgart.de, mathis.kelm@iws.uni-stuttgart.de

Two-Phase flow in porous media is relevant for many applications and accurately capturing of interfacial effects in an effective model is central to its modeling. The flow morphology can vary significantly for different physical settings and impact the effective behaviour.

We use phase-fields to model two-phase flow on the pore scale with an advective Allen-Cahn formulation coupled to a Navier-Stokes equation. We aim to specialise this model for different characteristic flow behaviours and investigate the upscaling of such models. Using periodic homogenization we arrive at macroscopic equations and microscopic cell-problems that yield effective parameters.

Based on experimental microfluidic data we characterise fluid morphologies exhibited in porous medium flows. These allow for specialisation in the micro-scale model and its upscaling process, yielding a more specific micro-macro model to better capture the effects of microscopic interface behaviour on the larger scale.

We implement our phase-field model for two-phase flow in DuMu^X, using a finite volume discretization. It features staggered control volumes and a combination of cell- and facecentered variables, which communicate using a multidomain coupling manager. This serves as a solver for cell-problems in the two-scale formulation that results from upscaling.

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Time Block A (09:00-12:00 CET)

Participation:

Online

MS15 / 48

Estimating permeability of real-rock micro-CT images by physics-informed neural networks

Author: Stephan Gärttner¹

Co-authors: Faruk Omer Alpak ; Andreas Meier ; Nadja Ray ²; Florian Frank

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In recent years, convolutional neural networks (CNNs) have experienced an increasing interest for fast approximations of effective hydrodynamic parameters in porous media research. In this talk, we present a novel approach to improve permeability predictions from micro-CT scans of geological rock samples.

A well-known method to enhance the quality of CNN predictions is the supply of additional information about the input data, leading to the field of physics-informed CNNs. Most commonly for permeability predictions from rock samples, porosity and/or (specific-) surface area are made available to the CNN as auxiliary data. However, these quantities become only loosely correlated to the target permeability for complex 3D geometries posing a poor information basis for the CNN to perform predictions.

Increasing the relevance of the additional physical information provided, we supply a highly correlated graph-network-based quantity to our CNN, namely the maximum flow value. Consequently, detailed information about confined structures dominating overall fluid flow is encoded in this additional input. As a result, high prediction accuracy and robustness for permeability prediction are observed across a variety of sandstone types.

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Time Block B (14:00-17:00 CET)

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MS06-B / 49

Nanoscale visualization of dissolution and precipitation at calcite-oil-brine interfaces upon aging at variable salinity

Author: Frank Megens¹

Co-authors: Mohammed B. Alotaibi ²; Subhash C. Ayirala ²; Ali A. Yousef ²; Igor Siretanu ¹; Frieder Mugele ¹

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While wettability alteration is arguably the dominant factor controlling low salinity IOR in sandstones, the relative importance of mineral dissolution and wettability alteration through modified organic-mineral interaction for carbonate reservoirs is still under debate. In this study, we present a new method to directly visualize local dissolution/precipitation in model systems upon aging crude oil drops in brines of varying composition.

Calcite samples covered in crude oil droplets were aged for up to two weeks at room temperature in brines of varying salinity, ranging from high-salinity formation brine to various low-salinity smart brines. After aging, the oil droplets were removed by toluene washing and the samples were dried. Subsequently, the calcite surface was scanned with Atomic Force Microscopy (AFM), characterizing the topographical differences between locations previously covered by oil and the immediate surrounding area that was directly exposed to the brine.

During aging, optical microscopy showed no change in the location or shape of the droplets (as seen from above), hinting at pinning of the three-phase contact line for each droplet. Height maps taken by AFM at droplet locations, show the locations of the original oil-calcite interfaces as mesas above the ambient substrate level for samples aged in undersaturated ambient brines of low salinity, whereas holes below the ambient substrate level are seen for supersaturated ambient brines. At the same time, the surface underneath the original droplet resembles the freshly cleaved calcite. This suggests that the oil protects calcite from being accessed and altered by the surrounding brine, while calcite is either dissolved or precipitated from the brine next to drop leading to the altered substrate levels. In accordance with their Saturation Index, high-salinity formation brine caused precipitation whereas low-salinity smart brines caused dissolution. Precipitation was limited to tens of nanometers observed at all timepoints (2 days – 2 weeks), whereas dissolution continued over time up to of hundreds of nanometers. Addition of SO₄(2-) had little effect on the dissolution; increasing the Mg(2+) content slightly inhibited mineral dissolution.

Our results provide a direct microscopic demonstration of mineral dissolution and precipitation upon aging calcite in various brines in the presence of crude oil. The method is easily adapted to elevated temperatures and possibly natural rock samples. Our observations contribute to the understanding of the relevance of mineral dissolution for smart water IOR in carbonate reservoirs.

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS05 / 51

Mechanisms driving intermittency in preferential flow paths in porous media biofilms

Author: Dorothee Luise Kurz^{None}

Co-authors: Eleonora Secchi ¹; Francisco Carrillo ²; Ian C Bourg ³; Roman Stocker ¹; Joaquin Jimenez-Martinez ⁴

¹ *ETH Zürich*

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³ *Princeton University*

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Biofilms, surface-attached bacterial communities, are abundant in many environmental and industrial porous media such as soils or filters. Fluid flow through the porous medium affects the biofilm development through shear stress and nutrient supply while in turn the biofilm affects the fluid flow. This interplay can lead to the formation of preferential flow paths (PFPs) through the bio-clogged porous medium as well as strong intermittency. The intermittency manifests itself by the rapid opening and slow closing of the preferential flow paths which leads to drastic changes in the local fluid flow and mass transport.

We unravelled that the mechanism driving PFP intermittency is the competition between microbial growth and shear stress. Microfluidic experiments in analog porous media allowed us to quantify *Bacillus subtilis* biofilm formation and behavior for different pore sizes and flow rates. This combined with a mathematical model accounting for flow through the biofilm and its rheological properties enabled us to reveal the underlying mechanisms. We find that the closing of PFPs is driven by microbial growth and the opening of PFPs is driven by flow-induced shear stress. We thereby demonstrate that in bio-clogged porous media, the competition between microbial growth and shear stresses can lead to strong temporal variability in transport and flow conditions.

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Participation:

Unsure

MS13 / 52

Water transfers (imbibition, drying) in cementitious materials followed by MRI (Magnetic Resonance Imaging)

Authors: Hicham DIALLA¹; Alban GOSSARD²; Benjamin MAILLET³; Jean-Baptiste CHAMPENOIS⁴; Philippe COUSSOT³

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Nowadays, cement-based materials are widely used, whether in construction or even in the conditioning of radioactive waste. However, the performance of these materials could be substantially affected by the penetration of water. Indeed, the infiltration of water facilitates the ingress of aggressive agents such as Cl, CO₂, etc. and can cause many types of degradation such as chloride infiltration and freeze-thaw damage [1] [2]. Therefore, a comprehensive understanding of water transport in cement-based materials is fundamental. For that aim, we focus on the physical mechanisms that control water transfers in mortar. More precisely, we study in detail the mechanisms of water imbibition and drying of a simple mortar sample. We in particular take advantage of visualization in time of the spatial distribution of water inside the sample by (non-invasive, non-destructive) MRI.

The imbibition tests observed by MRI show that for some samples the penetration of water can be heterogeneous, i.e. the water appears to follow some paths through the structure, temporarily not invading some regions. As a consequence, in such case, the imbibition dynamics is not described by the standard Washburn model [3]. When the imbibition is homogeneous, i.e. when a saturating front progresses in the material, the Washburn model applies under the assumption of a less than nanometric pore size. This process might also be described by a diffusion process.

The results obtained for drying are even more surprising. We systematically observe a homogeneous desaturation, which is usually the hallmark of dominant capillary effects, but at the same time, the drying rate continuously decreases and is essentially independent of the air flux velocity, which are usually the hallmarks of the development of a gradient of concentration at the approach of the free surface. In order to reconcile these contradictory observations we suggest that the extraction of water results from a diffusion process through the structure, but with two very different coefficients depending on the saturation: for relatively large saturation (say, more than 0.5) the diffusion coefficient has some approximately constant value; for lower saturation it strongly drops to a much lower value. This would allow the development of a saturation gradient in a thin layer close to the free surface, not visible by MRI, but yet a homogeneous desaturation in the rest of the sample still having a larger saturation.

The mechanical water penetration and extraction from a mortar appear to follow more complex processes than standard capillary processes. Diffusion from one site to another, easier at large saturation could be the main driving effect.

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References:

[1] R. M. Ghantous, M. K. Moradillo, H. H. Becker, M. T. Ley, et W. J. Weiss, « Determining the freeze-thaw performance of mortar samples using length change measurements during freezing », *Cement and Concrete Composites*, vol. 116, p. 103869, févr. 2021, doi: 10.1016/j.cemconcomp.2020.103869.

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design of concrete structures in Hong Kong–Zhuhai–Macau sea link project », *Structural Safety*, doi: 10.1016/j.strusafe.2014.11.002.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 53

Challenges for Microfluidic Devices in Representing Flow in Geological Formations

Authors: Simon Cox¹; Afshin Davarpanah¹; William Rossen²

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Microfluidic devices offer unique opportunities to directly observe multiphase flow in porous media. However, as a direct representation of flow in the 3D pore networks of geological formations, conventional microfluidics face several challenges.

One is the ability of microfluidic networks to represent steady two-phase flow without fluctuating occupancy of locations in the network. The ability of two phases to form steady, intertwined flow pathways is a key property of 3D pore networks (King and Masihi, 2019). This is not possible a two-dimensional network (Fisher, 1961) unless the flow paths of the two phases can cross at some locations in the network. Crossings are possible in a microfluidic network if wetting phase can form a bridge across the top and bottom of a gap between grains at a pore throat while non-wetting phase flows through the throat.

We examine the conditions under which this is possible using the Surface Evolver software (Brakke, 1992) to determine fluid interface shapes in several different throat geometries. Specifically, we determine the capillary pressures P_c at which strongly nonwetting phase penetrates a throat, and then the lower values of P_c at which wetting phase forms a bridge between grains, and the yet-lower values of P_c at which wetting phase re-invades and blocks the throat ("snap-off").

For relatively long straight or curved throats, the capillary pressure for bridging is the same as that for snap-off. Microfluidic networks designed to represent flow in geological formations that feature throats of this geometry cannot support steady two-phase flow without fluctuating occupancy of the pore space. In other words, flow is forced into the high-capillary-number regime where phases displace each other in the network.

Concave throats, as between cylindrical pillars, can support bridges over a substantial range of capillary pressure. Steady two-phase flow would be possible in networks of pores with throats of this geometry. The range of capillary pressures at which bridging is stable increases as throats become more strongly concave (i.e., pillar radius decreases) and for narrower throats. Strongly concave throats can also prevent "Roof" snap-off as nonwetting phase penetrates a pore body through a narrow throat.

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M.E. Fisher. Critical probabilities for cluster size and percolation problems. *J. Math Phys.* 2: 620–627 (1961).
P.R. King and M. Masihi. *Percolation Theory in Reservoir Engineering*, World Scientific Publishing Europe Ltd., 2019

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS17 / 54

Three-dimensional Rayleigh-Darcy convection at high Rayleigh numbers

Authors: Marco De Paoli¹; Francesco Zonta²; Sergio Pirozzoli³; Alfredo Soldati⁴

¹ *TU Wien, Institute of Fluid Mechanics and Heat Transfer*

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We perform large-scale numerical simulations to study Rayleigh-Darcy convection in three-dimensional fluid-saturated porous media up to Rayleigh-Darcy number $Ra=80,000$. At these large values of Ra , the flow is dominated by large columnar structures - called megaplumes - which span the entire height of the domain. Near the boundaries, the flow is hierarchically organised, with fine-scale structures interacting and nesting to form larger-scale structures called supercells. We observe that the correlation between the flow structure in the core of the domain and at the boundaries decreases only slightly for increasing Ra , and remains rather high even at the largest Ra considered here. This confirms that supercells are but the boundary footprint of megaplumes dominating the core of the domain. In agreement with available literature predictions, we show that the thickness of the thermal boundary layer (d) scales very well with the Nusselt number (Nu) as $d \sim 1/Nu$. Measurements of the mean wave number - inverse of the mean length scale - in the core of the flow support the scaling $Ra^{0.49}$, in very good agreement with theoretical and numerical predictions. Interestingly, the behaviour of the mean wave number near the boundaries scales as $Ra^{0.81}$, which is distinguishably different from the presumed linear behaviour. We hypothesise that a linear behaviour can only be observed in the ultimate regime, which we argue to set in only at Ra in excess of 500,000, whereas a sublinear behaviour is recovered at more modest Ra . The present results are expected to help the development of long desired reliable models to predict the large- and fine-scale structure of Rayleigh-Darcy convection in the high- Ra regime typically encountered in geophysical processes, as for instance in geological carbon dioxide sequestration.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS06-A / 55

Predicting and measuring pore-scale capillary pressures associated with meniscus movements during slow imbibition

Author: Sharon Ellman¹

Co-authors: Arjen Mascini²; Tom Bultreys³

¹ *Universiteit Gent*

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³ *Ghent University*

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Multiphase flow in porous rock is of vital importance to several issues facing the world at present. It is key to contaminant transport and subsequent remediation, subsurface energy storage and carbon dioxide capture and sequestration. Subsurface flow is typically characterized by having a low capillary number. The fluid displacement is therefore controlled by the capillary pressure across the fluid interface. Being able to predict the capillary pressures that lead to pore-by-pore displacement events is therefore vital to understanding the displacement patterns.

Since drainage consists predominantly of piston-like displacements, the capillary pressures resulting in these displacements can be estimated using the cylindrical Young-Laplace formulation in pore throats. Imbibition is a more complex displacement process[1], necessitating capillary pressure models for snap-off and cooperative pore filling events that require more complex formulations[2], [3]. However, it is still unclear whether these models can be used to sufficiently describe imbibition in e.g. pore network models (PNMs). Here, we address this by measuring the capillary pressures of imbibition displacement events imaged using dynamic micro-CT imaging in a glass beads pack by Schluter et al.[4], and comparing these on a pore-by-pore basis to capillary pressure calculations commonly used in quasi-static PNMs. A crucial challenge to do this, is that local contact angles and the geometry of the pore space are needed. Therefore, we determined image-based contact angles using the conventional geometric[5], thermodynamic[6], force-based[7] and local geometric[7] contact angles. The latter was deemed most suitable for use as input in the capillary pressure models as its distribution was narrower than that of the other types of contact angles, suggesting it accounts for the local hinging of contact angles which occurs during imbibition. Furthermore, (semi-)analytical capillary pressure models require a simplification of the local geometry. We used a maximum inscribed sphere[8] PNM as well as a watershed segmented (Avizo 2020.3 Thermo-Fisher Scientific) PNM to supply this. The results obtained from each PNM were compared to assess the impact they have on the output.

The analytical models were compared to local capillary pressure measurements prior to each displacement event, derived from the curvatures of the fluid interfaces in the μ CT images. This makes it possible to pin down the leading cause of errors in simplified multiphase flow models and improve them in the process. The improvement of pore-scale multiphase flow models has implications for carbon dioxide sequestration, contaminant transport, etc.

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Country:

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References:

- [1] R. Lenormand, C. Zarcone, and A. Sarr, "Mechanisms of the displacement of one fluid by another in a network of capillary ducts," *J. Fluid Mech.*, vol. 135, p. 337, Oct. 1983, doi: 10.1017/S0022112083003110.
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In person

Poster / 56

Steady State Two-Phase Flow Relative Permeabilities in Microfluidic Devices

Authors: Ewald Obbens¹; William Rossen¹; Simon Cox²

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Microfluidic devices allow direct observation of multiphase flow in porous media. However, as a direct representation of flow in the 3D pore networks of geological formations, conventional microfluidics face a challenge in representing steady two-phase flow without fluctuating occupancy

of locations in the network. In a separate presentation (Cox et al., 2022) we show that such flow is possible in networks with concave pore throats, such as between cylindrical solid pillars. Here we investigate the range of relative permeabilities possible in such a two-phase flow without fluctuating pore occupancy.

We use phase configurations at capillary pressures at which such two-phase flow is possible (Cox et al., 2022), determined using the Surface Evolver program. Then, using COMSOL software, we solve for conductivity for flow through pores and pore throats in different phase configurations: fully saturated with wetting phase; occupied by nonwetting phase with wetting phase occupying the corners around pillars; and at bridges where two phases cross flow paths at pore throats. Such crossings are necessary for steady flow in 2D microfluidic networks (Cox et al., 2022). The wetting phase must also navigate around pore bodies occupied by nonwetting phase through connections between corner regions occupied by wetting phase at the top and bottom of pillars (shown in attached figures). This work is an extension of previous work (Rossen et al., 2020) that used crude estimates of interface shapes in these cases.

We compute the overall conductivity for each phase through a 32x32 network with pore throats between pillars, using wrap-around boundary conditions. We begin with invasion percolation of the network by nonwetting phase, which disconnects the wetting phase. We then model re-imbibition of the wetting phase until its flow path is reconnected by bridging. We do so using the conductivities determined from COMSOL for segments of the complex network paths occupied by each phase. We repeat the calculations for 12 realizations of the network.

Relative permeabilities for both phases are extremely low. Moreover, the fractional flow of wetting phase that can be maintained is low, especially in gas-liquid flow. In addition, large pressure differences occur at pore throats blocking large stagnant clusters of nonwetting phase, providing another mechanism for fluctuating occupancy of pores and pore throats.

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References:

S. Cox, et al. Challenges for Microfluidic Devices in Representing Flow in Geological Formations. ms. submitted to J. Colloid Interface Sci., <https://arxiv.org/abs/2108.05144>

W. R. Rossen, et al., Conditions Allowing Steady Two-Phase Flow in Microfluidic Devices. Presentation at InterPore Annual Conference, Qingdao, China, 2020

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS13 / 57

Molecules diffusing and relaxing in macro, meso and microporous materials: An NMR approach for studying the behaviour of fluids confined in nanoporous media

Author: Carmine D'Agostino¹

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Transport and dynamics of fluids in nanoporous networks play a significant role in many applications of porous materials, most notably catalysis, separation and adsorption technologies. Yet, direct experimental measurements of such phenomena at a pore-scale/microscopic level is challenging and key parameters such as diffusion or adsorption coefficients are often extrapolated using indirect macroscopic measurements. In this context, nuclear magnetic resonance (NMR) methods offer some key advantages since they are non-invasive, chemically selective and allow generally fast acquisition of the experimental data. Traditional applications of these methods have been in the area of reservoir engineering and oil/water/rock systems.[1]

In recent years, new applications of such methodologies have been extended to systems such as heterogeneous catalysts, membranes for gas separation as well as soft materials. In this work, the latest developments in these areas are presented. In particular, both high-field as well as newly developed low-field bench-top NMR techniques are used to unravel the behaviour of challenging systems such as photocatalysts and heterogeneous organocatalysts for chemical manufacturing, soft materials for drug delivery as well as mixed matrix membranes for gas separation.[2,3,4] In-situ multi-nuclear (^1H , ^{13}C and ^{19}F) NMR spectroscopy, diffusion and relaxation methods able to provide new and exclusive insights into reaction, diffusion and dynamics of fluids at the solid interface within the pores are used to rationalise and optimise the design of such porous materials, with a particular attention to the structure-transport-activity relationship.

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[1] Quantitative In Situ Enhanced Oil Recovery Monitoring Using Nuclear Magnetic Resonance, J. Mitchell, J. Staniland, R. Chassagne, E. J. Fordham, *Transport in Porous Media*, 94, 683–706 (2012)

[2] Light-driven, heterogeneous organocatalysts for novel C-C bond formation towards valuable perfluoroalkylated intermediates, G. Filippini, F. Longobardo, L. Forster, A. Criado, G. Di Carmine, L. Nasi, C. D'Agostino, M. Melchionna, P. Fornasiero, M. Prato, *Science Advances*, 6, eabc9923 1-10, (2020)

[3] Tailoring pore structure and surface chemistry of microporous Alumina-Carbon Molecular Sieve Membranes (Al-CMSMs) by altering carbonization temperature for optimal gas separation performance: An investigation using low-field NMR relaxation measurements, L. Forster, C. D'Agostino, M. A. Llosa-Tanco, V. Spallina, C. Brencio, F. Gallucci, M. Lindley, S. J. Haigh, D. A. Pacheco-Tanaka, *Chemical Engineering Journal*, 424, 129313 (2021)

[4] Oxidative coupling of aldehydes with alcohol for the synthesis of esters promoted by polystyrene-supported N-Heterocyclic Carbene: Unravelling the solvent effect on the catalyst behavior using NMR relaxation", G. Di Carmine, D. Ragno, A. Massi, C. D'Agostino, *Organic Letters*, 22, 4927-4931 (2020)

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

Poster / 58

Agrochemical Transport in Heterogeneous Agricultural Soils

Authors: Mackenzie Dughi¹; Veronica Morales¹

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The fate and transport of contaminants associated with agricultural soils have important implications for groundwater quality and public health. Intricacies of the pore structure control how water flow is distributed and consequently how dissolved chemicals are transported in the subsurface. We hypothesize that the structural heterogeneity generated by different agricultural land management practices (ploughed vs no-till) will affect the transport behavior of agrochemicals in these soils. We test this hypothesis with data from direct numerical simulations of tomographic images of soil samples obtained from a long-term agricultural field station in the United Kingdom. The flow in each soil domain is resolved from the full Navier-Stokes equations and transport is simulated from tracking of massless particle tracers. A statistical analysis of the Lagrangian tracks is presented to compare the velocity distribution, velocity correlation length, breakthrough curve, and evolution of displacement moments that characterize each land management practice. Our findings show that for low Peclet numbers, representative of natural water infiltration, the two soil treatments have comparable transport behavior with mild anomalous characteristics. Conversely, for high Peclet numbers, representative of infiltration rates from Ag-Managed Aquifer Recharge, transport in ploughed soil is significantly more anomalous than in no-till soils. An improved understanding of the controls for contaminant transport in agricultural soils and of the predictive tools to model contaminant transport are key to helping decision makers implement more sustainable strategies in agriculture.

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Time Block C (18:00-21:00 CET)

Participation:

Online

MS10 / 59

Use of advanced imaging techniques as a valuable tool to analyze the freeze-drying process in more detail in situ

Author: Sebastian Gruber¹

Co-authors: Maximilian Thomik²; Nicole Vorhauer-Huget²; Frederik Coppens³; Evangelos Tsotsas²; Petra Först¹

¹ *Technical University of Munich, Chair of Process Systems Engineering*

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Lyophilization or freeze-drying is commonly applied to stabilize (bio-)pharmaceutical substances and high value foods for long-term storage. The freeze-drying cycle typically consists of three stages: i: freezing ii: primary drying and iii: secondary drying [1]. The freezing step is the most crucial one because the performance of the overall process vastly depends on the freezing step. Since the freezing parameters fixes the morphological structure of the dried material, they directly influence the pore size distribution and the connectivity of the porous matrix. Hence, it affects the heat and mass transfer trough the dried cake, which effects the drying rates of both, the primary and secondary drying stages [1,2].

While the influence of pore size on the freeze-drying process is already known, surprisingly other structural parameters like pore orientation or shape is still not sufficiently investigated. Next to the microstructure, process design as well as critical properties of the formulation are important. Drying above critical parameters can lead to changes in microstructure and thus, directly influence the overall drying process and product quality [3].

In this study we will present the influence of the pore structure on the overall drying kinetics and how the pore structure will change during drying. This investigation is carried out in a lyomicroscope. Furthermore, for the first time our self-developed freeze-drying stage [3,4] inside a 4D μ -CT (DynaTOM, TESCAN) to observe structural changes in 3D with a high temporal resolution in-situ is used. Here, maltodextrin and sucrose solutions with different solid concentrations ($c = 0.05$ w/w, $c = 0.2$ w/w and $c = 0.3$ w/w) were used as model substances. In order to estimate the structural changes during the drying process, an in-house image processing code is applied to analyze microstructural parameters like pore size, orientation and shape. The change in the morphological structure at the different drying stages is discussed. The experimental data will further be transformed into irregular pore networks and used for further modelling of drying. The results will lead to guidelines for a faster freeze-drying process with high product quality.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Micro-macro models for reactive two-mineral systems

Authors: Nadja Ray¹; Stephan Gärttner²; Peter Frolkovic³; Peter Knabner⁴

¹ *Friedrich-Alexander Universität Erlangen-Nürnberg*

² *Friedrich-Alexander-Universität Erlangen-Nürnberg*

³ *Slovak University of Technology*

⁴ *University Erlangen-Nürnberg Department Mathematics*

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Porous media naturally exhibit a heterogeneous structure including two different spatial scales: The pore/micro-scale is the fundamental scale, on which flow and reactive transport processes take place whereas the macro-scale, i.e. the scale of the porous medium itself, is of practical relevance for many geoscientific applications. (Periodic) homogenization has been successfully applied for several decades to bridge these scales and to arrive at macroscopic (upscaled) models, which only keep the microscopic information by means of a decoupled computation of 'effective' parameters on a so-called unit cell. However, the situation becomes more intertwined, if competing minerals dissolve and precipitate and consequently dynamically alter the porous medium's structure and its bulk properties.

In this talk, we discuss the formal upscaling and numerical investigation in such a situation. We start from a pore-scale model for reactive flow and transport in an evolving porous medium being composed of two distinct minerals. We derive an effective micro-macro model by formal two-scale asymptotic expansion in a level-set framework. For such a micro-macro model, the macroscopic equations (reactive flow and transport equations) and the equations posed at the unit cell are fully coupled: At each macroscopic point a unit cell is attached and the solution to the equations on the unit cell depends on the macroscopic solution at that point. This is due to the fact that the macroscopic concentration triggers mineral reactions, which alter the unit cells' geometrical structure. On the other hand, the macroscopic solution depends on the microscopic solutions by means of 'effective' hydrodynamic parameters such as porosity, reactive surface, diffusion, and permeability.

Finally, we present numerical simulations of the fully coupled micro-macro problem with application to dissolution of calcite and dolomite. Our results can be found in [1-3].

[1] S. Gärttner S., P. Frolkovič, P. Knabner, N. Ray. "Efficiency of micro-macro models for reactive two-mineral systems." accepted in SIAM Journal of Multiscale modeling and Simulation, 2021

[2] S. Gärttner, P. Frolkovič, P. Knabner, and N. Ray. "Efficiency and Accuracy of Micro-Macro Models for Mineral Dissolution/Precipitation." Water Resources Research 56(8), 2020.

[3] N. Ray, J. Oberlander, and P. Frolkovič. "Numerical investigation of a fully coupled micro-macro model for mineral dissolution and precipitation." Computational Geosciences 23, 2018.

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References:

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS13 / 61

Elasticity of Liquid Nitrogen in Nanoporous Vycor Glass

Authors: Klaus Schappert¹; Rolf Pelster¹

¹ *Universität des Saarlandes, Department of Physics*

Corresponding Authors: k.schappert@mx.uni-saarland.de, rolf.pelster@mx.uni-saarland.de

Experimental and theoretical research has shown that several factors influence the elastic properties of fluids confined in nanopores [1,2]. Previous experimental studies on the longitudinal modulus of confined fluids were mostly limited to the adsorbate argon. Here we study the longitudinal modulus of liquid nitrogen in the nanopores of Vycor glass at various temperatures using ultrasonic measurements. With the aid of an effective medium analysis we determine the modulus of the confined nitrogen, $\beta_{N_2,ads}$, from the measured effective longitudinal modulus of the system consisting of porous matrix and filled nanopores. In addition to the temperature dependence of the modulus at saturation vapor pressure, we investigate the impact of nanoconfinement on the pressure dependence of $\beta_{N_2,ads}$.

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References:

[1] Christopher D. Dobrzanski, Boris Gurevich, and Gennady Y. Gor, Elastic properties of confined fluids from molecular modeling to ultrasonic experiments on porous solids, *Appl. Phys. Rev.* 8, 021317 (2021).

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS11 / 62

Microfluidics-based analysis of dynamic contact angles relevant for underground hydrogen storage

Author: Willemijn van Rooijen¹

Co-authors: Leila Hashemi²; Maartje Boon²; Rouhi Farajzadeh¹; Hadi Hajibeygi²

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The contribution of renewable energy, specially wind and solar, is expected to increase significantly in the future global energy mix [1]. However, due to the intermittent nature of these energy resources, development of large-scale (TWh) energy storage systems is essential [2]. Underground hydrogen storage (UHS) in porous media, such as depleted oil and gas reservoirs and aquifers offer feasible solutions [3, 4, 5, 2].

A good understanding of H₂/water transport properties such as relative permeability and capillary pressure is needed to ensure the safety of UHS, as well as to optimize injection and withdrawal cycles [6, 7, 8, 9, 10, 2]. Relative permeability and capillary pressure functions are highly dependent on the wetting properties of the system [11,12,10]. The wettability in H₂/brine/rock systems can be characterized by the contact angle between the rock-brine and the brine-H₂ interfaces.

Recently, several different techniques, including the captive-bubble cell and the tilted plate technique, have been applied to measure or derive contact angles relevant for UHS [13, 14, 6]. Although, water-wet conditions were reported in all these studies, inconsistencies exist between the reported data. This could possibly be explained by differences in the measurement techniques and types of rocks and fluids used in the experiments.

To help shedding new lights on characterisation of this crucial interface property, we have measured contact angles in microfluidic systems. Microfluidic chips resemble actual subsurface systems much closer compared to tilted plate techniques or captive bubble cells, because of the dynamic and micro-channel-based nature of the flow conditions. The experiments were carried out at P = 10 bar and T = 20 °C using a microfluidic chip with channel widths ranging between 50 - 130 μm. Advancing and receding contact angles of H₂/water, N₂/water and CO₂/water systems were measured. The results indicate strong water-wet conditions with H₂/water advancing and receding contact angles of respectively 13 - 39°, and 6 - 23°. It was found that the contact angles decrease with increasing channel widths. Little hysteresis was measured, and consequently, the results are not in line with Morrow's curve. The receding contact angle measured in the smallest channel width (50 μm) agrees well with the literature coreflood tests on the Vosges Sandstone [13], suggesting that this channel width is representative of actual subsurface systems. The N₂/water and CO₂/water systems showed similar behaviour to the H₂/water system and no significant differences in contact angle were observed for the three different gases.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS05 / 63

Time evolution of biofilm permeability field in porous media and control on fluid flow velocities

Authors: Dorothee Luise Kurz^{None}; Eleonora Secchi¹; Roman Stocker¹; Joaquin Jimenez-Martinez²

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In soil ecology, as well as in environmental and industrial applications such as bioremediation and filters, it is of growing importance to understand the interplay between biogeochemical processes

and hydrodynamics in porous media. In the latter, microorganisms can form surface-attached communities, known as biofilms. Biofilms lead to bio-clogged pores, which causes modified pore geometries, redirecting the fluid flow and impacting the spatial distribution of velocities within the porous medium. To quantify this impact, both in space and time, numerous experimental and numerical efforts have been done. However, the quantification of the permeability of the highly heterogeneous biofilm still presents a challenge.

We designed a microfluidic platform to study the influence of different flow rates and pore size on biofilm development in porous media systematically. Using the experimental images obtained, we developed a method to obtain the permeability field within the biofilm. We then simulate the fluid flow dynamics within the entire bio-clogged porous medium at different stages of biofilm development using a continuous approach. Time-resolved probability density functions of permeabilities and of the resulting velocities were computed. While the variance in the fluid flow velocities showed a steady increase in hydrodynamic heterogeneity, the variance of the permeability of the bio-clogged porous medium decreased.

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Time Block B (14:00-17:00 CET)

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Poster / 64

The influence of gas bubble interfaces on the acoustic properties of partially saturated poroelastic media

Authors: Patrick Kurzeja¹; Holger Steeb²

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² *Universität Stuttgart*

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The present work focuses on the impact of gas bubble dynamics on effective acoustic properties in partially saturated poroelastic media. It's key objective is the bubbles' interface mechanics on various length scales. The analysis starts from a single air bubble embedded in surrounding water. The classical Minnaert solution [Minnaert 1933] is covered by first taking into account the bulk compressibility. Turning the view towards smaller scales, we extend the description by surface tension and capillary effects [Leighton 1994, de Gennes 2003]. This does not only modify the bubbles' stiffness, it also introduces new oscillation modes. The length-scale analysis of the interface mechanics is eventually completed by incorporation of higher-order curvature effects [Helfrich 1986] such as the Tolman-length [Tolman 1949].

A macroscopic acoustic model is then derived for multiple gas bubbles in saturated porous media. The system thus contains a poroelastic frame (e.g., rock) [Biot 1956a,b], a continuous wetting phase (e.g., water) and a discontinuous non-wetting phase (e.g., air bubbles). Homogenization of the gas bubble ensemble yields a set of continuum equations that account for the individual bubbles' resonance frequencies and damping [Frehner 2010, Steeb 2012, Kurzeja 2014a,b]. Like in Biot's theory, the model accounts for two propagating P-waves and one shear wave, respectively. In addition to classical poroelasticity, the discrete (discontinuous) bubble oscillation contribute to the dispersive behaviour of the system.

The evolution of wave speed and intrinsic attenuation of waves is illustrated numerically for water-saturated rock with air bubbles of various size and distribution. Respective assumptions and limitations are summarized in this process to provide a quick reference for choosing the best compromise between a model's complexity and applicability. Opportunities and limitations of the predictions are discussed with respect to characterization. Open questions in terms of material parameters and simplifying assumptions will conclude the discussion and shall motivate subsequent investigations across disciplines.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS07 / 65

An efficient preconditioning framework for the coupled simulation of contact mechanics with hydraulically active fractures

Authors: Laura Gazzola¹; Andrea Franceschini¹; Massimiliano Ferronato¹

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The coupled simulation of frictional contact mechanics and fluid flow in fractured porous media is attracting more and more attention in many subsurface applications, such as geothermal energy production, carbon dioxide sequestration, and underground gas storage. In these contexts, large computational domains are usually required to achieve the desired accuracy, along with high resolution representations of the geological structures and their heterogeneous properties. A natural consequence is the growing demand towards the development of sophisticated models of increasing size, for which computational efficiency is an issue. A key factor is the availability of an efficient linear solver, which is usually the most time-consuming component of a simulation. In this talk, we focus on the development of a scalable and efficient preconditioning tool for the linearized system arising from the discretization of the coupled flow-deformation problem in fractured media.

We consider a model that relies on the explicit discretization of fractures, with Lagrange multipliers used to impose the contact constraints. Low order finite elements are used for the linear momentum balance in the continuous domain with a cell-centered finite volume scheme for the mass balance in the fracture network. Fracture-based Lagrange multipliers are also cell-centered. This mixed formulation does not require any interpolation between different fields, but needs to be properly stabilized to satisfy the inf-sup condition. The arising linearized Jacobian is a nonsymmetric and indefinite matrix, with a 3x3 block structure.

We propose two different approaches exploiting the natural unknown subdivision and a state-of-the-art aggregation-based multigrid solver. The key idea is to restrict the system to a single-physics problem, approximately solve it by an inner algebraic multigrid approach, and finally prolong it back to the fully-coupled problem. The two approaches are analysed and tested. Moreover, theoretical bounds for the eigenvalue distributions of the preconditioned matrices are identified. The comparison allows to find the best strategy among the two proposed. Finally, numerical results prove the algorithmic scalability, the influence of the relative weight of fracture-based unknowns and the performance on a realistic complex problem.

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Time Block C (18:00-21:00 CET)

Participation:

Online

MS01 / 66

A micro-scale analysis for wettability characteristics of H₂ in heterogeneous geological media

Author: Maartje Boon¹

Co-authors: Leila Hashemi¹; Willemijn van Rooijen²; Rouhi Farajzadeh²; Hadi Hajibeygi¹

¹ *TU Delft*

² *Delft University of Technology*

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Underground Hydrogen Storage (UHS) has the potential to play an important role in the transition towards renewable energy resources [1,2]. In many industrial applications, initially a mixture of hydrogen (H₂) and methane (CH₄) will be introduced to the grid and storage facilities [3]. Secure and efficient UHS requires accurate characterization of the cyclic movement of the H₂-CH₄ gas mixture through the reservoir which highly depends on the wettability of the system [4].

To get a better understanding of the wettability behavior of cyclic stored H₂-CH₄ gas mixtures, and the factors that contribute to contact angle hysteresis, we measure intrinsic contact angles and dynamic contact angles during drainage and imbibition, for H₂, CH₄ and their mixtures, in contact with brine under a range of pressure, temperature and salinity conditions using the captive-bubble cell approach [5,6] and microfluidics approach [7], respectively. The microfluidic experiments allow us to look at the impact of different heterogeneity structures on the contact angle hysteresis, while the captive-bubble cell approach is used to investigate the impact of pinning. In the captive bubble cell method, the rock sample (Bentheimer) is placed in a high P, T cell, filled with brine. Gas bubbles are released from the bottom of the cell and buoyantly rise through the brine until they reach the rock surface. The gas bubbles slowly dissolve into the brine while images are taken every minute. The images are processed with our in-house code to calculate the contact angles. The captive bubble cell approach is traditionally seen as static measurement, however, due to the dissolution of the gas into the brine the bubble size decreases with time. This dynamic behavior is mimicking the imbibition process where water is displacing the non-wetting phase and allows for the visualization and the characterization of the effect of pinning on the contact angle.

Our preliminary results show that pinning can significantly increase the contact angle and more pinning is observed in the higher salinity brines. Furthermore, no contact angle hysteresis is observed in homogeneous micro-fluidic systems. Overall, H₂, CH₄ and their mixtures, show similar wettability behavior independent of pressure, temperature and salinity. To further explore the observed behavior, a theoretical analysis based on the Young-Laplace equation is carried out for the captive-bubble cell method. This analysis shows that the contact angle depends on 1. the density difference between the brine and the gas, 2. the interfacial tension and 3. the bubble radius, of which the combined effect can be characterized with the Bond number. Moreover, we theoretically validate that under similar Bond numbers and similar bubble radii, the contact angles of H₂ and CH₄ bubbles and their mixtures are indeed comparable. Our work suggests that in real field processes in which buoyancy and capillary are the main acting forces, H₂, CH₄ and their mixtures, will have similar wettability behavior independent of pressure and temperature. More details about this part of the work can be found in the journal manuscript [6].

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- 3) RAG, UNDERGROUND SUN STORAGE 2030. 2021
- 4) L. Hashemi, M. Blunt, H. Hajibeygi, Pore-scale modelling and sensitivity analyses of hydrogen-brine multiphase flow in geological porous media, *Scientific reports* 11 (2021) 1–13. URL: <https://doi.org/10.1038/s41598-021-87490-7>.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS09 / 68

Dynamic Pore-Network Modeling of Solvent Vapour Extraction

Author: Merouane Khammar¹

Co-author: Vahid Niasar²

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Solvent Vapour extraction (Vapex) of bitumen from oil sands is a promising technology for in-situ bitumen recovery. It is analogous to steam assisted gravity drainage (SAGD) where solvent is used as a substitute to heat to reduce bitumen viscosity. In the Vapex process, two parallel wells are employed. Solvent is injected in the upper well and recovered diluted bitumen is produced from the bottom well. GHG emissions and the environmental impact of bitumen extraction in Vapex are improved compared to the SAGD process.

In Vapex, solvent and oil mix by a combination of molecular diffusion, mechanical dispersion and capillary redistribution of fluids. The mass transfer layer between the vapour chamber and oil consists of a dynamic vapour-liquid capillary mixing zone and a single phase liquid-zone where dispersive forces mix solvent and oil. Oil production in Vapex experiments carried in porous media were found

to be significantly higher than model predictions. This was attributed to increased surface contact in porous media, surface renewal at the bitumen front and capillary imbibition. It was reported that capillary imbibition is a dynamic pore-scale mechanism that draws diluted oil away from the solvent vapour-bitumen interface and contributes to periodic interface renewal and mass transfer rate enhancement.

In this work, a pore network model is used to describe the dynamics of two-phase flow and mass transfer during solvent vapor based extraction of bitumen from a two dimensional randomly generated porous medium. Thermodynamic equilibrium is assumed in the pores and a two-phase flash calculation is performed to compute phase composition. Solvent diffusion and dispersion, capillary imbibition and dynamic two-phase flow of diluted bitumen and solvent vapour in the pores are modeled. The model presented in this work can be used to investigate the impact of operating conditions on bitumen recovery and obtain macroscopic parameters for reservoir scale models of the Vapex process.

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Time Block C (18:00-21:00 CET)

Participation:

Online

MS03 / 70

Matrix-fracture flow transfer in fractured porous media: experiments and simulations

Author: Jiafan Guo^{None}

Co-author: Zhechao Wang

Corresponding Authors: guojiafan2020@gmail.com, wang_zhechao@hotmail.com

The matrix-fracture flow transfer is one of the most important characteristics of flow in fractured porous media. Matrix-fracture flow transfer experiments in fractured porous media were carried out using a self-developed experimental device and simulation. The matrix-fracture flow transfer was analyzed in fractured porous media with regular fractures and irregular fractures at different matrix-fracture pressure differences. The matrix-fracture flow transfer rate accounted for 26%~72% of the matrix inlet flow rate, and the flow transfer rate presented a nonlinear increasing trend as the matrix-fracture pressure difference increased. We have observed the influence of heterogeneous pressure and inconsistent transfer direction on flow transfer in experiments and simulations. The influence of the heterogeneous matrix-fracture pressure difference increased with increasing fracture aperture and fracture/matrix permeability ratio and decreased with increasing trace length and density. The matrix-fracture flow transfer term obtained in the experiment and simulation was analyzed using the shape factor theory and the generalized transfer model we have previously proposed. In FPM with a regular fracture distribution, the fitting effect of the shape factor model and the generalized model was approximately the same. However, in FPM with irregular fracture distribution, the flow transfer rate predicted by the generalized model was more accurate than that predicted by the shape

factor model. The flow transfer rate predicted by the traditional shape factor model may have been overestimated because it ignored the effect of the heterogeneous matrix-fracture pressure difference. The findings of this study can help for better understanding of matrix-fracture flow transfer to predict groundwater flow field in naturally fractured porous media.

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MS12 / 72

NMR characterization of critical boundary of pore fluid in shale

Authors: Xu Dong¹; Bo Liu¹; Lijuan Cheng¹; Yangchuan Lin¹; Yue Jin¹; Xue Han¹

¹ *Northeast Petroleum University*

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Pore fluids are generally classified into movable fluid and irreducible fluid by one or two NMR T2 cut-offs (T2C). Fluid mobility in shale may not be accurately characterized by pore size-based classification methods solely because of the complex pore structure and heterogeneity in pore size. In this study, we propose a nine-grid dual T2C model to characterize critical boundary of fluid and calculate the percentages of free fluid (FF), capillary-bound fluid (CAF), and clay-bound fluid (CBF). The pore size distributions and capillarity boundaries are converted from T2 and mercury injection capillary pressure (MICP). Three T2 spectra (TFF, TCAF, and TCBF) under water saturation, centrifugation, and heat-treatments are measured to classify pore fluids as FF, CAF, and CBF according to the pore capillary force needed to displace them. T2C1 and T2C2 are calculated to classify pores into three size categories. Finally, the nine-grid dual T2C model that is composed of the three T2 distributions and two T2C is applied to explain results of a N2 displacement test and evaluate fluid mobility in shale samples. The results suggest that the conventional classification method based on fixed T2C results in the underestimation of CAF and overestimation of CBF. The macro-pores range in size of $T2 > T2C1$ and have lower pore capillary pressures. Micro-pores ($T2 < T2C2$) are smaller, and have high capillary pressures. Compared with conventional methods, the introduced model interprets the pore capacity-related displacement process well, especially for the remarkable displacement ratio of medium pores. The co-effect of fluid types and pore sizes in gas-displacing-water tests indicates that the process is primarily governed by fluid-matrix interaction and the connections among pores, rather than a simple sequential displacement of larger-to-smaller pores.

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Time Block A (09:00-12:00 CET)

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MS07 / 73

Simulation of reactive transport in heterogeneous porous media with a Newton-Krylov method

Authors: Laila Amir¹; Michel Kern²

¹ *Laboratoire d'Ingénierie Informatique et Systèmes*

² *Inria*

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Reactive transport modeling in porous media involves the simulation of several physical and chemical processes: flow of fluid phases, transport of species and chemical reactions between species. After discretization, one obtains a highly nonlinear system of partial differential for transport, coupled to algebraic equations for chemistry.

In [1], we have presented a globally coupled approach, where transport and chemistry are solved in a fully coupled manner, while transport and chemistry modules are kept separate. The method uses the same fixed point formulation than the Standard Iterative Approach, but, at each time step the nonlinear system of algebraic equations that couples all chemical species at all mesh points is solved by a Newton-Krylov method. The linear system at each Newton step is solved by the GMRES method, with a Jacobian free implementation where the required matrix by vector product may be approximated by a finite difference quotient or computed exactly.

Linear and nonlinear preconditioners must respect the block structure of the system in order to remain matrix-free. We have shown that block Gauss-Seidel preconditioners is closely related to a non-linear elimination method, and that both give a method where the number of both Newton and GMRES iterations do not grow when the mesh is refined [2].

In this talk, we recall the main features of the method, and we present an extension to handle mineral precipitation and dissolution reactions using an interior point Newton method [3]. We also study the performance of the method on 2D heterogeneous geometries.

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Laila Amir, Michel Kern, “A global method for coupling transport with chemistry in heterogeneous porous media”, *Computat. Geosci.*, 14 :465–481, 2010.

Laila Amir, Michel Kern, “Preconditioning a coupled model for reactive transport in porous media”, *Int. J. Numer. Anal. Model.*, 16(1) :18–48, 2019.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

Poster / 74

Low-field NMR studies to investigate the effects of salinity in the behaviour of brines within porous media.

Author: Aristarchos Mavridis¹

Co-author: Carmine D’Agostino²

¹ *University of Manchester*

² *The University of Manchester*

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Nuclear magnetic resonance (NMR) techniques have been used extensively for studying fluid behaviour in porous rocks, mainly through complementing other experimental processes, such as core flooding, as well as through NMR logging techniques. Common applications of these methods include determining the pore size distribution of the porous media, wettability characterization and fluid identification (Guo et al., 2020).

In this study, simple porous materials have been used as a substitute for rock samples, in order to look at the fundamentals behind the behaviour of brines within different porous media, which is of particular importance in applications such as enhanced oil recovery and CO₂ sequestration. Specifically, NMR relaxation/diffusion experiments have been performed on silica gel and alumina catalyst pellets, saturated with NaCl brines of various salinities (from pure water to 25% w/v NaCl) in order to investigate the effects of salinity on the water behaviour in terms of thermal diffusion and adsorption within the pore structures.

The ratio between the longitudinal and transverse NMR relaxation times T_1/T_2 is known to be proportional to the strength of the surface interactions between the fluid and the solid surfaces of the porous medium (D’Agostino et al., 2014). In our experiments, by increasing the salinity of the brines, a steady decrease in T_1/T_2 has been observed for the brines within the alumina samples, while a slight increase has been observed in the T_1/T_2 values of the brines within the silica samples. The results therefore suggest that increasing the NaCl concentration weakens the surface interactions between the brines and the alumina, while it strengthens the interactions between the brines and the silica pore surfaces.

A steady decrease in the NMR diffusion coefficients of the brines has also been observed in both alumina and silica porous media. This implies that the presence of NaCl within the solution hinders the mobility of the liquid within the pore structures. These results are consistent with the increase

in viscosity due to increased NaCl concentration as observed by other studies (Kwak et al., 2005), but could also be partially attributed to salt precipitation/deposition blocking the pore pathways.

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References:

Guo, J.-C. et al. (2020) 'Advances in low-field nuclear magnetic resonance (NMR) technologies applied for characterization of pore space inside rocks: a critical review', *Petroleum Science*, 17(5), pp. 1281–1297. doi: 10.1007/s12182-020-00488-0.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS20 / 75

Reduced-order model to investigate cell-scale hemodynamics through disordered porous networks of the human placenta

Authors: Eleanor Doman¹; Qi Zhou²; Miguel O. Bernabeu³; Timm Krüger²; Oliver E. Jensen⁴; Igor Chernyavsky⁵

¹ *University of Manchester*

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⁵ *Department of Mathematics & Maternal and Fetal Health Research Centre (School of Medical Sciences), University of Manchester, UK*

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The circulatory system in the human placenta consists of the separate maternal and fetal blood flows which are interlaced across a complex multiscale domain of porous regions and capillaries. As imaging techniques improve, we are able to construct representative porous domains, for organs such as the placenta, with a higher degree of accuracy [1]. High-resolution characterization of the human placenta can enable a greater understanding of the effect of pathologies on the placental transport of oxygen and nutrients. These transport mechanisms are fundamentally interlinked with

the geometry and topology of the placental porous domain and the dynamics of red blood cells (RBCs) within this space [2].

One possible avenue to utilize emerging imaging data is via high performance computing, which can be used in conjunction with lattice Boltzmann and immersed boundary methods to simulate the motion of a suspension of highly deformable RBCs through porous domains [3]. However, these simulations are computationally costly, restricting the domain size over which these simulations are tractable. An alternative method comes from the classic work of A. R. Pries and T. W. Secomb, who developed empirical laws for hemodynamics in microvasculature [4]. These laws are widely used in biomedical models, however they are developed based on experimental observations in long cylindrical vessels. As we explore more complex biological tissues, these empirical laws are less accurate and can lead to unphysical predictions of blood flow and oxygen distribution.

New techniques are needed to describe the flow of blood as a suspension of RBCs through porous domains. Pore-network models have long been used to describe flow through disordered irregular domains in areas such as geophysics. These reduced-order models are able to couple complex multiscale mechanics with scalability over a range of different domain sizes [5]. Here we demonstrate how pore-network models can be extended to include a description of particulate blood flow.

Principal component analyses of the RBC flow using lattice Boltzmann simulations suggest a clear dependence on non-dimensional geometric factors which differ from those within the Pries-Secomb formulation. We infer a novel reduced-order model utilising this new data. Disordered 2D porous networks are constructed by randomly placing non-overlapping discs on a plane and using Voronoi tessellation to identify pores and the throats connecting them. We test the reduced-order model by simulating flow through both regular and disordered 2D porous networks and by comparing the results against the quasi-3D lattice Boltzmann simulations.

Pore-network models are a powerful tool enabling us to model suspension flows through complex domains. Informed by recent progress in imaging, this work extends pore-network approach to nonlinear hemodynamics in disordered porous media. The developed methodology can be used to examine the structure-function relationship in the human placenta and other complex microvascular systems.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS08 / 76

Three-Dimensional Imaging of Density-Driven Convection in Unconsolidated Glass Packings and Consolidated Rock Samples Using X-Ray CT Scanning

Author: Anna-Maria Eckel^{None}

Co-author: Ronny Pini¹

¹ *Imperial College London*

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The determination of realistic rates of CO₂ dissolution associated with geological CO₂ storage in deep saline aquifers requires an understanding of the mixing process that takes place during the emplacement of CO₂ into these formations. The mixing process is triggered by the local density increase in the ambient brine following the CO₂ dissolution. As a result, gravitational instabilities occur, and perpendicular elongated finger-like patterns form that are enhancing the mixing between CO₂ and water compared to a purely diffusive process. This density-driven mixing process is important because it accelerates the CO₂ dissolution into brine and could eventually form a stable stratification in the aquifer, thereby reducing the chances of leakage.

Owing to the difficulty of imaging the time-dependent convective process, experiments so far have largely focused on two-dimensional systems (e.g., Hele-Shaw cells), which inherently limit the lateral spreading of the downwelling plumes. Here, we present the development of an experimental approach to investigate the evolution of the convective mixing process in three-dimensional porous media using X-ray Computed Tomography. To this end, we have considered both homogeneous glass-packs as well as consolidated rock samples, for which observations have thus far been lacking. To imitate the dissolution process of CO₂ in brine under laboratory conditions, a salt is used with a high X-ray attenuation coefficient that dissolves in water and creates a heavier solution than pure water. We explore a range of Rayleigh numbers and compute from the images the temporal evolution of several global quantities, including the total mass, the vertical centre of mass and the dilution index. The results on the uniform packings enable a direct comparison against results obtained with two-dimensional porous media and the associated scaling laws. We further observe that the mixing structures, that arise upon dissolution in the consolidated rock samples, differ strongly among those. To evaluate the porous media in terms of overall mixing efficiency, we compute the dilution index at the time of the onset of shutdown and we find a correlation of the dilution index with the characteristic length of the pore space. This suggests that mixing on the microscopic level plays a significant role and, apart from characteristics of the advective transport (such as permeability, included in the Rayleigh number), other microstructural features are influencing the overall mixing.

These observations provide therefore more representative information towards the investigation of convective mixing in the context of CCS as well as the selection and evaluation of sequestration sites.

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Time Block A (09:00-12:00 CET)

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MS10 / 77

3D X-ray velocimetry for pore-scale flows in geological and industrial porous media

Authors: Tom Bultreys¹; Stefanie Van Offenwert¹; Wannes Goethals¹; Jan Aelterman¹; Matthieu Boone²; Veerle Cnudde¹

¹ Ghent University

² Ghent University - UGCT

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Fluid dynamics in porous materials plays an important role in nature and in industry, e.g. groundwater flow in aquifers or the performance of filtration devices and porous catalysts. The intricate confining pore geometries in such materials can lead to complex flow phenomena, particularly during e.g. multiphase and non-Newtonian flows, which are difficult to reproduce in numerical or experimental model systems. A crucial impediment to investigate such phenomena is the current lack of methods to measure 3D, unsteady, pore-scale flow fields in most materials –despite advances in micro-particle velocimetry for optically transparent porous media (Roman et al. 2015, Datta et al. 2013) and MRI-based velocimetry for steady flows (De Kort et al. 2019). Here, we present new 3D micro-particle velocimetry results on flows in optically opaque porous media, based on time-resolved X-ray micro-computed tomography (micro-CT). We imaged the movement of X-ray tracing micro-particles suspended in single-phase flow, using laboratory-based fast micro-CT at frame rates on the order of tens of seconds and voxel sizes on the order of 10 μm . A Lagrangian particle tracking algorithm was then used to determine individual micro-particle paths through the pores, from which the 3D, 3-component velocity field in the pore space could be interpolated. The experimental methodology was validated by testing the workflow on simulated micro-CT datasets based on ground-truth particle tracks, and by comparing the experimental results to computational fluid dynamics results. The new method is readily extendable to even higher spatial and temporal resolutions, enabling its application to complex, unsteady flows in a wide range of porous materials of scientific and industrial relevance. It thus has the potential of causing a breakthrough in the study of flow in porous media.

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de Kort, D. W. et al. Under-sampling and compressed sensing of 3D spatially-resolved displacement propagators in porous media using APGSTE-RARE MRI. *Magn. Reson. Imaging* 56, 24–31 (2019).

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS06-A / 78

From Darcy flow to fingering instabilities in a fluid-driven silo**Authors:** Miles Morgan¹; David James¹; Martin Monloubou²; Bjornar Sandnes¹¹ *Swansea University*² *ENSTA Bretagne***Corresponding Authors:** b.sandnes@swansea.ac.uk, martin.monloubou@ensta-bretagne.fr, d.w.james@swansea.ac.uk, m.l.morgan@swansea.ac.uk

The flow of granular matter in silos has been extensively studied, largely due to its prevalence in industry. However questions remain, for instance regarding the nature of the velocity field, while work considering submerged, fluid-driven systems is somewhat scarce. In this work, fluid-driven granular drainage was performed in a quasi-two-dimensional silo with grains submerged in fluid. A variety of behaviours were observed, including Darcy flow through the static packing of the silo at low flow rates, Gaussian grain velocity profiles at moderate flow rates and finger-like instabilities at the upper grain boundary that penetrate the packing at high flow rates in addition to the occurrence of other transient phenomena. The transitions between these regimes are discussed and explored with the aid of phenomenological models.

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References:**Time Block Preference:**

Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 80

Microfluidic model of micro-haemodynamics in porous media**Authors:** Qi Chen¹; Naval Singh¹; Kerstin Schirrmann²; Igor Chernyavsky¹; Anne Juel¹¹ *University of Manchester*

² *The University of Manchester*

Corresponding Authors: anne.juel@manchester.ac.uk, igor.chernyavsky@manchester.ac.uk, qi.chen-27@postgrad.manchester.ac.uk, naval.singh@manchester.ac.uk, kerstin.schirrmann@manchester.ac.uk

The human placenta is an essential organ for the developing fetus, which relies on well-orchestrated haemodynamics to deliver its multiple functions [1]. The geometrical complexity of the placenta and lack of appropriate animal models mean that biomimetic laboratory models offer a powerful tool to investigate haemodynamics and haemorheology in the human placenta and other complex biological tissues [2, 3]. The placental microstructure is effectively a porous medium where the particulate nature of red blood cells (RBCs) is important. However, particle transport and its influence on permeability remain unexplored.

We use droplet and capsule suspensions in planar microfluidic porous media to explore the transport of deformable particles, with the aim of characterising rheology in this setting. Droplets are the simplest RBC analogues but they lack the shear elasticity of the real RBC. In addition, undesired coalescence and breakup limit their use in experiments. A better biomimetic model of RBC is provided by polydimethylsiloxane (PDMS) capsules of adjustable diameter and wall thickness, which are microfabricated using a 3D nested glass capillary device [4]. Their elastic modulus can be varied by an order of magnitude by adjusting the chemistry and the capsules can further be deflated by osmosis to match the area to volume ratio of real RBCs. We test the aptitude of these objects to mimic the motion and large deformations of single red blood cells and of suspensions of RBCs in straight capillaries and arrays of contractions and expansions. Planar porous media of controlled geometry, porosity and different levels of disorder are then constructed by positioning cylindrical pillars in different spatial arrangements within a Hele-Shaw channel. Suspension flows are characterised in terms of the dynamic capsule distribution, flow resistance and permeability as functions of hematocrit (concentration of capsules), capsule geometry, disorder of the medium and capillary number, which provides a measure of the importance of viscous shear forces relative to elastic forces.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

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Poster / 81

Particle migration and deposition at the pore scale: Eulerian-Lagrangian approach

Authors: Saeid Sadeghnejad¹; Frieder Enzmann²; Michael Kersten²

¹ *Department of Petroleum Engineering, Faculty of Chemical Engineering, Tarbiat Modares University, Tehran, Iran*

² *Johannes Gutenberg-University Mainz, Germany*

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Solute transport containing particles is essential in various applications, including filtration industry, subsurface contaminant transport in hydrology or environmental engineering, formation damage in the petroleum industry, and subsurface biocolloids or microorganism transport [1-4]. The evolution of pore-scale structure because of particle retention is a complicated process, which is a function of pore-scale heterogeneity and non-linear coupling of particle transport and fluid flow. Deposited particles alter the fluid flow fields at the pore scale, increase pore space heterogeneity, and impair the porosity and permeability of the porous medium. Pore-scale studies enable us to find effective mechanisms during particle transport.

Various modelling approaches were introduced to explain the retention mechanism of particle transport in porous media. Continuum-based numerical models can be used at representative elementary volume to explore solute transport in porous media. By solving the advection-dispersion equation, these models blur microscopic details and employ simplifying assumptions in the averaging process [5]. At the pore scale, the Lattice Boltzmann method (LBM), computational fluid dynamics (CFD), and pore network models (PNM) can be implemented to predict flow field variations. To track particles, the discrete element method (DEM) and Lagrangian CFD approaches are usually coupled with flow field predictors. Coupled methods enable us to study velocity fields, particle trajectory, spatial distributions, and residence time [2, 6].

This study incorporated the Eulerian-Lagrangian approach at the pore scale to investigate the spatial and temporal deposition of solute transport with particles. The velocity field and trajectory of particles were determined by solving the Navier-Stokes and momentum balance equations, respectively. When particle diameter is smaller than image voxel size, handling deposited particles can be challenging because many particles are required to occupy a pore voxel. Pore voxels adjacent to solid voxels are dynamically updated to trapped voxels when particles touching them have a comparable velocity to the adhesion forces of solid surfaces. The model was developed in Python and validated with the experimental data. Using an image-based technique, the portion of retained particles by surface deposition and clogging mechanisms were discriminated during various experimental simulation scenarios. Mean injection velocity, particle size and concentration, surface adhesion forces, and surface roughness are considered as sensitivity parameters. The results show that the role of the clogging mechanism rises by increasing the particle size, particle concentration, and surface adhesion forces much more than surface deposition. Hydrodynamic particle bridging can reduce structure permeability substantially compared to surface deposition. Particle retention at a critical velocity is maximum where the spatial deposition switches from filter cake development to homogeneous retention across the structure.

Acknowledgement

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS06-A / 82

Direct prediction of fluid-fluid displacement efficiency in ordered porous media using the pore structure

Authors: Tian Tian Lan^{None}; Ran Hu¹; Wei Guo¹; Guan-Ju Wei^{None}; Yi-Feng Chen¹; Chuang-Bing Zhou^{None}

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Fluid-fluid displacement in porous media is common in many natural and engineering settings. Extensive studies investigated the transition of displacement patterns, but the direct prediction of the displacement efficiency using the pore structure is lacking. Here, we propose a method to directly predict the displacement efficiency with no need of solving the Navier-Stokes and the Hagen-Poiseuille equations in ordered porous media. The predictive method originates from the pore-scale filling events, which can be divided into two directions such as the bulk flow direction and the transverse direction. For the bulk flow direction, the pore-filling event (burst) dominates the fluid invasion, and the invading phase forms a thin fingering channel. For the transverse direction, we introduce three invasion modes (compact, taper, and widen) to quantify fluid invasion. We can predict the finger width in each column, and the displacement efficiency can be predicted through the weighted average of the predicted finger width. We evaluate the predictive method using microfluidic experiments and pore-network simulations, confirming that the predictive method can reasonably predict the displacement efficiency in ordered porous media. The predictive method can directly predict fluid invasion according to pore structure, thus greatly improving the computational efficiency and is of significance in multiphase flow control.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS06-A / 84

Temperature Dependency of Steady-State Relative Permeability Curves: Aquistore CO₂ Storage Site, Canada

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Large-scale subsurface CO₂ storage has been recognized as a promising technology to mitigate carbon emissions in the atmosphere. Relative permeability with phase saturation is an essential flow parameter for quantifying and modelling injectivity, gas storage capacity, and containment of geological formations for CO₂ storage. The drastic impact of temperature fluctuations, due to CO₂ injection cycles in deep (hot) saline aquifers (e.g., Aquistore CO₂ storage site, Canada), on hydro-mechanical properties of rock has been well-established. However, experimental studies on temperature-dependent relative permeability have reported conflicting results regarding the consistency of shifts in end-point saturations and mobility. We implemented a series of core-flooding experiments on the deadwood sandstone (Aquistore) using the modified Hassler method in which two fluids are simultaneously injected into the core at declining brine fractional flow rates. Using this method, we present steady-state isothermal drainage relative permeability at three temperatures (20, 45, and 70°C) and 30 MPa effective confining stress. We find a systematic rightward shift in relative permeability curves in response to an increase in temperature. We further find a 10% and 48% increase in irreducible brine saturation and end-point gas mobility, respectively, increasing temperature from 20°C to 70°C. Intuitively, these results indicate an increment in rock's affinity to the brine (i.e., increase in hydrophilicity) with temperature. These experimental observations underscore the significant effect of temperature on multiphase fluid flow in porous media, leading to a more accurate characterization of fluid-fluid displacement mechanisms for CO₂ injection in deep saline aquifers.

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MS22 / 85

How to design a 3D ordered microstructure for redox flow batteries: A pore network modeling study

Author: Javad Shokri¹

Co-authors: Masoud Babaei¹; Vahid Niasar¹

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Amid growing energy demand and the progressive contribution of intermittent renewable energy, the need for large-scale energy storage systems have become critical. Redox flow batteries can be a

legitimate choice to store a huge amount of energy, subject to further improvement in their components, specifically the porous electrode. 3D printing technology is a viable method to manufacture porous electrodes with an engineered design and controllable properties. Attaining this goal requires an understanding of the effect of electrode microstructure which this study strove to provide. The effect of different parameters, including pore size, throat size, frequency of lattice units, and permeability anisotropy in the through-plane and in-plane directions were investigated in the flow-through as well as interdigitated batteries.

Pore network modeling was utilized to investigate the effect of microstructure on the performance of Hydrogen-Bromine (H₂-Br₂) flow batteries. Simulations were carried out under steady-state conditions for electrolyte transport, species transport, and charge transport. To isolate the role of microstructure on the performance of the battery, simulations were performed at the constant flow condition in which the advective force was constant.

The simulations were validated against the experimental study using an unstructured pore network, extracted from a tomography scan of a commercial carbon paper. A 3D printed ordered cubic lattice with the same permeability of the carbon paper showed a better performance. This was mainly achieved by better mass transport as a result of higher advection, diffusion, and lower tortuosity of the ordered lattice.

It was found that a combination of bigger pores and smaller throats at constant permeability, facilitated the diffusion rate especially in the in-plane direction, as well as, increased the specific surface area of the network. It was also shown that a larger number of lattice units, resulted in a higher surface area, consequently a higher current generation.

For both of the flow-through and interdigitated flow fields, permeability change in the through-plane direction (x-direction and y-direction) at the constant flow rate condition, almost did not affect the performance of the battery. However, the latter drastically changed the required electrolyte supplying pressure that could translate into a more economically feasible process. The permeability variation in in-plane direction reinforced or hampered the diffusion and also the current generation. Finally, an improved design of microstructure for the flow-through and interdigitated batteries were proposed and investigated. The specific surface area, permeability, and flow rate were kept constant to solely observe the role of microstructure on the battery performance. Results presented the superior performance of the improved microstructure in both flow fields. It was achieved by deviating the electrolyte main flow path, to the proximity of the membrane, where more reactions were taking place. This study took an initial step and provided insight into designing and manufacturing a porous electrode using 3D printing technologies. However, it can be continued in various paths including using complex 3D pore structures rather than simple cylindrical lattice to optimize the hydrodynamic behavior of the electrolyte and the specific surface area of the electrode.

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MS02 / 87

Effects of charring temperature on physicochemical properties of wheat straw biochar

Author: Mardin Abdalqadir¹

Co-authors: Tannaz Pak¹; Sina Rezaei-Gomari¹

¹ Teesside University

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Environmental management through the effective utilisation of biowaste has attracted significant attention in recent years. The production of biochar and its use in agriculture can play a vital role in climate change mitigation and support improve the management and quality of forestry and agricultural waste. Biochar is the carbonaceous, porous material that can be obtained from the conversion of bio-based waste commonly via the pyrolysis process at elevated temperatures. Variation in pyrolytic temperature affects the yield and nutrient composition of biochar. The selection of optimum pyrolytic temperature is crucial before using it for agricultural and environmental purposes.

This study examines the effect of pyrolysis temperature on the physical and chemical characteristics of biochar (BC) derived from wheat straw. The feedstock sample was heated at 100 °C/min to different temperatures of 300, 400, 500, 600, 700 and 800 °C and held at that temperature for 15 min (residence time). The samples are then cooled back down to room temperature.

The produced biochar samples at different temperatures were characterised for their pore structures, chemical functionalities, and mineral compositions to understand their physiochemical behaviour. We show that pyrolysis temperature plays a significant role in the formation of biochar microstructure. These biochar samples were utilised without any additional purifications/ treatments for their practical application as support materials for soil improvement and water treatment.

The results show that by increasing temperature, the biochar yield declines rapidly with the final yield of biochar of about 25% at 800°C. This can be attributed to a greater biomass 's decomposition at elevated temperatures. Furthermore, our analysis shows that at the higher pyrolysis temperatures the functional groups alter more significantly indicated by the relative change in the degree of polarity [(O+N)/C and O/C] and aromaticity (H/C) ratios. The existence of some inorganic components such as crystalline SiO₂ and CaCO₃ have been also detected. A higher amount of alkaline metals is found in biochar that is produced at above 500°C temperature (Mg, K and Ca). The SEM images demonstrated that as the temperature increased, the biochar particles became smaller and lost more of their original cell structures. However, BET Analysis showed that the surface area and micropore volume of biochar can be increased with charring temperature. The altered structure of biochar at elevated temperatures offers a large surface area, which is crucial in enhancing the soil arability, texture, and retention of nutrients and while also promoting the growth of beneficial microorganisms.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS07 / 88

A phase-field approach to model evaporation in porous media: Upscaling from pore to Darcy scale

Author: Tufan Ghosh¹

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¹ *Institute for Modelling Hydraulic and Environmental Systems (IWS), University of Stuttgart*

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We develop a phase-field model for evaporation in a porous medium by explicitly considering a vapor component together with the liquid and gas phases in the system. The phase-field model consists of the conservation of mass (for phases and vapor component), momentum, and energy. In addition, the evolution of the phase field is described by the Allen-Cahn equation. In the limit of vanishing interface width, matched asymptotic expansions reveal that the phase-field model reduces to the sharp-interface model with all the relevant transmission conditions at the moving interface. An energy estimate is derived, which suggests that for the diffusion-dominated regime, energy always decreases with time. However, this is not always the case for other regimes. The phase-field model is upscaled to the Darcy scale using periodic homogenization for the diffusion-dominated regime. The effective parameters at the Darcy scale are connected to the pore scale through corresponding cell problems.

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MS06-A / 89

Sol-gel transition in porous media by drying

Author: Romane Le Dizès^{None}

Co-authors: Leo Pel¹; Sara Jabbari Farouji²; Noushine Shahidzadeh³

¹ *Eindhoven University of Technology*

² *University of Amsterdam*

³ *University of Amsterdam -Institute of Physics*

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An important part of our cultural heritage, such as artefacts, statues or historical monuments, is exposed to chemical and physical degradation over time. The degradation can lead to fractures and loss of cohesion among the individual particles forming the porous materials used for their construction. Nowadays, the most promising route for consolidation of such weakened porous materials is the addition of colloidal solutions which undergo a sol-gel transition through evaporation of the solvent [1][2][3][4]. The consolidation treatment should not only restore the mechanical properties of the stone but also not change their physical appearance and other properties such as porosity or permeability. Therefore, an homogeneous distribution of the gel in the porous network of the material is very important. While the kinematics of transport and drying of Newtonian fluids in porous media have been widely studied by both experimental and theoretical approaches [5], the case of non-Newtonian fluids remains largely unexplored. This work focuses on viscoelastic fluids which undergo sol- gel transition upon drying.

Here, we present a multiscale study of the drying kinetics of solutions during the sol-gel transition in different type of porous materials. At the microscale, 2D micromodel porous media are fabricated and used to follow the dynamics of gelation during drying [6]. At the macroscale, the drying kinetics are studied on real stone samples of different porosities and pore size distribution. Highly advanced techniques such as NMR imaging and X-ray microtomography are used (Figure 1). The saturation profiles during drying and the localization of the sol-gel transition zones in the stones are investigated. Different drying regimes compare to Newtonian fluids are identified. Our results show that the duration of these different regimes remains strongly dependent on the intrinsic properties of the stones. Based on our NMR and X-ray micro tomography results, we discuss how a front that separates the liquid region from the gelified region can develop in the porous network and progress from the surface to the inner part of the stones. We show that the porosity, the pore sizes and the evaporative surface are strongly influencing the dispersion of the dry gel in the materials. Environmental factors (relative humidity and temperature) have also a big impact on the mechanisms of the gel formation, which can result in a non-homogenously distribution of consolidant in the treated stone.

We will also discuss the macroscopic mechanical properties such as the Young Modulus and the stress at break of the material before and after treatment. They reveal a significant mechanical strengthening and hence an efficient consolidation of the treated porous media.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 90

Digital Rock Techniques to Study Physical Properties of Hydrate-Bearing Sediments: Considering Hydrate Distribution Patterns

Authors: Yuqi Wu^{None}; Keyu Liu¹; Senyou An²; Chengyan Lin¹

¹ *China University of Petroleum (East China)*

² *University of Manchester*

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It is of great significance to study the physical properties of hydrate-bearing sediments (HBSs) for improving the recovery of the gas hydrate resource. Previous studies reveal that the hydrate distribution patterns and saturations affect the physical properties of HBSs. However, the experimental techniques are difficult to investigate the effects of hydrate distribution patterns and current numerical modeling methods cannot precisely control the hydrate saturations and distribution patterns. Therefore, a new hybrid and robust modeling method (CT-MO-QSGSM) for generating different distribution patterns and specific saturations of hydrates in digital models was proposed, which integrates the X-ray CT technique, morphological operation algorithm, and quartet structure generation set method. The presented method is used to produce a series of digital models containing pore-floating, cementing, and bridging hydrates with predefined saturations. Based on the digital models, a comprehensive investigation of the effects of the hydrate distribution patterns and saturations on pore/throat radius, coordination number, correlation functions, permeability, electrical conductivity, and elastic moduli of HBSs is implemented. The results indicate that the pore-floating hydrates lead to the most rapid decline in the pore/throat radius and correlation probability of pore space among the three types of hydrates, but they increase the average coordination number while others decrease the number. Moreover, the cementing and pore-floating patterns bring about the weakest and strongest damages to the permeability and electrical conductivity of HBSs containing low hydrate saturations, respectively. Among three patterns, the bridging type results in a rapid decline in these two properties when the hydrate saturation is high. Furthermore, the pore-floating and bridging patterns cause the largest and smallest increase in the elastic moduli. In addition, the physical properties of HBSs from the numerical simulations are consistent with the laboratory measurements, which proves that the generated digital models containing different hydrate distribution patterns are reliable.

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Poster / 91

Cr(III)-entrapped Nanocapsules Obtained via W/O/W Double Miniemulsion Nanoprecipitations of Hydrophobic Polymers for Delaying HPAM Gelation

Author: Jingyang Pu^{None}

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The main objective of a gel treatment in most mature oil fields is to improve the homogeneity of the reservoir by blocking highly permeable channels or fractures without damaging productive zones. In recent decades, Cr(III)-polyacrylamide (HPAM) gels have been extensively applied as blocking agents for sweep efficiency improvement. However, the gelation time of the current gels is not long enough for in-depth placement. This study systematically describes a novel approach of using nanocapsules to entrap and delay the release of crosslinking agents (Cr(III)) to extend gelation time. The nanocapsules are successfully prepared by a controlled nanoprecipitation of hydrophobic polymers onto stable aqueous droplets in a water-in-oil-in-water (W/O/W) double miniemulsion. The stable aqueous nanodroplets are obtained by inverse miniemulsions with an aqueous Cr(III) solution dispersed in an organic medium of solvent/nonsolvent mixture containing the hydrophobic polymer for the shell formation and an oil-soluble surfactant. The nanoprecipitation occurs when heating the mixture at 50°C which led to the evaporation of solvent and precipitation of the polymer into the interface of the aqueous droplets. Another water-soluble surfactant can also be pre-added into the aqueous Cr(III) solution to improve the precipitation efficiency of the polymer. The achieved nanocapsules show the size range from 200-1500 nm depending on the surfactant(s) type and concentration. A Cr(III) loading ratio of 5-20% is obtained by varying initial Cr(III) contents and polymer contents which is detected by Inductively coupled plasma - optical emission spectrometry (ICP-OES) measurements. Besides, the nanocapsules can be easily transferred into water and mixed with the HPAM solution. Gelation results prove that capsuled Cr(III) significantly delays the formation of the HPAM gel whose modified gelation time is dependent on pH and temperature.

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MS13 / 93

Gas Flow Simulation in Multiscale and Multimineral Digital Rocks of Shale Samples

Authors: Yuqi Wu^{None}; Keyu Liu¹; Chengyan Lin¹¹ *China University of Petroleum (East China)***Corresponding Authors:** 1650852619@163.com, wuyuqi150348@163.com, ycdzycmsi@126.com

The exploration and development of shale gas require accurate characterization of shale samples and modeling of gas flow. Digital rocks have been widely used to characterize the shale samples, predict their petrophysical properties, and understand the pore-scale transport mechanisms in micrometer and nanometer pore systems. Previous studies from numerous geologists have indicated that the shale samples involve multitype minerals and multiscale pore systems. Therefore, such factors must be considered when shale models are constructed and characterized. Nevertheless, the imaging techniques such as X-ray CT scanners and FIB-SEM have to make a balance between high resolution and large field of view. In other words, current 3D imaging techniques either cover the large-scale structures at a low resolution or cover a small region at a high resolution. To address this issue, this study proposes a novel modeling technique (DEM-QSGSA), called process-based modeling, which combines the discrete element modeling method (DEM) and quartet structure generation set algorithm (QSGSA). The proposed technique can generate various types of minerals (such as quartz, feldspar, calcite clay minerals, and pyrite) and pore structures (interparticle pores, intraparticle pores, and organic-matter pores) in digital models of shale samples.

On the other hand, numerous techniques such as the lattice Boltzmann method, molecular dynamics, direct simulation Monte Carlo, and pore network modeling have been used to study the transport mechanisms of shale gas. Among them, pore network modeling can precisely characterize the geometric and topological properties of pore space and consider the micro- and nanometer pore systems. However, the previous pore network modeling method cannot take all the mechanisms into consideration. Therefore, this talk will present a new pore network modeling method, which does not only account for the viscous flow, Knudsen diffusion, and surface diffusion, but also consider the shape and multiscale characteristics of pores and throats and phase behavior.

Finally, the gas flow will be simulated by the pore-network modeling method in the multiscale and multimineral digital models constructed by DEM-QSGSA. In order to evaluate the performance of the algorithms, multiple digital models of shale samples were constructed. The modeling accuracy of the methods was tested by comparing the petrophysical properties from the constructed digital models and experimental data.

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MS06-A / 94

A quantitative study of oil mobilization induced by water diffusion in n-alkane phases: from pore-scale experiments to molecular dynamic simulation

Author: LIFEI YAN^{None}**Co-authors:** Yuanhao Chang¹; S. Majid Hassanizadeh²; Senbo Xiao¹; Amir Raoof²; Carl Fredrik Berg³; Jianying He¹¹ *Norwegian University of Science and Technology (NTNU)*² *Utrecht University*³ *NTNU***Corresponding Authors:** jianying.he@ntnu.no, s.m.hassanizadeh@uu.nl, senbo.xiao@ntnu.no, a.raoof@uu.nl, carl.f.berg@ntnu.no, l.yan@uu.nl, yuanhao.chang@ntnu.no

Low-salinity water flooding is a promising technique for enhanced oil recovery in sandstone and carbonate reservoirs. Numerous mechanisms have been proposed to untangle the effect of a low concentration of dissolved salts in the flooding medium. Among the mechanisms, it is suggested osmosis may explain the observed remobilization of residual oil. However, the process of water transport through the oil phase, due to a salinity contrast, and its contribution to oil remobilization is not fully understood. In our study, we used three aqueous solutions and two alkanes in a series of microfluidic experiments with hydrophobically coated glass micro-chips for mimicking the low-salinity waterflooding process in an oil-wet rock formation. With three steps of liquid injection, we created multiple systems of low-salinity water/alkane/high-salinity water in the porous micro-model, and, afterward, continuously monitored the domain for 70 hours. The acquired images gave a direct pore-scale observation of the dynamic expansion in the trapped high-salinity water regions and its influence on the oil movements. Through the quantitative approximation, we noted that ionic strength and the hydrocarbon chain length both played important roles in water diffusion. A salinity contrast of 1.7 g/L-17 g/L caused higher water flow rates than 50 g/L-17 g/L for both alkanes. The difference in water flow rates between the case of 1.7 g/L- 17 g/L and the case of 50 g/L-17 g/L were not proportional to the salinity contrast during the experimental period. There was no a simple relationship between the chain length of hydrocarbon and water flow rate.. Moreover, to investigate the effect of salinity on water behavior in heptane, we conducted molecular dynamic (MD) simulations by considering three different concentrations in the high-salinity water region featuring our experiments. The results indicated that high salinity limited the diffusion of water from the high salinity region into the oil phase and reduced the possibility of water entering the heptane phase. Therefore, the net flux of water from the pure water side to the salty waterside was enhanced. MD simulations thus provided a better understanding of how water diffuses through an alkane phase due to the solubility difference and helped us explain the expansion of high-salinity water in microfluidic experiments.

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MS06-B / 95

Impact of Aqueous-phase Ions on Asphaltenic Crude Oil-Water Interfaces

Author: Ahmed M. Saad¹**Co-authors:** Stefano Aime ²; Sharath Mahavadi ³; Yi-Qiao Song ⁴; Maxim Yutkin ¹; David A. Weitz ⁵; Tadeusz Patzek ¹¹ KAUST, Saudi Arabia² ESPCI Paris, PSL University, France³ Schlumberger-Doll Research, USA⁴ Massachusetts General Hospital, USA⁵ Harvard University, USA**Corresponding Authors:** stefano.aime@espci.fr, weitz@seas.harvard.edu, smahavadi@slb.com, maxim.yutkin@kaust.edu.sa, ahmed.mohamedsaad@kaust.edu.sa, ysong5@mgh.harvard.edu, tadeusz.patzek@kaust.edu.sa

Displacement of crude oil with brine is one of the most widely implemented methods of oil production. The process is governed by the competition of surface and viscous forces. The polar components of crude oil adsorb at the oil/water interfaces, developing viscoelastic films that affect emulsion stability and adhere to reservoir rock minerals, making them more oil-wet and hindering oil extraction. Despite the substantial research conducted in this area, the underlying mechanisms are still unclear.

We look into the formation of crude oil/water interfacial films and show that it is a complex process ruled by competition among distinct species of polar molecules. Varying the chemical composition of the aqueous phase and the concentration of polar species in the oil, we demonstrate the impact on adsorption kinetics and the film elasticity. This study highlights the relation between the interfacial rheology and the chemical composition of the developed films. Also, the role of different salts in determining the composition of the interfacial films and the potential to tune this composition by adjusting the aqueous phase chemistry will be presented. Thus, this study provides insight into the mechanism behind rock wettability and emulsion stability, which are key in enhancing the oil recovery from mixed-wet reservoirs.

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Time Block B (14:00-17:00 CET)

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Poster / 96**Molecular Dynamics Study of Carbonated Water Confined in Nano Slit Illite Pore: Effect of the Layer Charge**Author: Masashige Shiga¹¹ *Geological Survey of Japan, National Institute of Advanced Industrial Science and Technology (AIST)***Corresponding Author:** mdridista.ms0323@gmail.com

Wettability is an essential property in terms of structural trapping, which is considered to be the primary mechanism of CO₂ geological storage [ref. 1]. Illite, a dioctahedral 2:1 phyllosilicate of common occurrence in soils and sedimentary rocks, is one of the main components of the caprock [ref. 1]. In this study, we focused on the interface of carbonated water and illite. This interfacial system is expected to occur when CO₂ dissolution has progressed for some time after injection, or when CO₂-dissolved water is injected. It is known that water forms a stable adsorption film [e.g., ref. 2-4] because water molecules interact strongly with the clay mineral surface. However, few studies have been performed to investigate the effect of the layer charge. How the water film is affected by the CO₂ concentration and the behavior of CO₂ is still not well understood.

This study investigated the interfacial structure and dynamics of carbonated water by using molecular dynamics simulations for illite slit systems with different layer charges.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

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Poster / 97

A multi-dimensional parametric study of variability in multi-phase flow dynamics during geologic CO₂ sequestration accelerated with machine learning

Authors: Hao Wu¹; Nicholas Lubbers¹; Hari Viswanathan¹; Ryan Pollyea²

¹ Los Alamos National Laboratory

² Virginia Tech

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Successful geologic CO₂ storage projects depend on numerical simulations to predict reservoir performance during site selection, injection verification, and post-injection monitoring phases of the project. These numerical simulations solve non-linear sets of coupled partial differential equations, while accounting for multi-phase fluid dynamics on the basis of constitutive equations that are embedded into the solution scheme. As a consequence, individual simulations often require tens to hundreds of hours to complete on high-performance computing clusters. Moreover, laboratory experiments reveal that parametric functions for capillary pressure and relative permeability exhibit substantial variability, even within the same rock type. This combination of computational expense and wide-ranging parametric variability means that there remains substantial uncertainty in the behavior of multi-phase CO₂-water systems, particularly in the context of feedbacks between relative permeability and capillary pressure. To bridge this knowledge gap, we develop a novel workflow that utilizes physics-based numerical simulation to train an artificial neural network (ANN) emulator for interrogating the multivariate parameter space that governs both capillary pressure and relative permeability. With this approach, the ANN is trained to emulate both fluid pressure distribution and CO₂ saturation, which are then interrogated quantitatively to generate parametric response surface mappings with high-fidelity resolution. Results from this study initially show that capillary entry pressure is the dominant control on both CO₂ plume geometry and fluid pressure propagation when considering the combined effects of capillary pressure and relative permeability, particularly when phase interference is low and residual CO₂ saturation is high. Moreover, the ANN emulator provides tremendous computational speed-up by computing 2691 individual simulations in several minutes; whereas, the same simulation ensemble would have required ~3 years of simulation time using only physics-based simulation methods (25,000 times speed up).

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MS03 / 98

Simulation of CO₂ mineral trapping and permeability alteration in fractured basalt: Implications for geologic carbon sequestration in mafic reservoirs

Authors: Hao Wu¹; Richard Jayne²; Robert Bodnar³; Ryan Pollyea³

¹ *Los Alamos National Laboratory*

² *Sandia National Laboratory*

³ *Virginia Tech*

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Basalt formations are potentially attractive targets for carbon capture and sequestration (CCS) on the basis of favorable CO₂-water-rock reactions, which result in permanent CO₂ isolation through mineral trapping. Recent pilot-scale experiments in Iceland and Washington state, USA, provide promising results that indicate rapid carbon mineralization occurs within basalt reservoirs. Nevertheless, transitioning these pilot-scale results to large-scale industrial CCS operations is fraught with uncertainty because fluid flow in basalt formations is governed by fracture-controlled hydraulic properties that are highly heterogeneous and difficult to map in situ. This uncertainty is exacerbated by feedbacks between multi-phase fluid dynamics (CO₂ and water) and fluid-rock reactions, which may result in a reinforcing feedback comprising CO₂ mineralization, permeability alteration, and fluid mobility. To begin to understand the feedbacks between multi-phase fluid flow and mineralization in fractured basalt, this study uses reactive transport simulation methods to model CO₂ infiltrating a meter-scale, synthetic basalt fracture overlying a storage reservoir while accounting for porosity change due to mineralization and its corresponding effect on permeability and fluid mobility. Results show that (i) carbonate and clay mineralization tends to occur downgradient of a fracture intersection, (ii) mineralization reduces porosity, which leads to permeability reduction and slows free-phase CO₂ migration, (iii) stronger porosity-permeability coupling increases the proportion of mineralized carbon while reducing CO₂ mass that can enter fracture, which may lead

to self-sealing behavior as fluid mobility approaches nil, and (iv) errors caused by unknown porosity-permeability relationships are small in comparison to errors that arise by omitting mineralization-induced permeability reduction when simulating CO₂ sequestration scenarios in basalt reservoirs.

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MS15 / 99

Multi-scale reconstruction of porous media from low-resolution core images using conditional generative adversarial networks

Authors: Yongfei Yang¹; Fugui Liu^{None}; Jun Yao¹

¹ *China University of Petroleum (East China)*

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Various rocks such as carbonate, coal or shale contain both micro- and macro-pores. To accurately predict the fluid flow and mechanical properties of these porous media, a multi-scale characterization of the pore space is of key importance. Hybrid superposition methods perform well in such multi-scale reconstructions, however, input images with two resolutions (high and low) and different reconstruction methods are required. In addition, the superposition algorithms are complex and human factors can introduce serious bias. Here we thus propose an effective approach based on conditional generative adversarial network (cGAN) for efficient and reliable multi-scale digital rock reconstruction based only on low-resolution core images. High-resolution core images with narrow field of view (FOV) and their corresponding large structure images were thus used to train the cGAN model. The model was validated with real sample images, and the model-generated images exhibited great agreement with the real pore structures. We also demonstrate that the cGAN model can generate images independent of the structure size. This work provides an advanced image-generating model based on deep learning, and therefore aids in better and wider pore-scale characterization and process modeling, to improve understanding of subsurface science and engineering processes.

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MS11 / 100

Geometric criteria for the snap-off of a non-wetting droplet in pore-throat channels with rectangular cross-sections**Author:** Chiyu Xie¹**Co-authors:** LUMING CHA²; Qihong Feng³; Matthew Balhoff⁴¹ *University of Science and Technology Beijing*² *China University of Petroleum*³ *China University of Petroleum (East China)*⁴ *University of Texas at Austin***Corresponding Authors:** fengqihong@126.com, coc1993@163.com, balhoff@mail.utexas.edu, chiyu.xie@gmail.com

Snap-off is a phenomenon that occurs when a non-wetting fluid is displaced by wetting fluid in pore-throat channels, leading to the breakup of droplets at the throat. Snap-off plays a key role in many industrial processes involving immiscible multiphase flows, such as aquifer remediation, carbon capture and geological storage, recovery of hydrocarbons. Here we derive geometric criteria for the capillary snap-off at the pore-throat junctions in 2D microchannels with rectangular cross-sections. The criteria are theoretically presented in three categories according to the range of the throat depth, h . We find that if h is smaller than the throat width, snap-off will be inhibited, if h is larger than the pore width, snap-off may occur but it is independent of h , and if h is in between the throat width and the pore width, a critical depth exists for the occurrence of snap-off. These criteria are verified using numerical CFD simulations and validated using microfluidic experiments. These results indicate the conditions for snap-off in the pore-throat channel with rectangular cross-sections, which clarify previous debates in the literature. One application of this work is for micromodels, which are porous microfluidic chips used as tools to observe multiphase flow in porous media at the pore scale. Most micromodels are two-dimensional (2D), which have rectangular cross-sections with uniform depth. The geometric criteria derived here provide guidelines for the design of micromodels used in the study of multiphase flow processes in porous media.

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MS15 / 101

Data-driven production optimization utilizing multi-objective particle swarm algorithm based on ensemble-learning proxy model

Author: Shuyi Du¹

Co-authors: Hongqing Song²; Chiyu Xie ; Wang Jiulong¹

¹ *University of Science and Technology Beijing*

² *Beijing University of Science and Technology*

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Production optimization plays an extremely significant role in closed-loop management of reservoirs, affecting the sustainability and profitability of reservoir development directly. Due to the uncertainty of geological structure and the complexity of multiphase flow, traditional physics-based numerical simulator methods tend to suffer from insufficient calculation accuracy and excessive time-consumption. This research establish an ensemble proxy-model-assisted optimization framework in a data-driven approach, combined Random Forest with Bayesian algorithm and multi-objective particle swarm optimization algorithm innovatively. It can optimize production quickly and effectively under the premise of ensuring safety as much as possible. After experimental testing, the ensemble proxy model of the injection-production system based on the BRF algorithm shows better performance in the prediction of dynamic parameters, which can replace the traditional numerical simulator. Compared with deep learning, the proxy model not only has higher prediction accuracy, but the time required for training is only 1/9 of the deep learning. In addition, relying on the ensemble proxy model, the injection mode adjusted by the multi-objective particle swarm optimization algorithm can reduce the gas-oil ratio and increase the oil production by more than 10% for carbonate reservoirs. Meanwhile, Pareto Frontier analysis can provide more options for project decision-makers to balance oil production and gas-oil ratio considering physical and operational constraints.

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Poster / 102

A novel microfluidic PEM water electrolyzer cell for the study of counter-current two-phase flow at the anode side

Authors: Nicole Vorhauer¹; Supriya Bhaskaran^{None}

Co-authors: Evangelos Tsotsas²; Tamara Miličić²; Vikranth Kumar Surasani³

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Driven by the aims to drastically reduce CO₂ emissions in several different sectors within the next decades, such as in the transport or the industrial production sectors, the substitution of fossil fuels by “green”hydrogen is widely considered. The hydrogen is “green”when it is produced emission-free and based on the use of renewable energy sources. Electrochemical splitting of water inside polymer electrolyte membrane water electrolyzers (PEMWEs) is one possibility for efficient and sustained production of “green”hydrogen. However, its efficiency is still limited by the coupled kinetics of flow and reaction that occur at the anodic side of the PEMWEs. Especially the microstructure inside the anodic porous transport layer (PTL) plays a major role for the counter-current transport of the feedstock water and the product oxygen.

In this work, a prototype model of a microfluidic PEMWE cell was tested with the purpose to experimentally examine the two-phase flow in the anodic PTL (Fig. 1). The cell is made of transparent PMMA (Poly-Methyl-Methacrylate) in order to allow monitoring of the fluid flow. The anodic PTL is represented by a quasi 2D pore network with distributed pore sizes, similarly as in previous work [1, 2]. However, in contrast to previous works, the microfluidic device is realized as a full electrochemical cell. Thus, the gas phase is not injected at a discrete point, but generated at an electrically activated catalyst coated membrane with iridium oxide on the anode side and carbon supported platinum on the cathode side. Platinum meshes were used as current collectors on both sides.

The microfluidic electrochemical cell is used to study the correlation of gas-liquid invasion patterns in dependence of the pore network structure as well as of the applied current densities and stoichiometry of flow rates. In contrast to more advanced measurements like operando neutron imaging [3], the simplified quasi 2D structure allows to study the invasion profiles directly. In addition to that, very good comparison of the experimentally recorded profiles to simulation results, e.g. from Lattice Boltzmann simulation [4], is given.

Keywords: PEMWE; microfluidic cell; anodic porous transport layer (PTL); counter-current transport; invasion regimes; current density; pore-scale physics.

Figure 1: Schematic representation of PEMWE cell

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Participation:

In person

MS06-A / 105

The influence mechanism of pore structural properties on gas hydrate saturation and permeability via micro-CT technology

Authors: Huaimin Dong¹; Jianmeng Sun²

¹ *School of Geological Engineering and Geomatics, Chang'an University*

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Gas hydrate, as an alternate hydrocarbon source, has attracted significant attention in past decades. A precise estimation of permeability of the gas hydrate-bearing formation is essential for predicting the flow behaviors and the associated gas production performance. In this research, the influence of gas hydrate saturation on pore structural properties and then affect permeability was investigated using a three-dimensional micro-CT dataset that records an experiment of xenon hydrate formation in a sand pack at selected times during the experiment. Unlike the previous work, the goal of this work is to characterize pore space evolution, during gas hydrate formation, using a set of key microscopic pore characteristics, i.e. pore and throat radii, pore throat ratio, coordination number and tortuosity, by applying pore network analysis, on larger and therefore more representative sub-volumes. The same segmented volume of that dataset was used in this work to estimate gas hydrate saturation and permeability, recalculated by the lattice Boltzmann method, on those larger sub-volumes at selected snapshots. Besides, the analysis provides further insights into the links of gas hydrate localities and local pore characteristics and therefore their controls on the permeability. New evidence of semi-quantitative nature emerges that grain-coating gas hydrate formed at low gas hydrate saturations play a crucial role on reducing permeability, while pore-filling and/or cementing gas hydrate become dominating at high gas hydrate saturations, and these can be explained by gas hydrate formation mechanisms.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

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MS05 / 106

Visualizing biofilms within porous media using contrast-enhancing staining agents

Author: Laurenz Schröer¹

Co-authors: Tim De Kock²; Tim Balcaen³; Greet Kerckhofs⁴; Karel Folens⁵; Nico Boon⁵; Veerle Cnudde⁶

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Bacteria colonize almost every habitat, including porous media such as rocks, sediments and soils. They are usually attached to the surface and agglomerated in biofilms. The location, extent and composition of the biofilm depend on the environmental conditions and chemical and physical characteristics of the material (Miller et al., 2012). They affect the material properties and influence fluid transport by obstructing the pore space, reducing the permeability and hydraulic conductivity (Baveye et al., 1998). Their influence is investigated for numerous industrial fields as they could contribute to wastewater treatment (di Biase et al., 2019), bioremediation of groundwater (Meckenstock et al., 2015) and carbon dioxide sequestration (Ebigbo et al., 2010).

It is important to visualize biofilms within a porous rock, know their location, and understand their effect on fluid flow inside the pore system. Within porous media, this could be achieved by X-ray

micro-computed tomography (μ CT). However, distinguishing biofilms from the pore fluid, such as water, is hard due to a similar X-ray attenuation coefficient. Contrast-enhancing staining agents (CESAs) could enhance the X-ray attenuation, and a few CESAs such as particulate BaSO₄ (Davit et al., 2011), silver-coated microspheres (Iltis et al., 2011), 1-chloronaphtalene (Rolland du Roscoat et al., 2014) proved to be successful. However, these CESAs have some drawbacks, such as sedimentation, heterogeneous distribution of the particles and the fact that they change the pore fluid properties, such as the viscosity and wettability (Carrel et al., 2017). FeSO₄ could overcome these drawbacks (Carrel et al., 2017), and other CESAs, like Mono-WD POM and Hf-WD POM, could be interesting as they proved to be powerful staining agents for tissues (de Bournonville et al., 2020).

Within this research, numerous CESAs (KBr, FeSO₄, BaCl₂, Hexabrix, CA⁴⁺, Mono-WD POM, Hf-WD POM and Hexabrix) were tested that bind to the biofilm, and which could afterwards be replaced by the original pore fluid. These CESAs were screened for their potential to stain bacterial biofilms in between sand grains and on stones. The biofilms were imaged by HECTOR at the Centre for X-Ray Tomography (UGCT) of Ghent University (Masschaele et al., 2013).

In our experiments, most CESAs had a limited effect on the X-ray attenuation of the biofilms. However, Hf-WD POM and isotonic lugol were very promising CESAs for biofilm visualization using μ CT. Both were able to visualize cyanobacterial biofilms on rocks. Isotonic lugol led even to the visualization of (bundles of) filaments, and provides opportunities for future 3D microbial mat visualization. Moreover, it was possible to image and quantify the spatial distribution of biofilms inside a sand column.

Hf-WD POM and isotonic lugol create thus new possibilities to increase our understanding of the effect of biofilms on the pore scale. It could be possible to directly visualize their effect on flow paths, flow velocities and pressure gradients during a dynamic μ CT experiment. Moreover, μ CT could link the presence or absence of biofilms with changes in the pore system, including dissolution or precipitation.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

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Poster / 107

Experimental evaluation of percolation in evolution of flow

Authors: Samaneh Vahid Dastjerdi^{None}; Nikolaos Karadimitriou¹; S. Majid Hassanizadeh²; Holger Steeb³

¹ *Institute of Mechanics (CE), Stuttgart University*

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Many real-life applications are dependent on the physics of multiphase flow in porous media. Some important examples are geological carbon sequestration [1], enhanced oil recovery [2], and remediation of groundwater/soil contaminated by a non-aqueous phase liquid (NAPL) [3]. The predictability and efficiency of the aforementioned scientific and industrial applications rely on developing a robust constitutive theory of two-phase flow in porous media. However, currently-used theories [4, 5], which involve capillary pressure and saturation, are not capturing the process- and history-dependent nature of the flow adequately.

To address this deficiency, some theories of porous media have been extended during the last decades. For instance, Hassanizadeh and Gray [7, 8] developed a macroscale theory for two-phase flow, in which they introduced the interfacial area between the three phases as additional state variable in describing two-phase flow ($P^c = f(a^{ns}, a^{ws}, a^{wn}, s^w)$). Later, Hilfer and Doster [9] showed that with a phenomenological approach they are able to reproduce experimental findings for capillary pressure and saturation, by differentiating between a percolating and a non-percolating saturation for the fluid phases. Although there has been extensive improvement in reproducing the hysteretic behaviour of the processes, the numerical and experimental investigations about the mentioned theories have not been able to prove their unconditional validity and show that they are dependent on the displacement process, the capillary number and the viscosity ratio under which the study was performed [6, 10].

In this work, we aim at examining the two aforementioned theories [7, 8, 9] by combining microfluidic experiments, optical microscopy and image processing techniques. We put the hypothesis of a potential synthesis of these theories at test, by investigating the role of interfacial area as a separate state variable, while making the distinction between connected and disconnected to the reservoir phases (percolating and not). We performed flow-controlled microfluidic experiments, consisting of sequential drainage and imbibition cycles. Subsequently, the images recorded during the experiments were processed and, among other parameters, the interfacial area, the curvature and contact angle of the terminal menisci were extracted. Using Young-Laplace equation, the capillary pressure associated with each wetting/non-wetting interface was calculated and averaged over interfacial area. Then, a simple, but physically-motivated, function was fitted to the experimental data for phase saturation, capillary pressure, and interfacial area. This was done once for all terminal menisci

between the wetting and the non-wetting phase, and then separately for the percolating phase only. Our experimental results so far show that by taking the disconnections as a topological measure into account, we are capable of modelling the apparent hysteresis between capillary pressure and saturation more effectively than only having interfacial area as a state variable. The fitting seems to be valid for quasi-static as well as dynamic conditions irrespective of the displacement process, the capillary number and the viscosity ratio. We hypothesize that there can potentially be a single unique surface for a certain solid-fluids system, on which all triplets, for all combinations for the capillary number and viscosity ratio would land.

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Participation:

Unsure

Poster / 108

Experimental Studies on Permeabilities of Thin Fibrous Materials

Authors: Luwen Zhuang^{None}; S. Majid Hassanizadeh¹

¹ *Utrecht University*

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Knowledge of hydraulic properties is crucial for understanding and modeling fluid flow in thin porous media. In this work, we have developed a new simple custom-built apparatus to measure permeabilities of a single thin fibrous sheet in in-plane direction. The permeability was measured for two types of thin fibrous porous materials using either water or gas phase. For each thin fibrous layer, the measurements have been done for different fiber alignments with flow. The results have shown that the measured permeability values using gas phase were slightly larger than the ones obtained using water phase. The largest permeability value was found when the flow direction was paralleled to the orientations of most fibers.

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MS22 / 110

Optimisation and characterisation of a dual porosity medical grade porous medium for personalised inkjet printed dosages applications

Authors: Hamed Aslannejad¹; Tamanna Lashkari^{None}; Elmin Breejen^{None}; Robbert Jan kok^{None}; Rainer Helmig²; Oliver Röhrle²; S. Majid Hassanizadeh³

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Personalized medicine enables tailored therapy, best response, and lowest side-effects to ensure better patient care. By means of inkjet printing technology, personalized medicine can be provided precisely, efficiently and affordably. In this work, we introduce a methodology based on inkjet printing which uses a porous substrate as carrier for Active Pharmaceutical ingredient (API). The porous substrate needs to have certain properties to uptake the API fast, distribute it uniformly, and realize it based on desired profile. To meet these criteria, a set of experiments has been designed and conducted. A list of required ingredients, granulation and tableting methodology have been identified to produce a Dual porosity porous tablet which fulfills required above-mentioned criteria as well as necessary mechanical strength before and after print. The pore network of the tablet was characterized to extract porosity, pore size distribution, connectivity, and permeability of the domain. Furthermore, the pore network of the tablet was extracted to be used in pore-scale two-phase

flow simulation to study the movement of API inside the domain. The results of the model, yielded in appropriate printing process parameters.

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MS11 / 111

Influence of solute transport and capillarity on bubble evolution in porous networks

Authors: Nerine Joewondo¹; Valeria Garbin²; Ronny Pini¹

¹ *Imperial College London*

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Understanding the temporal and spatial evolution of bubbles in porous media is key to applications such as gas storage in subsurface rocks, air-entrained concrete, and contaminants transport in soil. In the simplest case of a spherical bubble in unconfined bulk liquid, the evolution of the bubble can be predicted by considering its capillary pressure and the solute concentration in the liquid layer adjacent to the bubble/liquid interface. The presence of a porous medium complicates the growth and dissolution process, by introducing two controlling factors. First, as a bubble grows beyond the size of a pore body, its capillary pressure depends not only on its volume, but also on the local network geometry [1,2]. Second, the pore network limits transport fluxes from/to the bubble and leads to local concentration development, yielding a non-uniform solute concentration field [3]. The experimental evidence of the evolution of bubble lattices in porous media have been so-far quite limited.

Here, we investigate the mechanisms controlling the evolution of a bubble lattice in a porous network by comparing simulation results from a pore-network model [3] to microfluidic experiments. The pore-network simulation couples solute transport and bubble dissolution processes and outputs the temporal evolution of bubble radius and solute concentration on a pore-by-pore level. The experiments were performed with CO₂ and water at isothermal, ambient conditions within three distinct two-dimensional glass micromodels that feature a regular pore-network differing solely in the throat diameter. An image processing routine was developed to extract the temporal evolution of size and local curvatures of each bubble. We observed distinct modes of bubble growth and dissolution. The relative differences between the capillary pressure of a bubble and the value of its immediate neighbours were computed at each time. We analysed the relationship between the rate of change of the bubble volume and this “relative” capillary pressure to identify both linear and non-linear regimes. The absence of a linear regime during bubble dissolution (or growth) provides direct evidence that

the process is not solely controlled by capillarity, but also by transport and accumulation of solute in pores.

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS04 / 112

A shrinking pore network model for drying porous media

Authors: Xiang Lu^{None}; Abdolreza Kharaghani¹

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In the context of pore network modeling of drying porous media, the pore structure of porous media is often assumed to remain stationary during the drying process. Based on this simplification, several studies have been conducted that resolve and also raise many interesting and important algorithmic and application questions. However, questions remain on how the pore structure of drying porous media changes over time and how much the overall rate with which liquid is evaporated from such media can be impacted. This work seeks to provide fundamental insights into this topic by means of a shrinking pore network model. This model accounts for intraparticle mass transfer in a drying porous medium, morphological changes of its pore structure, and the connection to the medium's surroundings. The pore network model is defined on, initially, a regular three-dimensional lattice of spherical pores and cylindrical throats, and it accounts for forces caused by the capillary pressure acting on the solid matrix. Under the capillary pressure, the effective force acting on the invaded throat increases the throat radius while the neighboring throat size decreases. Thus, some throats or pores may close. After each invasion, the liquid is redistributed, and pore/throat sizes are updated accordingly. Compared with stationary pore network models, the drying kinetics predicted by the shrinking pore network model shows a sharp drop in evaporation rate but a relatively longer first drying period. As regards the volume reductions, three periods can be distinguished: The change in the volume of the porous medium is not evident at the beginning and is followed by a linear

shrinkage, whereas the volume reduction rate decreases in the second drying period and approaches zero by the end of the drying process.

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MS04 / 113

Extraction of pore networks from X-ray images of single wood particles subjected to drying

Authors: Jing Chen¹; NingHua Zhan²; Xiang Lu^{None}; Rui Wu³; Abdolreza Kharaghani⁴

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Wood exhibits complex anatomical features that make it hierarchically structured, heterogeneous, and anisotropic material. To obtain realistic predictions of drying behavior of intricate porous media as such by computational means, it is crucial to develop intraparticle models of transport phenomena that account for the spatial heterogeneity of the medium properties and directional anisotropy to convective and diffusive fluxes. Multiple efforts to this end thus need to be undertaken. This work essentially seeks to properly characterize the intricate pore structure of single wood particles dried under different well-controlled conditions. Gravimetric drying experiments are carried out using a magnetic suspension balance. In-situ X-ray tomograms are deployed to determine the porosity, pore size distribution, specific surface area, and structural anisotropy of single particles. An image-based algorithm developed based on the concept of omnidirectional Euclidean distance is utilized for mapping pore networks onto the void space of single wood particles. This method of pore network extraction not only preserves the topological and morphological properties of anisotropic pores in wood samples but also is robust and insensitive to image noise.

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MS09 / 115

Pore-scale modelling of non-isothermal reactive transport based on the micro-continuum approach: application to coke combustion in a matrix-fracture system

Author: Qianghui Xu¹**Co-authors:** Junyu Yang¹; Zhiying Liu¹; Lin Shi¹¹ *Tsinghua University***Corresponding Authors:** xuqh12@tsinghua.org.cn, rxnsl@mail.tsinghua.edu.cn, liuzhiyi18@mails.tsinghua.edu.cn, yang-jy17@mails.tsinghua.edu.cn

Non-isothermal reactive transport in complicated porous media is diverse in nature and industrial applications. This study focuses on coke combustion during in situ crude oil combustion techniques, which is an advanced recovery technique to exploit heavy oil in the fractured reservoir. There are challenges in modelling the multiple thermal and physicochemical processes in the multiscale matrix-fracture system, which contains nanometer-range coke pores, micrometer-range matrix pores, and a sub-millimeter-range natural fracture. In the present study, a pore-resolved micro-continuum approach was used to couple the weakly compressible gas flow, species transport, conjugate heat transfer, heterogeneous coke oxidation kinetics and structural evolution. Image-based simulations were implemented on synthetic geological models, mimicking coke deposition habits based on tomography images. The sub-resolution nanoporous coke region was treated as a continuum, for which the random pore model, permeability model and species diffusivity model were integrated as sub-grid models to account for the unresolved reactive surface area, Darcy flow, and Knudsen diffusion, respectively. Combustion regime diagrams for coke combustion in the unfractured fractured media were mapped with axes of the ignition temperature and the air flux. They were compared to address the influence of the natural fracture on the oxygen transport and burning temperature. The oxygen diffusion mechanism was found to dominate the oxygen transport from the fracture into the matrix and lead to desirable smouldering combustion temperature regardless of the air injection rate. Effects of fracture geometries were quantified to demonstrate tortuous and discrete fractures, and well-matched air injection rates with fracture apertures can effectively suppress the air channeling risk. Possible discrepancies between lab measurements and field operations were demonstrated due to the inconsistent air flux so that the misinterpretation of experimental results for field applications can be avoided. The present pathway from tomography image to synthetic image and to numerical simulation extends the “image and compute” technique to solve multiscale and non-isothermal reactive transport.

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MS06-A / 116

Quantitative determination of the threshold pressure for a discontinuous phase to pass through a constriction using microscale simulation

Authors: Gloire Imani¹; Zhang Lei¹; Martin Blunt²; Xu Chao¹¹ School of Petroleum Engineering, China University of Petroleum, Qingdao, Shandong 266580, China² Department of Earth Science and Engineering, Imperial College London, SW7 2AZ, UK**Corresponding Authors:** m.blunt@imperial.ac.uk, 642608830@qq.com, zhlei84@163.com, migthebest27@gmail.com

The displacement of oil by water in a porous rock leads to a disconnection of the oil phase as a result of the competition of viscous and capillary forces. In this study, we performed two-dimensional numerical simulations where the Navier-Stokes equations are coupled with the phase field method to capture the dynamic behavior of a single oil droplet in a capillary channel with a constriction. We investigated the effects of contact angle, the radius of the constriction and droplet size, and their coupled effect. The numerical results indicate that the droplet can be pushed through the constriction at capillary numbers of approximately 10^{-4} for water-wet condition, while the droplet is observed to break for oil-wet condition at the same capillary numbers. Classical theory states that the viscous pressure must overcome the capillary pressure for a droplet to pass through a constriction. However, the analysis of the two forces have shown that the viscous pressure doesn't always have to overcome the capillary pressure for a droplet to pass through a constriction, for example in the case where the radius of the constriction of the pore space is less than four times the radius of the widest region, the capillary pressure is larger than the viscous pressure which is contrary to the classical theory. The pressure to be applied for the droplet to pass through the constriction is larger at small constriction radii and for larger droplets. This behavior becomes more significant when the wettability surface condition is strongly water-wet. Through regression analysis, a mathematical model to determine the threshold pressure required to displace the droplet is established.

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MS09 / 117

Lattice Boltzmann modeling of the interfacial mass transport and heterogeneous chemical reaction in the multiphase system: numerical models and applications**Author:** Junyu Yang¹**Co-authors:** Qianghui Xu¹; Zhiying Liu¹; Lin Shi¹¹ *Tsinghua University***Corresponding Authors:** yang-jy17@mails.tsinghua.edu.cn, rxysl@mail.tsinghua.edu.cn, liuzhiyi18@mails.tsinghua.edu.cn, xuqh12@tsinghua.org.cn

Multiphase reactive transport in porous media is widely encountered in natural and engineering processes. Pore-scale modeling is an effective means to understand the mechanism of the multiphase reactive transport, but the related models still need development. In the present work, we proposed a multiphase mass transport numerical model based on the lattice Boltzmann (LB) method, referred to as the CST-LB model. This model involved continuum species transport (CST) term into the mass transport LB model to simulate interfacial species transport within the multiphase system, which is compatible with different multiphase LB models. We combined the CST-LB model with the multicomponent multiphase pseudopotential model to simulate multiphase mass transport with a large solvent's density ratio and different solute's Henry coefficient. The boundary schemes were also proposed to simulate heterogeneous chemical reactions in the multiphase system. For the CST-LB model, a lattice-interface-tracking scheme of the heterogeneous chemical reaction boundary was provided. Meanwhile, the local-average virtual density boundary scheme for the multicomponent pseudopotential model was formulated to avoid the unphysical mass transport layer caused by traditional wetting boundary treatments. The solid structure evolution during the multiphase reactive flow was also concerned and the numerical implementation of multiphase flow, interfacial mass transport, and heterogeneous chemical reaction was coupled. A series of benchmark cases have been carried on to validate the accuracy of the present models, which showed excellent numerical performance. Finally, we applied the proposed models to simulate complicated processes of methane hydrate dissociation in the sediment and discussed the role of mass transport on the dissociation behavior. Different dissociation patterns were identified under various water saturation and fluid velocities. The limitation effect of mass transport on the dissociation rate was quantified and upscaling parameters such as permeability curves were obtained. The proposed numerical models provided the solution to investigate multiphase reactive transport in porous media, which can also be applied for numerous engineering scenarios.

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MS10 / 119

Three-dimensional imaging of pore-fracture propagation in Triassic tight sandstones of the Ordos Basin, Northern China**Author:** Songtao Wu^{None}**Co-authors:** Zhichao Yu ; Xiaohua Jiang ; Ling Su ; Hua Tian ; Fengrong Liao ; Cong Yu**Corresponding Authors:** yucong87@petrochina.com.cn, suling2200@petrochina.com.cn, jiangxiaohua69@petrochina.com.cn, tianhua86@petrochina.com.cn, yuzhichao@petrochina.com.cn, liaofengrong@petrochina.com.cn, 326685139@qq.com

The characteristics of fracture propagation in heterogeneous tight sandstones are critical to volumetric fracturing, which is the key to unlocking unconventional resources in tight sandstones. Quantification of the influence of pre-existing pore systems and particle arrangements on the propagation of fractures is challenging due to inadequate imaging of the internal void systems in tight sandstones from three-dimensional (3D) aspect. In this study, the 3D geometry of tight sandstones from the Upper Triassic Chang 7 member in the Ordos Basin is continuously imaged under different loading stresses, and the voxel resolution of the X-ray computed tomography is 2.5 microns. The data set captured in this process shows the changes in the samples at the microstructural level as they approach fracturing. The data are stored as a time series of 3-D images. The results demonstrate that: (i) fractures propagate progressively and gradually link with pre-existing pores, resulting in macroscopic fractures with a maximum width of 250 microns, while newly generated fractures could break up particles and may not follow the line of pre-existing fractures; and (ii) three stages were identified in the failure process of tight sandstones, with new fractures running at an angle of about 30° to the general direction of the stress of compression. The total volumes of both the sample and pore-fractures, and the damage index, which were extracted from the 3D images, all increased when approaching fracturing. The final volume of pore-fracture systems could be 11 times that of the initial pore volume. All of these observations provide valuable insights and design guidelines for hydraulic fracturing in unconventional tight sandstones, and a quantified model of the dynamics and the morphology of fracture propagation with increasing stress approaching failure, which may shed light on dynamic critical transitions in the Earth's crust.

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MS04 / 120

Modelling pharmaceutical tablet swelling using discrete element modelling and a single particle swelling model

Author: Mithushan Soundaranathan¹

Co-authors: Mohammed Al-Sharabi²; Thomas Sweijen³; Kendal Pitt⁴; Axel J. Zeitler²; S. Majid Hassanizadeh³; Blair Johnston¹; Daniel Markl¹

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PURPOSE

Typical pharmaceutical tablets are porous media made through the compaction of a powder blend that consists of a drug substance and excipients. Most tablets have to break up into smaller fragments when they come in contact with a physiological fluid to accelerate the release of the drug – a critical quality attribute of solid oral dosage forms. This break up is caused by the swelling of individual particles in a tablet that leads to the interruption of the interparticulate bonds. The swelling is initiated by the wetting of the particles in the porous tablet and therefore the liquid uptake process is a prerequisite to initiate the swelling and eventually the break up. Since these critical processes, i.e. liquid uptake, swelling and break-up, directly impact the performance of tablets, it is crucial to have a deep understanding about these mechanisms and how they are linked to the raw material attributes and manufacturing conditions. This study focused on modelling the swelling of a tablet using discrete element modelling (DEM) paired with a single particle swelling model [1,2] and experimental liquid penetration depth data.

METHODS

The modelling consists of three different steps: 1) simulation of compaction to generate a particle configuration in DEM to represent the tablet, 2) modelling swelling of a single particle [2] and 3) modelling tablet swelling by integrating the single particle swelling model in the DEM tablet model. The particle-particle interaction in the DEM compaction model was described by the Luding elasto-plastic contact model [3] using YADE-DEM [4]. The parameters of the Luding contact model were calibrated using experimental compaction data of the materials. The analysis was conducted for microcrystalline cellulose (MCC) (Avicel PH101, Roquette, Lestrem, France) and croscarmellose sodium (CCS, FMC International, Philadelphia, USA). Experimental data to test the model for tablet liquid penetration and swelling was measured by a flow through cell [5] coupled with a commercial terahertz system (TeraPulse 4000, Teraview Ltd., Cambridge, UK).

RESULTS

The DEM modelling parameters were calibrated for MCC PH101 and CCS with an RMSE of 0.022 (-) for a porosity of 15%. The calibrated parameters were tested for tablets with porosities of 10% and 20% giving an RMSE of 0.025 (-). The tablet swelling was experimentally measured as a change in height at a single point on the tablet surface which was replicated in DEM. Experimental results showed that tablets with higher porosity swelled faster than tablets with lower porosity, also liquid penetration rate was faster in high porosity tablets. The results from tablets consisting of a mixture of MCC PH101 and CCS showed that an increase of CCS content resulted in a lower tablet swelling, even though the swelling capacity of single particles of CCS is higher than of MCC PH101 [2].

ACKNOWLEDGEMENTS

The author would like to thank the National Manufacturing Institute for Scotland for funding this work.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS06-B / 121

Comparison between secondary and tertiary low salinity waterflooding in carbonates: pore-scale processes, wettability changes and recovery

Author: Ahmed Selem^{None}

Co-authors: Nicolas Agenet¹; Branko Bijeljic²; Martin Blunt³

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Improving oil recovery from existing fields is an essential element in the energy transition to help meet the world's energy demand in an efficient and sustainable manner while exploration for new fields is in decline. Many lab experiments and field trials have highlighted the potential of low salinity waterflooding (LSW) as a prominent enhanced oil recovery (EOR) technique. The main advantages of LSW over the other EOR techniques include its enhanced performance, and simple and environmentally friendly field implementation.

Previous experimental work investigating LSW was performed mainly at the core or atomic scales where there are limitations to understand the mechanisms responsible for the low salinity effect (LSE) on a natural rock at reservoir conditions. In this work, comprehensive experimental studies of both secondary and tertiary LSW were performed to shed light on the pore-scale processes and correlate them to wettability changes and oil recovery. To reach initial wetting conditions found in oil reservoirs, two limestone rock samples were continuously injected with crude oil at 1 $\mu\text{L}/\text{min}$ at high pressure and temperature for three weeks. In the secondary mode, the oil-saturated sample was injected with low salinity brine at increasing flow rates. In the tertiary experiment, low salinity brine was injected after a sequence of high salinity floods. X-ray micro-computed tomography (micro-CT)

was used to image in situ waterflooding. Pore-scale displacement processes, wettability alterations and oil recovery were captured and analysed using high-resolution micro-CT images.

Pore occupancy analysis showed oil redistribution during secondary LSW; oil was displaced from smaller to larger pores and eventually recovered as more pore volumes of brine were injected. In tertiary LSW, oil was observed in layers confined to pore walls and was trapped to pore corners after the high salinity floods. After switching to low salinity brine, oil was displaced by the growth of water micro-droplets (10s of μm in size) within oil, and the expansion of thin water films between the oil and rock surfaces. The water-in-oil droplets formed at the oil-brine and oil-rock interfaces. Water micro-dispersions were observed mainly in the tertiary mode, compared to secondary, as the high salinity brine is believed to have slowed down the osmosis process allowing the images to capture the development of these droplets. In comparison with tertiary mode, LSW resulted in higher oil recovery in the secondary mode. In both LSW modes, the changes in contact angle, curvature and capillary pressure values were observed mainly after low salinity brine injection indicating wettability alteration from oil-wet towards more water-wet conditions.

This comprehensive study provides insights into low salinity pore-scale displacement mechanisms previously observed only on micro-models. It highlights both fluid-fluid and fluid-rock mechanisms associated with the LSE. This study can, therefore, offer valuable input for the fluid selection criteria to design LSW-EOR.

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Time Block A (09:00-12:00 CET)

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MS08 / 123

Open-FOAM simulation and analysis of non-Fickian transport in truncated pluri-Gaussian permeability fields.

Authors: Eugenio Pescimoro^{None}; Matteo Icardi¹; Marco Bianchi²

¹ *University of Nottingham*

² *British Geological Survey*

Corresponding Authors: marcob@bgs.ac.uk, matteo.icardi@nottingham.ac.uk, eugenio.pescimoro@nottingham.ac.uk

Understanding flow and transport in porous media is of fundamental importance for the design of processes and management strategies in oil extraction, groundwater remediation, CO₂ storage, and many other applications. However, the applicability and validity of standard macroscale transport models for highly heterogeneous media is still widely debated. Our study focuses on the impact of the subsurface structure and properties on the transport of solute through heterogeneous geological domains by means of three-dimensional simulations based on an open-source C++ library, built on

top of the finite-volume library OpenFOAM®.

Since it is not always possible to characterise the heterogeneities in a deterministic way, we make use of standard geostatistical techniques and pluri-gaussian truncated random fields, generated through Fourier decomposition, to construct realistic domains for flow and transport simulations. Additional challenges are posed by the numerical simulation of such highly heterogeneous and discontinuous permeability fields. We study the numerical upscaling of dispersion models from the meso- (i.e. heterogeneity) to the macro- (i.e. reservoir) scale and we analyse the onset of non-Fickian or anomalous transport. The whole simulation workflow has been implemented using our open-source library whose implementation and capabilities will be illustrated. Flow and transport simulations results will be discussed and the impact of geostatistical metrics (e.g. correlation lengths, permeability contrast and Péclet numbers) on transport results (e.g. early solute arrival, solute peak and breakthrough curve statistical moments) assessed. Preliminary conclusions from our study highlight the role of high permeable channels in triggering non-Fickian transport behaviour by creating fast flow channels on which advection prevails over dispersion but also the importance of the interpolation method in estimating the macrodispersion parameters.

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS06-B / 124

Stochastic inverse modeling of transient core-scale three-dimensional two-phase flows

Authors: Andrea Manzoni¹; Alberto Guadagnini¹; Aronne Dell'Oca²; Martina Siena¹

¹ Politecnico di Milano

² politecnico di milano

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We present a computationally efficient methodology for stochastic inverse modeling of transient multi-phase flow at the core scale. We consider the availability of information combining temporal histories of pressure drop across a core sample as well as detailed three-dimensional spatial distributions of oil and brine saturations of the kind that can be observed through in situ X-ray detection. We study settings associated with an imbibition and a drainage scenario involving brine and a light oil or a heavy oil and brine, respectively. Considering the computational burden associated with stochastic inverse modeling aimed at characterizing the hydraulic attributes of a selected mathematical formulation of two-phase flow, we present a workflow that encompasses (a) stochastic model calibration and (b) global sensitivity analysis.

The workflow starts from a preliminary model calibration focused on identifying a plausible set of model parameters (in term of satisfactory representation of the available information) and a reference value of the objective function. This preliminary step is based on a parameter support space

resting on literature data and expert opinion. We then perform a detailed Global Sensitivity Analysis (GSA) of the simulated state variables (core-scale pressure drop and spatial distribution of oil saturation), which encompasses a model behavioral space based on the above mentioned inverse solution. The GSA results enable us to assess the influence of parameter uncertainty on the simulated state variables and (eventually) identify less-influential model parameters. Finally, we perform a stochastic model calibration aimed at obtaining the (conditional) probability density of the model parameters which are deemed as influential on the basis of the GSA, the remaining parameters are fixed to the value rendered by the preliminary model calibration. The ensuing reduction of the dimensionality of the model parameter space yields considerable saving of the overall computational burden.

For both scenarios analyzed we obtain a satisfactory agreement between the numerically simulated pressure drop and saturation distributions and their reference/observed counterparts. We then discuss the key traits of the obtained parameter distributions upon relating these to the behavior of the system, as encapsulated in the employed model formulation.

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Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 127

Study on laboratory measurement method of anisotropic permeability based on passive differential pressure ratio

Authors: Xuehao Pei^{None}, Yuetian Liu^{None}, Tengda Rang^{None}

Corresponding Authors: 572796099@qq.com, lyt51@163.com, pxhfly@qq.com

Permeability is a key parameter to control material and energy transport in porous media. However, the anisotropy of permeability makes it difficult to measure accurately in laboratory. In this paper, a detailed theoretical analysis of the anisotropic porous media flow process is carried out, and it is found that all physical quantities exhibit point-centered symmetry during the one-dimensional stable displacement of anisotropic porous media, while a passive pore fluid pressure difference is generated in the vertical direction of displacement. For an anisotropic sample with unknown principal axes, there are systematic errors in the designed method for adopting Darcy's law directly or calculating the components of the permeability tensor using the outlet fluid production profile. For anisotropic porous media, the permeability tensor cannot be solved by a simple analytical formula because the flowing state of each internal part is not completely uniform, and a standard plate can be established to fit the solution.

On this basis, a two-dimensional and three-dimensional anisotropic permeability tensor test method based on the passive differential pressure ratio is established, and the two-dimensional and three-dimensional passive differential pressure ratio plates are given based on conventional plates and Gaussian process regression, respectively. The permeability tensor can be obtained by measuring the pressure difference perpendicular to the direction of displacement in the one-dimensional stable

displacement process based on the constructed plots. The case test shows that the core test data are consistent with the theoretical analysis, and the method has high reliability and practicality.

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References:

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS07 / 128

Simulation of interface-coupled porous-medium applications using partitioned coupling methods

Author: Alexander Jaust¹

Co-author: Miriam Schulte¹

¹ *University of Stuttgart*

Corresponding Authors: miriam.schulte@ipvs.uni-stuttgart.de, alexander.jaust@ipvs.uni-stuttgart.de

Many real-world applications involve interface-coupled processes and porous media. Common examples are the hydromechanical coupling of liquid in a fracture under high pressure and the resulting deformation of the surrounding porous medium or coupled free and porous-medium flow. These examples play an important role in hydraulic simulations or simulations of filters. Moreover, the underlying problems can be split in two non-overlapping subdomains with different physical properties and mathematical models that are separated by a sharp interface. Solving such problems numerically leads to ill-conditioned (linearized) systems of equations if a monolithic solution strategy is used.

We circumvent the problem of ill-conditioned system of equations by solving the problems by partitioned black-box methods which are based on the idea of domain decomposition techniques. The individual problems are solved separately in an iterative manner. Suitable values for the coupling condition on the interface ensure that we recover the coupled behavior of the original problem. Additionally, we employ so-called accelerators based on interface quasi-Newton methods for stabilization and acceleration of the iterative coupling process. The black-box nature of the applied coupling method only relies on the data exchanged between the subdomains which simplifies the coupling of different solver (software) packages.

We investigate different black-box coupling methods for the mentioned porous-medium applications to show their versatility and to identify suitable accelerator configurations. The presented approach is based on the open-source library preCICE (www.precice.org) which, amongst other things, includes functionality to communicate data, to steer the coupling process, and to apply the acceleration to the coupling process.

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Time Block B (14:00-17:00 CET)

Participation:

Online

MS02 / 129

Climate change and primary soil salinization: A global scale perspective for the 21st century

Authors: Amirhossein Hassani¹; Adisa Azapagic²; Nima Shokri³

¹ NILU - Norwegian Institute for Air Research

² Department of Chemical Engineering, The University of Manchester

³ Hamburg University of Technology

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Soil salinization refers to the excessive accumulation of soluble salts in soil to a degree that adversely influences environmental, human, and animal health. Soil salinization poses an existential threat to ecosystem functioning, socioeconomic structure, and food security. The projected climate change will influence almost all key factors driving soil salinization. For example, rising temperature in summer will lead to higher evapotranspiration which in turn increases salt concentration in soil solution leading to expansion of the lands with higher salinity levels. Yet, quantification of the soil salinity response to projected climate change has been rarely investigated. Given the complexity of the processes influencing soil salinization at the regional to continental scales (Hassani et al., 2020), here we apply Machine Learning (ML) algorithms to build predictive models of naturally occurring soil salinity and estimate the variations of soil salinity in the world's dryland areas (lands with an Aridity Index ≤ 0.65), under different projected climate change scenarios by 2100 (Hassani et al., 2021). These predictive models map data-driven relations between the experimentally measured soil electrical conductivity (as a measure of soil salinity) and a set of purely spatial and spatio-temporal auxiliary data based on soil/land properties and output of Global Circulation Models (adopted from both Fifth and Sixth Phases of the Coupled Model Inter-comparison Projects, the so-called CMIP5 and CMIP6) to predict the soil salinity, expressed as saturated paste electrical conductivity at each time, location, and depth. Under different greenhouse gas concentration trajectories, analysis of the predictions made for the 2071 - 2100 period identifies the dryland areas of South America, southern and Western Australia, Mexico, southwest United States, South Africa, Spain, Morocco, and northern Algeria as the salinization hotspots, compared to the reference period (1961 - 1990). Conversely, we

project a decrease in the soil salinity of the drylands spread across the northwest United States, the Horn of Africa, Eastern Europe, Turkmenistan, and west Kazakhstan in response to climate change for the similar periods. The predictive tool developed here can be used for projection of other dynamic soil properties such as soil nutrients and pH under changing climate.

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Hassani, A., Azapagic, A., Shokri, N. (2020). Predicting Long-term Dynamics of Soil Salinity and Sodicity on a Global Scale, *Proc. Nat. Acad. Sci.*, 117(52), 33017-33027, doi.org/10.1073/pnas.2013771117.
Hassani, A., Azapagic, A., Shokri, N. (2021). Global Predictions of Primary Soil Salinization Under Changing Climate in the 21st Century, *Nat. Commun.*, 12, 6663. doi.org/10.1038/s41467-021-26907-3.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS07 / 130

Upscaling and Automation: Pushing the Boundaries of Multiscale Modeling through Symbolic Computing

Author: Kyle Pietrzyk¹

Co-authors: Svyatoslav Korneev²; Morad Behandish²; Ilenia Battiatto¹

¹ *Stanford University*

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In complex multi-scale system analysis, macroscopic differential equations are used to significantly increase computational efficiency and accurately model physical processes across multiple scales. Such equations can be systematically generated through rigorous *upscaling* techniques, which provide *a priori* error estimates and conditions under which the equations are valid (i.e., *applicability conditions*). However, the analytical derivations required in these techniques are time consuming, error-prone, and become quickly intractable for complex, multi-physical systems. To ease these complications, we propose a method of automatic upscaling through symbolic computation. By automating the analytical derivations, we democratize the utilization of upscaling techniques in practical applications and enable multi-scale model development in a feasible amount of time (i.e., seconds to minutes) with no requirements in analytical tractability, nor specialized expertise in mathematical model formulation. In this presentation, we demonstrate the ability of our software prototype, *Symbolica*, by reproducing homogenized advective-diffusive-reactive (ADR) systems from earlier studies and homogenizing a large ADR system deemed impractical for manual homogenization. We then discuss an application of Symbolica in Lithium ion battery packs to study heat transfer and thermal runaway.

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Pietrzyk, K., Korneev, S., Behandish, M., and Battiato, I. Upscaling and Automation: Pushing the Boundaries of Multiscale Modeling through Symbolic Computing. *Transp Porous Med* 140, 313–349 (2021). <https://doi-org.stanford.idm.oclc.org/10.1007/s11242-021-01628-9>

Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

Poster / 131**INFLUENCE OF SiO₂ NANOFLUID ON ENHANCED OIL RECOVERY INSIDE A TRANSPARENT MICROPOROUS MEDIA**

Authors: Afshin Goharzadeh¹; Yit Fatt Yap¹

¹ *Khalifa University*

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With the rapid development of the world economy, the demand for energy, especially oil, is increasing. Therefore enhanced oil recovery (EOR) has become an essential part of crude oil exploitation. EOR consists of a recovery process by the injection of materials not existing in the reservoir. At present, four primary techniques of EOR are available in industry: Gas flooding, thermal injection, microbial recovery and chemical process. Addition of nanoparticles to chemical reagents is a new chemical flooding method, which can enhance and improve certain properties at low volume concentrations of the dispersing medium. It has the following advantages: (i) increase the stability of dispersing medium because surface forces easily counteract the force of gravity and (ii) change the optical, thermal, stress-strain, electrical, magnetic and rheological properties that strongly depend on size and shape of the nanoparticles. Therefore, it is evident that there is significant practical meaning to develop nanofluids for oil and gas production. The objective of this study is to investigate the properties of a nanofluid (SiO₂) and its effect on Enhanced Oil Recovery (EOR) processes. The experimental setup consists of a digital microscope, transparent microporous media, a syringe pump (Cole-Parmer Dual Rate) and a beaker. To mimic a transparent porous media a network of squares was designed and fabricated inside a microchannel having the dimension of 750 μm × 150 μm × 35 μm (length × width × depth). The syringe pump is used to inject crude oil, DI-water and nanofluid into the microporous media made of PDMS. The flow rate can vary from 4 × 10⁻⁴ μl/h to 1 × 10⁺⁷ μl/h. Once the microchannel is filled with crude oil, DI-water (or nanofluid) is injected until breakthrough happened. During injection processes, oil saturation was monitored by taking high-resolution video. The flooding process was observed using a microscope (Leica DMS300) from the top of the horizontal microchannel. The magnification of the microscope is between 15 to 120 times. Video with a resolution of 1920 × 1080 pixels was recorded. To quantify the characteristics of flooding efficiency, the obtained images were analyzed (using MATLAB) to measure the residual oil inside the microchannel. Surface tension and viscosities of SiO₂ is measured by drop volume method and vibration string methods, respectively. Its stability and particle size were characterized using observational and dynamic light scattering method, respectively. The obtained experimental results reveal that with the addition of nanofluid in the brine, SiO₂ nanofluid trends to increase surface

tension. Performance of working fluid (DI-water or nanofluid) on flooding process are compared. It was observed that the recovery effects of SiO₂ is better than DI-water.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS01 / 132

Minimal surfaces in gas diffusion layers

Authors: Mohammad Javad Shojaei¹; Branko Bijeljic²; Martin Blunt¹

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Gas diffusion layers in fuel cells need to allow the simultaneous flow of gases and water. Empirically this is achieved by coating the naturally hydrophilic carbon fibres with a hydrophobic coating, usually PTFE. We have used high-resolution X-ray imaging to observe the configuration of water within gas diffusion layers with different degrees of PTFE coating, and to quantify curvature and contact angle.

We observe that the fluid menisci form minimal surfaces. These surfaces occur in equilibrium at pinned contact lines at the boundary between hydrophilic and hydrophobic parts of the fibres. Minimal surfaces have two desirable features for multiphase flow. Firstly, the pressure difference between the water and gas is zero, which means that no additional water pressure is required, preventing retention and clogging of the pore space. Secondly, from topological principles, minimal surfaces ensure well-connected phases: the water clusters contain many redundant loops which helps maintain the continuity of flow under operando conditions.

In our work we found minimal surfaces for gas diffusion layers with 5, 20 and 40% coating with PTFE. The layer with a 60% coating had a markedly lower porosity and was more characteristically hydrophobic with higher average contact angles and a negative capillary pressure –that is the water pressure was higher than the surrounding air. The presence of minimal surfaces suggests that the water and gas pressures are equal, allowing water to flow readily without a pressure build-up. From topological principles, the negative Gaussian curvature of the menisci implies that the fluid phases are well connected. The implication of the design of porous materials where the simultaneous flow of two phases over a wide saturation range is explored.

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References:

Reference

- (1) Blunt, M. J. Multiphase flow in permeable media: A pore-scale perspective; Cambridge University Press, 2017.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS08 / 133

Flow heterogeneity impact on dissolution reaction behavior in geologic porous media

Authors: Zoe Kanavas¹; Veronica Morales¹; John Nimmo²

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² *Unsaturated Flow Research*

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Two common structural patterns left by dissolution reactions in practical applications such as carbon sequestration are (1) uniform, in which the reaction spreads evenly throughout the medium and the reaction rate is relatively close to that measured in batch; and (2) wormhole, in which the reaction etches conductive pathways and the reaction rate is much lower than its batch measurement. The development of these patterns can be modeled from dimensionless transport (Peclet, Pe) and reaction (Damköhler, Da) characteristics. Specifically in dissolution behavior diagrams, one expects uniform dissolution in reaction-limited scenarios (low Da) and wormhole dissolution in transport-limited and advection-dominated conditions (high Da and Pe). However, in heterogeneous flow fields—characterized by contrasting fast velocity channels and stagnant flow regions—such dissolution behavior models often misclassify dissolution behavior. We hypothesize that flow heterogeneity, in addition to Pe and Da drives dissolution behavior and can be used to infer the reaction rate of the medium. In this work, we perform a meta-analysis of existing experimental studies on pore-scale dissolution in porous media to quantify the impact of flow heterogeneity. First, we collect the reported Pe , Da and reaction rates from existing studies and record the observed dissolution pattern. Next, we quantify each system's initial flow heterogeneity in dimensionless metrics and demonstrate the influence of flow heterogeneity on observed reaction rates. Lastly, the dimensionless flow, transport, and reaction metrics are used to parameterize a generalized linear model that can predict the reaction rate and classify the dissolution behavior. The findings of this work elucidate the emerging characteristics that control dissolution behavior during typical conditions for CO₂ sequestration in heterogeneous geologic media.

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MS22 / 134

Initial Yield Surface of Cellular Sheet TPMS Lattices

Authors: Nareg Baghous¹; Imad Barsoum¹; Rashid K. Abu Al-Rub¹

¹ *Khalifa University of Science and Technology*

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Due to the advancements in additive manufacturing and increased applications of additive manufactured structures, it is essential to fully understand both the elastic and plastic behavior of bio-inspired cellular materials, which include the mathematically-driven sheet/shell lattices based on triply periodic minimal surface (TPMS) that have received significant attention recently. The compressive elastic and plastic behaviors have been well established for many TPMS latticed structures, but not under multiaxial loading. Furthermore, TPMS lattices are computationally expensive to model explicitly (i.e., micromechanical) when used in latticing various structures for enhanced multi-functionality, and hence the need to develop an accurate yield surface function or criterion in order to model their plastic behavior in a homogenized approach. The majority of previous yield surfaces developed for cellular materials were developed for cellular foams [1, 2], and very few attempts has been made to develop a yield surface based on cellular lattices [3]. Furthermore, some of the few studies [4] that used the yield surfaces developed for foams to predict the yielding of cellular lattices, have found that such yield surfaces do not predict well the yielding of lattice structures under various multiaxial loading conditions. In this study, an initial yield surface is developed for sheet TPMS cellular lattices, which to our best knowledge has never been attempted before, and is compared to the major yield surfaces that have been developed for cellular materials.

The effect of different loading conditions on the effective yield strength of IWP sheet-based (IWP-S) TPMS lattice is numerically investigated. The simulations are based on a single unit cell of IWP-S under periodic boundary conditions, assuming an elastic-perfectly plastic behavior of the base material, for relative densities ($\bar{\rho}$) ranging from 7% to 28%. In order to account for the different loading conditions, the Lode parameter (L) is used [5]. The effect of L is studied over a range of mean stress values (σ_m) to understand the effect of both L and σ_m on the effective yield strength.

In the plane of the von Mises equivalent stress σ_{VM} verses σ_m , σ_{VM} is maximum at $\sigma_m = 0$ and reduces in a parabolic and almost symmetric manner with $\pm \sigma_m$ values. On the other hand, in the plane of σ_{VM} verses L , σ_{VM} is minimum at $L = 0$ and increases in a parabolic and almost symmetric manner with $\pm L$ values. Using these relationships, the effective yield surface for IWP-S is characterized by σ_{VM} , the mean stress σ_m , L and $\bar{\rho}$. In the 3D space of the principal stresses, this yield surface is best described as a cocoa pod. The current developed framework can be adapted for generating yield surfaces for other lattice topologies. As future work, tests on additively manufactured IWP-S lattices, under different loading conditions, will be conducted to validate the proposed yield surface.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS06-A / 135

Surface-Active Compounds Induced Time-Dependency and Non-Monotonicity in Fluid-Fluid Displacement in Porous Media

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Low salinity waterflood (LSWF) has proven to be an economic, environmentally friendly IOR method which leads to more oil recovery without adding additional chemicals into water [1-3]. However, the efficacy and the underlying mechanisms are still under debate and many mechanisms are proposed in literature. Many factors are believed to attribute to the additional oil recovery by low salinity water injection, which can be categorized into fluid-solid interactions and water-oil interactions. The lack of agreement is partially due to the complex composition of the crude oil used in previous studies. Surface-active compounds in the crude oil can render the naturally hydrophilic rock surface hydrophobic by adsorbing on fluid/solid interfaces [4-6]. Similarly, their desorption from the interfaces at low salinity can alter the surface back to hydrophilic [7]. The surfactant's redistribution and reactions with oil/water can potentially impact the macroscale water-oil two-phase flow dynamics in porous media.

In this paper, we investigate the impacts of surfactant concentration on the fluid-fluid displacement dynamics in porous media at both the macroscale and the microscale. We design the pseudo dual-component oils by mixing a non-polar mineral oil with different concentration of a non-ionic surfac-

tant (sorbitan monooleate). This way, we mimic the crude oil that contains natural, surfactant-like polar components. Deionized water (DI water) and a high salinity brine (8.6 wt% NaCl, 1.2 wt% KCl, 2.0 wt% CaCl₂) are used as the high salinity and low salinity in the displacement experiments. We visualize the macroscale water-oil displacements in inch-long micromodels and the oil droplet swelling processes in a dead-end pore. Interfacial tension between different oils and high and low salinity waters are measured. The oil swelling rates versus time at different surfactant concentrations are analyzed.

We observe that, at low salinity, the surfactant in the oil phase causes the water-in-oil emulsion and the droplet swelling and de-wetting, leading to the wettability alteration to a more water-wet state. Significant incremental oil displacement is obtained from the low salinity waterflood when the oil has high surfactant concentration. However, the impact of the surfactant on the incremental displacement efficiency is non-monotonic. This is caused by the two opposing effects of the increased surfactant concentration: stronger initial hydrophobicity which adversely affects the displacement and oil swelling which is beneficial for displacement. Two modes, *gradual invasion* and *sudden collapse*, are identified during the incremental displacements. They are explained by the evolution of local capillary force and global force imbalance, respectively. Both the microscale droplet geometry change and the macroscale two-phase displacement dynamics show time-dependency; the latter is characterized by a delay time of $\sim 10^1$ hours. The microscale droplet geometry change is over an order of magnitude faster than the macroscale displacement dynamics.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

Poster / 136

Pore-scale two-phase flow simulation of volcanic gas reservoir based on Volume of Fluid method

Authors: Yongfei Yang¹; Quan Xu^{None}; Xinze Li^{None}

¹ *China University of Petroleum (East China)*

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There are pore and fracture media in a volcanic gas reservoir, and two-phase gas-water flow is possible. However, there are few research on the effect of volcanic reservoir type, capillary number and wettability on 3D gas-water two-phase flow from pore scale. This paper aims to study the distribution, evolution and influencing factors of natural gas in different reservoir media during formation water flow at pore scale. The 3D pore scale model of volcanic rock was established by reconstruction of micron CT scanned images. Based on logging data and NIST(National Institute of Standards and Technology)database, the physical properties of fluids were obtained. The VOF (Volume of fluid) method was used to simulate the gas-water two-phase flow process at pore scale, and the flow laws of gas-water in different reservoir spaces are summarized. The capillary number and wettability were analyzed in the model. The results show that the residual gas in the pore is obviously larger than that in the fracture during the flow process. The increase of capillary number is beneficial to the removal of residual gas. With the increase of wettability angle, the distribution of residual gas at dead-end corners increases.

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Poster / 137

Toward integration of NMR and traditional centrifuge capillary pressure curves: A comparison study

Authors: George Yabesh¹; Stephen Banks²; Ausama Giwelli²; Lionel Esteban²; Ahmed Al-Yaseri²

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Capillary pressure is the difference in pressure across the interface between two immiscible fluids and is dependent on interfacial tension, pore size, and wettability. Understanding capillary pressure is crucial in determining hydrocarbons production, CO₂ and/or hydrogen underground storage. Capillary pressure laboratory measurement is performed by mercury injection, porous plate, or centrifugation. The latter “centrifuge” method has been widely accepted technique to establish capillary pressure curves, due to the time needed to complete a test and its non-destructive. Analysis of the centrifuge saturation measurement is usually performed using commercially available core analysis simulators (e.g., SENDRA or CYDAR) that function by either history matching of experimental behaviour or analytical solutions.

On the other hand, Green Imaging Technology proposed a protocol (trademarked as GIT-CAP) to obtain capillary pressure curves, through combining centrifuge method with Nuclear Magnetic Resonance (NMR) saturation distribution measurements on de-saturated core samples. The measured saturation profiles together with centrifugal force/spinning velocity enables the capillary pressure curve to be computed via correlations. This approach requires at least two, but preferably three, centrifuge speeds, while up to ten speeds might be needed if the traditional centrifuge technique is used alone. However, to the authors knowledge, the centrifuge displaced fluid measurements acquired during NMR GIT-CAP were never used to model local capillary pressure and compare to GIT-CAP. This was mainly due to the limitation of capillary pressure correlations implemented into the commercial core analysis simulators.

To that end, we have developed an in-house code (SBAG-CAP) in MATLAB to calculate drainage capillary pressure (with a view to add imbibition in future). The SBAG-CAP code has 5 models that were carefully selected due to their common acceptance by Energy companies and their compatibility with those used in GIT-CAP. The models work by finding a minimum of a constrained nonlinear multivariable function with default initial guesses provided by Adams 2016. This function is the difference between the experimentally determined average saturation at each speed during steady state/hydraulic equilibrium and that predicted by the chosen model.

Current work is meant to evaluate and validate SBAG-CAP and compare its capillary pressure results with the core analysis simulators, namely SENDRA and CYDAR. Thus, we used Vinci centrifuge to run a multi-speed drainage test on 5 outcrop sandstone and carbonate samples. Five speeds (300-1500 RPM) were selected, and each rotation was scheduled for 3 days, to ensure equilibrium. High-definition video camera (which is automatically adjusted to the rotational speed) was used to record the displaced water level in the transparent tank and then communicated to centrifuge software to calculate the displaced water volume every 30 sec. To achieve a “uniform” saturation profile, the samples were flipped and spun again at 1500 rpm for 3 hours. The recorded displaced water volume over time was used to generate local capillary pressures simulated in CYDAR, SENDRA and SBAG-CAP. Results show local capillary pressures obtained from SBAG-CAP were comparable to both SENDRA and CYDAR, indicating a close match and reliability of SBAG CAP, with very good capillary pressure curves similarity between CYDAR and SBAG-CAP.

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Enhanced Super Resolution Generative Adversarial Network (ES-RGAN) for improving the resolution of micro-CT images

Author: Mohamed Regaieg¹

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Mohamed Regaieg1*, Zakaria El Abid 2, Erwann Camberlin 3

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Digital Rock Physics (DRP) provides a new way to compute rock properties and carry-out related sensitivity analysis to complement laboratory measurements. In DRP, the first step is to obtain micro-CT images of a rock, this is then followed by segmenting the images to distinguish the rock from the pore space, and finally flow simulations are performed to compute advanced rock properties such as relative permeability and capillary pressure. Yang et al (2017) have proved that when the geometry of the pore space is well characterized, the flow simulators perform well.

However, the geometry of a real rock is not always well characterized, notably due to the lack of image resolution which in turn introduces uncertainty in the pore/throat geometry and consequently introduces errors in rock property computations. Furthermore, during image acquisition a compromise is often made between the speed of the image acquisition, the size of the scanned volume and the resolution obtained: increasing the resolution decreases the field of view, in turn limiting the quantity of information obtained from the image and thus making DRP simulations less representative.

Recent advances in deep learning methods have led to major advances in computer vision techniques, and notably in the field of super-resolution imaging. In this talk, we present such a strategy to digitally increase the resolution of 3D micro-CT using a deep learning approach called Enhanced Super-Resolution Generative Adversarial Network (ESRGAN). We first describe the ESRGAN method and our training strategy. Subsequently, we apply it to 3D micro-CT images of several rocks, and we compare the super-resolved images against the high-resolution ones of the same rock volume.

This is followed by presenting flow simulations performed on low resolution and super-resolved images showing how the ESRGAN can considerably improve the accuracy of DRP simulations. Large super-resolved images up to 4000 voxels cube were produced and the technique showed promising results when applied on low resolution micro-CT images. The super-resolved images were more realistic visually and produced better single and multiphase flow simulations results.

Keywords: Super-resolution, GAN, deep-learning, image processing, PNM, simulation

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MS09 / 139

Relative permeability computations using large Digital Rock Physics simulations

Authors: Mohamed Regaieg^{None}; Igor Bondino¹; Clément Varloteaux²; Titly Farhana Faisal³; Richard Rivenq⁴

¹ Total

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Mohamed Regaieg^{1*}, Igor Bondino¹, Clément Varloteaux², Titly Farhana Faisal³, and Richard Rivenq¹

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Abstract

Direct Numerical Simulation (DNS) on systems larger than few millimeters is too computationally demanding. Pore Network Modeling (PNM) is a practical way to study the flow at pore scale on larger volumes while keeping reasonable running times. Recent numerical developments in digital rock physics, known as Generalized Network Modelling (GNM) (Raeini et al 2017), allow to reconstruct an upscaled version of the 3D segmented image of a rock in the form of a network of pore elements where the single-phase flow conductances in each pore are derived by solving the Stokes equation in the original geometry. In engineering terms, this hybrid solution allows to capture relevant flow information from the original Micro-CT image whilst keeping the overall cost of multi-phase computation manageable. In this work, OpenFOAM is called for the Stokes flow solution inside a pore network extraction platform called Gnextact (Raeini et al 2017), and TotalEnergies's pore-scale network simulator DynaPNM (Regaieg et al 2017) is used in quasi-static mode after having been made fully parallel. All codes are run on TotalEnergies's supercomputer PANGEA.

In the first part, we give an overview of TotalEnergies's two-phase flow simulation workflow. Then, we describe how simulation runs in parallel mode allow to perform large uncertainty studies (thousands simulations / day) on images as large as (8480x8480x10000) voxels representing a rock volume of 46 cm³. We document the very large statistical dispersion in relative permeability results (due to the microscopic arrangement of oil-water contact angles) that is normally achieved when images as small as 1200x1200x1200 are used in simulation. We show how this finite size effect can be drastically reduced by simulating much larger and representative images, greatly improving the precision of the numerical result. Finally, relative permeability curves are computed compared to validation experiments.

Keywords: PNM, plug scale, quasi-static, speed-up

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MS10 / 141

Characterizing Ice Melting Dynamics in Porous Media with NMR-MRI

Authors: Natnael Haile¹; Hongxia Li¹; Yadong Zhang¹; Nahla AlAmoodi¹; TieJun Zhang¹

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Recent advances in nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) technology are paving ways to probe physical insights into transport phenomena in porous media, without destroying opaque materials structure or disturbing phase change processes. In this work, we utilize low-field NMR-MRI technology to capture in-situ melting dynamics of ice in homogeneous and heterogeneous porous media. Two different heating scenarios are applied in ice melting experiments, side-wall heating and top-surface heating. By regulating the heating temperature, transient phase change behaviors during ice melting are characterized through the NMR transversal relaxation time T₂. T₂ results from the interaction of the atomic nucleus with the magnetic field, and its distribution is proportional to pore characteristics, particularly pore size distribution. Meanwhile, transient and spatial distribution images of water in the entire porous medium are also captured by MRI. Based on the water content variation with time, the melting rate of ice in porous media is used to evaluate the melting speed and profile under two heating scenarios. Finally, the influence of heterogeneity in grain size and pore structure is investigated by using controlled non-uniform porous samples.

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MS17 / 142

Flower-like Porous Structure for Solar Thermal Distillation and Brine Treatment

Authors: Mohamed Abdelsalam¹; Muhammad Sajjad¹; Aikifa Raza¹; Faisal AlMarzooqi¹; TieJun Zhang¹

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Conventional desalination processes generate a flow of clean water and almost equivalent volume of excessively saline brine solution, which is harmful to the aquatic life. In order to mitigate environmental concerns, innovative solar thermal distillation technology are expected to produce freshwater without brine rejection. Herein, we have fabricated scalable petals-like porous structure for solar vapor generation and brine treatment with zero liquid discharge that is driven by localized heating and interfacial evaporation. The proposed porous structure shows an excellent wicking performance while having good light absorptivity. Under one-sun irradiance, our device is able to obtain a stable evaporation rate when dealing with synthetic seawater with a salinity of 3.5 wt%. The proposed solar evaporator can also achieve directional salt precipitation by controlling the surface wettability of the porous structure. The device is currently under evaluation with real concentrated brine (24 wt%) to attain cost-effective and eco-friendly solar thermal brine treatment.

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Poster / 143

Bubble Dynamics on Hierarchical Porous Nickel Phosphide Electrode for Electrocatalytic Water Splitting

Authors: Lin Yuan¹; Xinnan Lu¹; Shubra Lalwani¹; Faisal AlMarzooqi¹; TieJun Zhang¹

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The hydrogen/oxygen evolution reaction (HER/OER) has been well-studied for design and synthesis of efficient electrocatalysts. To further enhance electrode performance, the hierarchical porous architecture is used to obtain large surface area and efficient mass transport. Recent studies were

performed to reveal the impact of porous/mesh electrode surface wettability on bubble dynamics, which governs the overall interfacial mass transport during gas-evolving reactions and the associated overpotential. In fact, the quantitative relationship between the electrochemical process and bubble dynamics on porous electrodes is still unclear due to the sophisticated structure and difficulty in imaging bubbles at microscale. Here, we report the bubble dynamics and overpotential loss on hierarchical porous nickel phosphide electrode during electrocatalytic water splitting. The three-dimensional hierarchical structure of porous Ni₅P₄ powder coated Ni foam (p-Ni₅P₄@Ni) includes nano-pores ranging from 50-500 nm (from porous Ni₅P₄ powder) and micro-pores ranging from 200-600 μm (from Ni foam), and this porous structure is able to achieve outstanding catalytic performance with an overpotential of 145 mV for HER and 197 mV for OER at 10 mA/cm². Our high-speed imaging results on p-Ni₅P₄@Ni show that the bubble departure size is about 10-50 micron, and the bubble number density and departure frequency increase linearly with the current density. Nano-pores of Ni₅P₄ provide abundant cavities to H₂ bubble nucleation and subsequent inertia-controlled growth, especially under high current densities. This is totally different from H₂ bubbles, nucleating and growing in a diffusion-controlled mode, on smooth surface of macro pores of clean Ni foam. For our porous Ni₅P₄@Ni electrodes, both the low transport and intrinsic overpotential contribute to the exceptional electrocatalytic performance.

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MS22 / 144

Direct Solar Membrane Distillation Device with Micro-3D Printed Spacer and Titanium Mesh

Authors: Abdulrahman Khrbtli¹; Hongxia Li¹; Alaa Shaheen^{None}; Faisal AlMarzooqi¹; TieJun Zhang¹

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Creative and sustainable desalination solutions are needed to meet the world's vast demand for drinking water, one of which is direct solar membrane distillation (DSMD). High-resolution 3D printing can be used to manufacture spacer with complex porous structures, such as triply periodic minimal surface (TPMS), for DSMD. In this work, we propose a hybrid light-absorbing spacer by micro-3D printed assembling TPMS structure with titanium mesh. A direct solar MD setup is developed to monitor the pressure drop, inlet and outlet temperatures and permeate flux and also evaluate the desalination performance. From our experimental results, we find that the TPMS structures have better flow mixing and thus higher permeate flux in comparison with the commercial spacer. The effect of pore sizes of TPMS structures are also evaluated in terms of pressure drop and permeate

flux. By incorporating titanium mesh in the DSMD device between the porous spacer and the membrane, the feed water and heat can be localized near the membrane surface for high-efficient water vaporization. This work will provide a new solar desalination solution to relieve the undergoing freshwater stress.

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MS05 / 145

Transport of *Sporosarcina Pasteurii* in porous saturated sands and applications on soil improvement

Authors: Guijie Sang¹; Rebecca Lunn²; James Minto²; Gráinne El Mountassir¹

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² *University of Strathclyde*

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Microbial-induced calcite precipitation (MICP) has been regarded as a promising bio-grouting technique for soil stabilization, remediation of concrete and subsurface rocks, wellbore sealing, among others. One of the most extensively utilized bacteria for MICP is *Sporosarcina pasteurii* (*S. pasteurii*), which enables to catalyze the hydrolysis of urea to carbonate and ammonia via the production of urease enzyme, resulting in an increase in pH and precipitation of calcite if calcium is available. Understanding of the transport of *S. pasteurii* in porous sands is fundamental to delineate its fate and distribution, so as to provide clues to optimize the treatment strategy for soil improvement. The study attempts to elucidate the transport and retention mechanisms of *S. Pasteurii* in saturated sands based on a series of column breakthrough experiments under different physical-chemical-biological conditions including ionic strengths (ISs), flow velocity, bacterial optical density, column length. A two-site kinetic model, defining (1) physicochemical attachment on grain surfaces, and (2) straining at the crevices and constrictions, is applied to fit the column breakthrough curves. The experimental and modelling results show that bacterial breakthrough declines from 88% to 5.4% with IS increasing from 0.5mM (tap water) to 1M (NaCl), resulting from that higher ionic strength tends to weaken the electrostatic repulsion between negatively-charged bacteria and sands, and hence to enhance both physicochemical attachment and straining (due to flocculation). Besides, lower flow velocity, lower bacterial density, and longer column correspond to a higher bacterial retention. Under physicochemical perturbations, the injection of 0.5M CaCl₂ with stronger IS stabilizes the pre-attached and pre-strained bacteria while the elution of deionized water with lower IS causes the bacterial release.

In addition, a radial flow cell (diameter: 1 m, thickness: 0.15 m) is constructed for MICP treatment in two types of sands, one well-graded and the other less well-graded. After 9 cycles of MICP treatment,

the unconfined compressive strength of the treated sands (initially loose) is achieved up to several MPa. The permeability of the well-graded sands drops by one order of magnitude from 2.0×10^{-12} m² to 2.5×10^{-13} m², while the permeability of the less well-graded sands shows a minor drop from 1.3×10^{-11} m² to 7.9×10^{-12} m². The post-treated well-graded sands also show greater spatial heterogeneity in permeability, calcite distribution and strength due to the migration of fine particles and induced preferential flow paths. Our study shows the viability of MICP application in soil improvement as well as some opportunities and challenges for upscaling and optimizing MICP soil improvement in the field.

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Participation:

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MS16 / 147

Surface-washing of contaminated porous substrates

Author: Francesco Paolo Conto¹

Co-authors: Merlin Aragon Etzold²; Emily Butler³; Julien R. Landel³; Stuart B. Dalziel¹

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The cleaning of porous surfaces is a challenging problem in everyday life and industrial practice since it can lead to redistribution of the absorbed contaminant within the porous material instead of a complete removal of the unwanted agent. The role of decontamination is particularly crucial when contaminants (such as chemical weapons agents and pathogens) pose serious risks to human health [1].

In this work, we present surface-washing experiments modelling the decontamination of porous substrates.

Firstly, we report a protocol to manufacture mechanically stable porous media by sintering soda-lime glass ballotini (< 1 mm) to form free-standing homogeneous porous plates or composite structures where a porous matrix is sintered onto solid glass backing and surrounds. The ability to incorporate directly a solid glass backing provides a method of preventing any liquid leaks through their rear.

These samples are then integrated into a surface-washing apparatus [2] equipped with camera-based and in-line UV-Vis diagnostics. A dyed fluid is placed onto the porous substrate to simulate the region of contamination. The surface-washing is simulated by a thin (~ 1 mm) gravity-driven film of water flowing over an inclined porous-glass surface.

The resulting interaction between the cleansing film flow and the contaminating dye is then tracked

using direct image analysis based on dye-attenuation techniques, enabling us to study the space-time evolution of the contaminant field over the porous medium. Moreover, the camera visualization is complemented with a UV-Vis spectrometer monitoring in real-time the contaminant concentration in the effluent during the washing.

Our experiments provide insights on the role of initial conditions (wet/dry substrate, ingress of contaminant, contamination-washing time gap), the impact of cleaning strategies on industrial performances (e.g., amount of cleansing resources and decontamination time), and the relevant transport mechanisms of the contaminant (gravity/capillary-driven advection, diffusion, and dispersion in both liquid and porous phases). Importantly, they demonstrate a decontamination-induced redistribution of the contaminant within the porous matrix.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS07 / 148

An enhanced branch and bound algorithm for phase stability testing of multicomponent mixtures

Authors: Martin Jex¹; Jiří Mikyška¹

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The stability of matter is one of the fundamental problems of physics. In this contribution, we examine phase stability. From the mathematical point of view, the problem of coexistence or separation of phases can be formulated as a global optimization problem. We consider *VTN*-stability testing, i.e. the phase composition of a mixture under fixed concentrations and temperature. Our goal is to predict whether the phase composition of a mixture is stable or unstable. In other words, if the mixture stays in a single phase or splitting into multiple phases occurs. Mikyška and Firoozabadi (Mikyška, J.; Firoozabadi A. 2012) derived a criterion for the *VTN*-phase stability which leads to solving an optimization problem. Mikyška and Smejkal (Smejkal T.; Mikyška J. 2020) proposed to solve this problem with the branch and bound algorithm with the use of a convex concave split. In this contribution, we are going to improve the algorithm with more effective bounding strategy. This improvement is achieved using the necessary condition of optimality. In the bounding step of the algorithm, before solving an underestimated convex optimization, we check whether the pressure (given by the Peng-Robinson equation of state) is feasible. If it is not the case, we can exclude the

corresponding part of the feasible set from the search. The Peng-Robinson equation of state is not convex and therefore leads to a non convex optimization which is computationally expensive. We propose to use a less precise estimate of the global minimum of the pressure. This estimate can be found by comparing the finite number of the values of the tangent plane to a concave overestimate of the Peng-Robinson equation of state. Another benefit of this additional step is to avoid the optimization of an underestimated objective function. Suggested method is tested on several concrete examples.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS15 / 149

Towards Pore Super Segmentation on Artificially Enhanced SEM Images of Opalinus Clay by Voting Classification

Authors: Marco Brysch¹; Ben Laurich¹; Christoph Schettler¹; Monika Sester²

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For the safe underground storage of radioactive waste, it is crucial to carefully determine the porosity of the host rock as pores control all of its physical properties, such as the essential low permeability. Specialized scanning electron microscopy (SEM) is an established method in the analysis of Opalinus Clay and used in many studies, e.g. [Houben et al., 2013], [Laurich et al., 2018], and [Keller, 2021]. In the studies, the pores are characterized and evaluated by size, orientation, and frequency using

binary segmentation masks. However, the creation of these masks entails some difficulties, such as interpretation limitations, non-standard procedures, and in particular, the nanoscale resolution limit of the SEM. In addition, the overlap of gray values between grains and pores makes conventional methods like the gray value thresholding method not applicable.

Over the past decades, technical achievements in image analysis and machine learning have led to the development of new methods. Especially methods based on self-learning algorithms show the potential to perform even sophisticated analyses. From a geoscientific point of view, the goal is to analyze high-resolution information from sample material in large quantities.

This requires at least a semi-automatic analysis workflow.

This work presents a method that enhances the original micrograph's resolution and improves the quality of pore identification. First, the resolution of the SEM images is artificially increased. Our approach uses an Enhanced Super-Resolution Generative Adversarial Network (ESRGAN) [Wang et al., 2018] trained in the upsampling of SEM images. The enhanced images show much more detailed pores and pore edges so that even small pores can be identified with greater clarity. This step is followed by a voting algorithm that combines several machine learning classifiers (MLC) and calculates a probability field on that basis. Nine different MLC's were trained in this process. This training allows the derivation of different confidence levels that reduce false pore segmentation and capture the pore edges more smoothly and consistently.

The proposed method is able to detect pores in Opalinus clay that were previously undetected or poorly segmented. Thus, even small pores are now detected with better quality and a clear edge identification, which makes it possible to lower the practical truncation limit [Bonnet et al., 2001]. We discuss the results and further ongoing work to improve the reliability of MLC's with ESRGAN images.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

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MS06-A / 150

Investigating the pore scale mechanism of miscible phases mixing in porous medium 2D

Author: Yahel Eliyahu-Yakir¹

Co-authors: Tal Ballas ; Ludmila Abezgaüz¹; Yaniv Edery¹

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The process of a fluid replacing a separate miscible fluid in a porous medium is present in many industrial and natural systems, such as enhanced oil recovery, CO₂ sequestration and salt-fresh water interfaces in the ground. While the replacement can be approximated with the Darcy law, the mechanisms of the miscible phases mixing to the displacement remain unclear, specifically as the heterogeneity of the domain increases. As this mixing influences the reaction pattern between the fluids, it is important to estimate it using indirect measurements that are available, such as pressure and flux measurements. We propose a set of experiments that allow us to observe and measure the displacement and mixing process in high resolution and with the use of image analysis we can distinguish between the mechanisms. We can clearly see how the heterogeneous rate of the pore structure influences the mixing pattern, rate, and duration. Surprisingly, we found a clear and typical “mark” of the mechanisms on the flow rate, under constant pressure, which allows us to relate heterogeneity level of the structure to the ratio of displacement to mixing.

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MS06-A / 151

A mathematical model of oil-water spontaneous imbibition with dynamic contact angle in the fractal porous media of tight reservoirs

Authors: Yongfei Yang¹; Lixin Kang¹; Lei Zhang²; Jun Yao¹

¹ *China University of Petroleum (East China)*

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Corresponding Authors: kanglixinupc@163.com, yangyongfei@upc.edu.cn, zhlei84@163.com, shenliu603@163.com

Spontaneous imbibition is an important mechanism of improving oil recovery in tight reservoir. Oil-water contact angle is one of the most important factors affecting spontaneous imbibition process, but the dynamic change of contact angle during imbibition is ignored in most studies. Considering the dynamic change of contact angle, the flow equation for the oil-water spontaneous imbibition with dynamic contact angle in a capillary is derived, and the flow velocity, imbibition distance and capillary pressure during the spontaneous imbibition process are characterized. Then, based on fractal theory, a capillary bundle model was constructed by using the porosity, pore distribution function in a tight sandstone core. A core-scale mathematical model for the oil-water spontaneous imbibition with dynamic contact angle in a tight sandstone core is developed. The effects of contact angle, fluid viscosity and surface tension on quantity of flow during the spontaneous imbibition process are studied and validated with simulation data and experimental data from the literature. The results show that the fluid flow can increase the contact angle and reduce capillary pressure. The imbibition flow calculated by the model is smaller than that calculated by L-W model. a relatively good match in imbibition profiles obtained by the mathematical model with dynamic contact angle and experiments at the long stage of air-water spontaneous imbibition. This study may thus provide new insights into studying the oil-water flow in tight reservoirs.

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MS09 / 152

Particle-Strength-Exchange methods for Lagrangian 3D DNS of rheological and reactive fluids with evolving interfaces at the pore-scale

Authors: Sarah Perez¹; Philippe Poncet¹

¹ *University Pau & Pays Adour, France*

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This talk will show the latest developments in Lagrangian/particle methods for the computation of complex fluid dynamics in real 3D geometries at the pore-scale. This involves the consideration of shear-thinning fluids from [2,5] and reactive solid rock matrix [1], using the Lagrangian transport developed in [2], whose physical considerations have been validated in [3].

These models couple the diffusion and transport of chemical species in the pore space of a rock matrix itself reacting with the fluids. The hydrodynamics of the fluid is then strongly coupled to

species concentrations, especially in the non-Newtonian context for which the viscosity of the fluid depends non-linearly on the concentrations.

Our practical applications focus on the methodology for computing these coupled phenomena in complex geometry and consequently we consider configurations with a minimal number of components: we consider reactions of the kind $A + B \rightarrow C + D$ (typically involving calcite), in a geometry built by microCT measures, with a Carreau law for the shear-thinning fluid (typically involving Xanthan).

Among all the mathematical terms involved in the partial differential equations modeling this coupled system, the Particle-Strength-Exchange method is dedicated to approximating the term $-\text{div}(L\nabla u)$. Using a particle description of the species velocity or concentration, the goal is to establish an exchange kernel σ between particle in their large neighborhood. Due to the substantial number of neighbor particles, especially for large 3D computations, a stencil generator Θ (here a spherically symmetric function with compact support) is considered: all the work required is to link L , Θ and σ . The exchange kernel σ is produced at second order, its weights being given by a straightforward formula, to the opposite of SPH methods which require the computation of weights at each particle and each time steps.

It results in an efficient numerical method, conservative by construction, second order and allowing large variations in the diffusion coefficients. This is especially convenient for two-scale porosity models (such as Koseny-Carman law), Archie's law of the rock matrix (modeling the tortuosity of the subscale pore space), and more generally for averaged equations modeling the effect of porosity in the rock matrix. This is also well-fitted to shear-thinning features of the fluid, exhibiting up to 5 orders of magnitude in the value of the viscosity. Future work will involve mechanical coupling using wall displacements, inspired from the wall laws introduced in [4].

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS07 / 153

Modeling of Multicomponent Flow in Porous Media using Higher-Order Methods

Authors: Petr Gális¹; Jiří Mikyška^{None}

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A numerical scheme of higher-order approximation in both space and time for the single-phase multicomponent flow in porous media is presented. The mathematical model consists of Darcy velocity, transport equations for components of a mixture, pressure equation and associated relations for physical quantities such as viscosity or density. The discrete problem is obtained using a combination of discontinuous Galerkin method for the discretization of transport equations with and of mixed-hybrid finite element method for the discretization of Darcy and pressure equations both using higher-order approximation. Subsequent nonlinear problem is solved with the fully mass-conservative iterative IMPEC method. Experimental order of convergence analysis (EOC) and some numerical experiments of 2D flow are carried out.

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Time Block A (09:00-12:00 CET)

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MS17 / 154

Experimental measurement of the heat transfer coefficients for gas flow through granular porous media

Author: Shaolin Liu^{None}

Co-authors: Azita Ahmadi¹; Cyril Levet²; Jean Lachaud³

¹ ENSAM - I2M

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Heat transfer phenomena through granular porous media are widespread in industrial fields e.g. energy storage technology and thermal process engineering. Numerous research focused on a uniform temperature distribution within the solid phase with small Biot numbers (Bi), see [1] for a review. The volumetric heat transfer coefficient (Hv) is used to represent the internal heat exchange between the fluid and solid phases. Here we obtained Hv and the solid effective thermal conductivity for large Biot numbers ($Bi \gg 0.1$) by using an inverse analysis [2] of experimental results with well-designed simulations. The experiment was conducted using a transient technique in a 1 m long, 194 mm diameter iron tube filled with uniformly sized glass spheres ($d = 16$ mm). The temperatures inside the iron tube are measured at seven central axis locations ($x = 5, 15, 25, 35, 45, 65, 85$ cm) and three radial locations. The wall surface temperature is also measured at four axial locations ($x = 5, 35, 65, 90$ cm). The inlet boundary condition for the pressure is calculated based on the velocity measured at the outlet assuming a constant mass flow rate in the porous sample. The inlet mass flow rate is variable in order to obtain a range of Reynolds (Re) in the experiment. The flow inside the granular porous medium is considered compressible, the coupling between gas density and temperature is implemented in the mass conservation equation. The velocity field is modeled by the Darcy-Forchheimer equation based on the Reynolds number ($Re \gg 10$). Heat transfer is described using a local thermal non-equilibrium (LTNE) model in which there is conduction in both phases and convection in fluid phase. The governing equations are solved in the Porous material Analysis Toolbox based on OpenFoam (PATO) [3]. Hv is calculated and optimized based on the Wakao correlations [4] between the Nusselts (Nu), Prandlt (Pr) and Re numbers in which a new coefficient f has been added, $Nu = 2 + f \cdot Pr^{1/3} Re^{0.6}$. The effective solid conductivity is treated as an anisotropic tensor due to the flow. The results show that Hv is a function of space and time within granular porous media. The distribution of Hv is consistent with the gas temperature distribution e.g., where the gas temperature is high, Hv is also high. The factor f in the Nu correlations will increase with the increase in the Re . The inverse analysis can be used to obtain Hv and effective solid conductivity in uniform sized spheres and random shape granular porous media.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS06-B / 155

Modeling of spontaneous imbibition in porous media from modified Lucas-Washburn equation

Author: Jianchao Cai¹

Co-authors: Chenhao Sun¹; Yang Liu²; Yin Chen²

¹ *China University of Petroleum, Beijing*

² *China University of Geosciences, Wuhan*

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Capillary-driven flow in porous media is prevalent in nature and in industry, such as petroleum and hydraulic engineering as well as material and life sciences. Due to the numerous types and complex structures of porous media, together with a number of influencing factors, the study of capillary-driven flow based on theoretical analysis and numerical simulation methods is now widely carried out to reveal the flow mechanisms and seepage laws behind them. Recent advances made over the last several decades in this field are systematically reviewed in this work. The progress in mathematical models that modify and extend the Lucas-Washburn (LW) equation for various microchannels and porous media, including heterogeneous porous media, discrete fractures and capillary tubes with different geometries, is comprehensively summarized. In addition, numerical simulation methods used for capillary-driven flow in porous systems, such as molecular dynamics method, pore network modeling, the phase-field method and the volume-of-fluid method, are thoroughly reviewed. Based on these, the comments on the future works and research directions on the capillary-driven flow in porous systems are made. The present work provides a systematic and detailed review of advances in capillary imbibition in numerous fields, which is useful for understanding the capillary imbibition in different types of porous systems.

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Poster / 156

Wave-induced fluid flow in fractal porous media

Author: Shanshan Jiang¹

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¹ *China University of Geosciences, Wuhan*

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Wave-induced fluid flow (WIFF), as an intrinsic attenuation mechanism, is a significant mechanism in causing seismic attenuation and dispersion in saturated porous media. However, the fact that the WIFF is related to the complex structure of porous media is always ignored. Since the fractal nature of rocks is revealed, make it possible to study the fluid flow in different scales in a flexible way. In this paper, a poroelasticity model considering fractal distribution of the grain radius is developed and the explicit expression of the quality factor is derived to study the attenuation and dispersion in saturated porous media. Further, the analytic properties of attenuation and dispersion are analyzed. It is shown in the case where the structure is a self-similar fractal medium, the quality factor Q is a power law in the wave frequency, while the exponent of this power law is related to the fractal dimension of the grain radius. These results provide theoretical basis to estimate the formation properties with the seismic data in the future.

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Poster / 157

Pore structure characterization and seepage law analysis of tight reservoir

Author: Liang Jiao¹

Co-authors: Jianchao Cai ²; Yuxuan Xia ¹; Xiangjie Qin ²; Kai Xu ²; Henglei Zhang ¹

¹ *China University of Geosciences, Wuhan*

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Tight oil and gas exploration and development has made important progress in the world, and its resource potential and prospect are widely concerned. However, tight reservoir network system formed by the development of pores, micro fractures and artificial fractures is complex, which makes it difficult to study the microscopic flow law of tight reservoirs. Combined with X-CT images, the cores are divided into three types: matrix, fracture and vugs. Based on the fractal theory and the High-Pressure Mercury Intrusion experiment, four fractal models were used to calculate the fractal dimension of rock samples. The relationship between the calculated fractal dimension and the physical properties of tight reservoirs is analyzed. Simultaneously, using the mathematical simulation

method, the single-phase flow intrinsic permeability model of fractal capillary bundle and the single-phase flow apparent gas permeability model of flow permeability tight reservoir with slippage effect were established. The validity of the model was verified on the basis of the experimental data of gas permeability and intrinsic permeability. Besides, according to the fractal characteristics of pore size distribution and tortuosity, a novel and more generalized two-phase flow relative permeability prediction model was established. Based on the relative permeability experiment, the validity of the model was verified. It is found that there is a strong consistency between the model prediction and the existing experimental data. At the same time, the factors affecting the relative permeability model parameters are analyzed. This study provides a theoretical basis for effective displacement and enhancement recovery of tight reservoirs.

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Poster / 158

Effect of grain size and distribution on the two-phase flow at pore scale

Author: Yin Chen¹

Co-authors: Jianchao Cai ²; Yang Liu ¹; Jiuyu Zhao ²; Yadan Mao ¹

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² China University of Petroleum, Beijing

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The size and distribution of grain have great influence on the micro-scale displacement mechanisms. Coupled Cahn–Hilliard phase field and Navier–Stokes equations were solved using finite element method to simulate two-phase flow in homogeneous and heterogeneous models, respectively. Several heterogeneous models were conducted with different heterogeneity intensity and distribution. In both models, the medium porosity and absolute permeability were kept unchanged, compared to the homogeneous case. The micromodels were initially saturated by oil, and the displacing fluids were prepared as aqueous water. The preferred paths and flow morphologies of these models were obviously different. The general trends of the oil recovery factor and macro-scale capillary pressure variations were similar during displacement under different wettabilities condition for different models. However, the homogeneous model showed higher displacement efficiency at water-wet conditions and lower capillary pressures at oil-wet conditions; due to less complexity of its pore network geometry. These findings extend our understanding of the effect of grain size and distribution on water flooding process.

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MS15 / 159

Data-Driven Physics-informed Interpolation Evolution Combining Historical-Predicted Knowledge for Remaining Oil Distribution Prediction

Authors: Jingwei Zhu¹; Chiyu Xie¹; Jiulong Wang²; Shuyi Du¹; Hongqing Song¹

¹ *University of Science and Technology Beijing; School of Civil and Resource Engineering*

² *Computer Network Information Center, Chinese Academy of Sciences*

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The remaining oil distribution plays an important role in enhanced oil recovery (EOR), which directly guides the development of an oil reservoir in the middle and later stages. However, it is still challenging to accurately and efficiently characterize the distribution of remaining oil due to the complex reservoir geology. We propose a data-driven physics-informed interpolation evolution algorithm combining historical-predicted knowledge (DPIE-HPK) for the prediction of remaining oil distribution. As a key step towards the remaining oil distribution, the production rates can be predicted as well. A physics-informed data supplement (PIDS) process is also presented to assist the DPIE-HPK algorithm. Both historical physics information and future information are used in the DPIE-HPK framework. The historical physical information is preprocessed by the PIDS, and future information is predicted by Long Short-Term Memory (LSTM) deep learning models. As a crucial interpolation evolution method, the Kriging method is also integrated into the framework to evolve the unknown spatial information. We test the DPIE-HPK framework for the prediction of the remaining oil distribution of a typical tight carbonate oil reservoir located in the Middle East. It is concluded that the DPIE-HPK framework is an accurate and efficient intelligence tool for predicting the remaining oil distribution.

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MS10 / 160

Multiscale pore structure evolution of shale induced by dilute acid**Author:** Sai Xu¹**Co-authors:** Jianchaoi Cai ²; Lei Wang ¹; Qi Zhang ¹¹ *China University of Geosciences, Wuhan*² *China University of Petroleum, Beijing***Corresponding Authors:** xus@cug.edu.cn, qizhang@cug.edu.cn, wanglei330@cug.edu.cn

Hydraulic fracturing to generate complex fracture networks is the most effective stimulation method to develop shale reservoirs. However, the stimulated reservoir volume (SRV) is limited due to the high stress difference, high breakdown pressure and undeveloped natural fracture. Acid treatment has been approved to be an effective way to enhance SRV by reducing shale rock mechanical strength and improving petrophysical properties. In this work, acid soaking experiments are conducted on Longmaxi shale samples to study the mechanism of acid treatment. Cylindrical and powdered shale samples were thoroughly immersed in 15 wt% hydrochloric acid for 10 days. X-ray micro-computed tomography (micro-CT) scanning and low-pressure nitrogen gas adsorption experiments are performed on cylindrical and powdered samples before and after acid treatment. Inductively coupled plasma mass spectrometry (ICP-OES) and X-ray diffraction (XRD) are used for elemental analysis during the acid rock reaction. The nanopore size distribution and pore structure parameters obtained from nitrogen adsorption/desorption isotherms are compared before and after acid soaking. The changes of microscale pores and fractures are directly visualized in micro-CT images. The mechanism of multiscale pore structure evolution during acid-shale interaction is quantitatively discussed. The results show that the pore diameter and pore volume increase significantly, nanopores in shale are enlarged after the acid soaking experiment. Some pores and fractures are generated due to the acid dissolution. The elemental analysis from ICP-OES and XRD indicates that carbonate minerals (calcite and dolomite) are partially dissolved, generating the pores and fractures. Only the pyrite near the fracture is dissolved due to the poor pore connectivity of shale. The findings presented in this work help understand the pore structure evolution mechanism during acid treatment in shale, which would have great significance in shale reservoir development.

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Poster / 161

Study on the dominant factors of rock permeability

Author: Kai Xu¹

Co-authors: Jianchao Cai ¹; Chenhao Sun ¹; Juncheng Qiao ¹; Xiangjie Qin ¹; Jiuyu Zhao ¹

¹ *China University of Petroleum, Beijing*

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Permeability is usually considered to be related to porosity. However, rocks with the same porosity may have different permeabilities in some cases, because of the variations in pore and throat size and pore space connectivity. It is vitally important to understand the effect of throat size on the transport property. In this work, five sets of regular pore network models and six core-based models are employed to study the effect of throat size on permeability. Four kinds of random distributions are utilized to generate reconstructed pore network models with varying pore size. Average pore coordination number is adjusted for the verification of the effect of connectivity on permeability. Random pore networks are also constructed to study the threshold point of permeability variation. Random forest and factor analysis methods are employed to study the dominant factors controlling permeability based on PNM extracted from core samples. The simulation results indicate that small throats play an extremely important role in determining permeability. The influence of pore coordination number on permeability is not obvious compared to that of small throat size.

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Poster / 162

Hydrate growth and electrical properties modeling based on digital rock techniques

Author: Haitao Tian¹

Co-authors: Jianchao Cai ²; Wei Wei ¹; Yuxuan Xia ¹

¹ *China University of Geosciences, Wuhan*

² *China University of Petroleum, Beijing*

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During the exploration of natural gas hydrate reservoirs, the macro-scale spatial heterogeneity of hydrate sediments is caused by the formation of hydrates, which makes it difficult to predict the hydrate saturation accurately. In this study, random simulation methods are used to construct digital rocks under three types of hydrate growth habits (Grain-Coating, Pore-Filling, and Patchy), and the finite element method is carried out to simulate the resistivity of digital rocks. By extracting the pore size distribution parameters and fractal dimensions of digital cores under different hydrate saturations, the differences in the influence of the microstructure evolution of the three types of hydrate distribution on the electrical properties of the sediments are analyzed. The results show that with the increase of hydrate saturation, the change of microstructure caused by Grain-Coating type growth has the most significant effect on the electrical conduction process at the same hydrate saturation. The pore structure changes caused by Pore-Filling growth have the least influence on the electrical conduction process; the different pore size distribution of sediment under different hydrate morphologies explain the electrical differences of the three types of hydrate morphologies. Finally, the applicability of the empirical value is further verified by comparing the dissolved gas method hydrate synthesis experiment in the laboratory. Combined with the in-situ resistivity logging data, the difference between the empirical parameter values under the laboratory and actual reservoir conditions is analyzed.

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MS03 / 163

Fractal characterization of time-dependent shape factor for counter-current imbibition in fractured reservoirs

Author: Lan Mei¹

Co-authors: Jianchao Cai ²; Qingbang Meng ¹; Yin Chen ¹

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The fluid exchange behavior for counter-current imbibition in fractured reservoirs can be quantitatively characterized by the transfer function in the numerical simulation. The time-dependent shape factor (TDSF) in the transfer function is one of the main factors controlling fluid transport, and it directly affects the result of ultimate oil recovery prediction. However, the current TDSFs proposed for counter-current imbibition assume that the microscopic pore structure has no impact on the fluid inter-porosity flow behavior, which is inconsistent with the actual situation. In this work, the fractal theory is employed to establish the TDSF of counter-current imbibition which is related to microscopic pore structure. The analytical solutions of average water saturation and imbibition rate under different conditions related to maximum pore diameter and tortuosity fractal dimension of the matrix are first obtained. The validity of the new analytical solution is ascertained by single-porosity model and experimental data. Then, the new analytical solution is applied to the two-phase transfer function to introduce the new TDSF for counter-current imbibition. The results demonstrate that the unsteady state duration of the TDSF is proportional to characteristic length and tortuosity fractal dimension of the matrix, and negatively proportional to maximum pore diameter of the matrix on the contrary. The influence of characteristic length, tortuosity fractal dimension and maximum pore diameter of the matrix on the value of constant shape factor under quasi steady state is exactly the opposite. This work fosters a better understanding of fluid exchange behavior during counter-current imbibition in fractured reservoirs.

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Poster / 164

The degree and law of the influence of microscopic pore structure on permeability in digital rocks

Author: Xiaobin Li¹

Co-authors: Wei Wei¹; Lei Wang¹; Jianchao Cai²

¹ China University of Geosciences, Wuhan

² China University of Petroleum, Beijing

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The three-dimensional digital core, which describes the microstructure of the rock on the pore scale, has become the basis for quantitative analysis of the pore structure and physical properties of the rock. The microscopic pore structure of rock greatly affects its seepage properties. Permeability is a parameter that characterizes the ability of a rock to conduct fluid, and it is one of the most important physical properties of rock. Using numerical simulation methods to study the influence of

microscopic factors on the permeability can make up for the deficiencies of traditional rock physics experiments and provide a bridge for quantitatively investigating the relationship between pore structure and permeability. In this paper, the degree and law of influence of microscopic factors on permeability are explored by using pore network model. Taking the X-ray CT rock and process-based model as the digital core material, the maximum ball technique is used to establish pore network model equivalent to the digital core, and their topological properties, pore throat size, and pore throat shape are analyzed. Based on the quasi-static principle and these digital cores, the influence of various factors (including grain skeleton, pore characteristics, fluid properties) on permeability is analyzed quantitatively. The primary and secondary factors can be judged by comparing the change times of the permeability of each pore throat parameter in the variation interval: throat size > coordination number > throat shape > pore size > pore shape. In addition, the relationship models between univariate factors and permeability parameters are established and analyzed. This research is helpful to understand the influence of micro-pore structure on permeability, find out primary and secondary factors, and provide more reference for reservoir logging prediction and petrophysical permeability model construction.

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MS10 / 165

Microstructural and mineral phase changes of reinforced concrete caused by high concentration CO₂

Authors: Quan Xue¹; Liwei Zhang¹

Co-authors: Kaiyuan Mei¹; Yan Wang¹; Pania Newell²; Manguang Gan¹; Xiaojuan Fu¹; Xiaochun Li¹

¹ *Institute of Rock and Soil Mechanics, Chinese Academy of Sciences*

² *Department of Mechanical Engineering, The University of Utah*

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At present, reinforced concrete is the most commonly used building material. Due to possible CO₂ reservoir leakage, reinforced concrete may be corroded by high concentration CO₂ (> 1 atm CO₂ partial pressure). In order to study the effects of corrosion time, CO₂ partial pressure and relative humidity (RH) on structural deterioration of reinforced concrete exposed to high concentration CO₂, reinforced concrete samples were prepared and corroded by 0.1, 0.5 and 1.0 MPa high purity CO₂ under water immersion, dry gas and 70% relative humidity conditions. The mineral phase changes of the samples were characterized by X-ray diffraction (XRD) and energy dispersive X-ray spectroscopy (EDS), and the structural changes of the samples with different corrosion times were characterized by micron computed tomography (μ -CT). The μ -CT images were analyzed by Avizo software, and the

images showed that the concrete corroded by CO₂ produced calcium carbonate, which was mainly deposited in pores. The reinforcement corroded by CO₂ produced iron oxide and iron hydroxide, mainly deposited on the contact interface between reinforcement and concrete. The corrosion products of reinforcement filled the pores around the reinforcement and penetrated into concrete with the development of corrosion time, which caused cracks to generate and expand. The corrosion degree increased with the increase of corrosion time and CO₂ pressure, and the corrosion of reinforced concrete samples immersed in water was the most serious.

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Poster / 166

A fast hybrid method of reconstructing 3D digital rock

Authors: Weichao Yan¹; Huilin Xing¹; Likai Cui²; Ping Feng³

¹ *Key Lab of Submarine Geosciences and Prospecting Techniques, MOE and College of Marine Geosciences, Ocean University of China*

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3D digital rock is widely used in the oil and gas industry to analyze pore structures and estimate petrophysical properties of rocks, such as permeability, elastic modulus, resistivity, and nuclear magnetic resonance response. Computed tomography (CT) images are the most common data for constructing 3D digital rock. However, the CT experiment is expensive, and rocks are not easy to obtain in some cases. It is still necessary to study the method of reconstructing 3D digital rock from one 2D slice.

In the presented work, we put forward a fast hybrid method of reconstructing 3D digital rock and investigated its effectiveness. We first reconstructed 3D digital rock (S1) with 200×200×200 voxels by the traditional sequential indicator simulation method (SISIM) from one 2D CT slice. Corrosion and expansion operations were then applied on the reconstructed 3D pore spaces to generate the new 3D digital rock. We determined whether the absolute error between the porosity of the newly generated digital rock and the actual porosity was less than 0.5%. If not, the corrosion and expansion were repeated until the absolute error was less than 0.5%, and then the final 3D digital rock was reconstructed (S2). Permeability, resistivity, and local porosity distribution function of the reconstructed digital rock were also calculated to verify the validity of the new method.

Results show that the 3D digital rock constructed by the hybrid method has good long-distance pore connectivity characteristics. Compared with the permeability of S1 (126.94 mD), the permeability of S2 is increased by at least seven times (889.19 mD), which is in better agreement with the actual result (970.73 mD). The saturation indexes of the digital rock models S1, S2 calculated by finite element method are 1.99 and 1.73, respectively. The actual saturation index is 1.64, which verifies the accuracy of the new method. The geometric mean of the local porosity distribution function of S2 (0.19 %) agrees well with the actual result (0.18 %), which also shows the reliability of the new method. It takes less than 3 minutes to generate a digital rock by using the new method, which is faster compared to the multiple-point statistics method and artificial intelligence methods.

The proposed methodology is simple and fast, which has the potential to attract more researchers to use it. Moreover, this hybrid method will be helpful in gaining insight into the relations between the pore structures and petrophysical properties by analyzing a large number of stochastic reconstructed digital rocks.

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Poster / 167

Molecular investigation on sorption-induced kerogen deformation and its impact on gas transport

Author: Jian Wu¹

Co-authors: Pengyu Huang¹; Luming Shen¹

¹ *The University of Sydney*

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Shale gas is becoming an increasingly important source in the global energy sector. The shale reservoir is characterized by the small porosity and ultra-low permeability, and the shale gas production decays rapidly with time. In the process of gas production, shale is expected to deform in response to gas adsorption and desorption, similar to many other nanoporous materials. Despite the potential effects on gas permeability and transport, the sorption-induced deformation remains poorly understood and is often overlooked in large-scale simulations.

In this study, we first use a hybrid Monte Carlo and molecular dynamics method to investigate methane adsorption and desorption in a flexible kerogen matrix (i.e., shale's primary organic matter). The volume of the simulation box is monitored during the process, and the volumetric strain is calculated at each pressure. Using a surface energy approach, a non-linear adsorption-strain model

is derived to describe the relationship between the methane adsorption amount and the volumetric strain by taking the methane adsorption and deformation coupling into consideration. Furthermore, methane flow is simulated by non-equilibrium molecular dynamics in both rigid and flexible kerogen slit pores with sizes ranging from 10 to 40 Å. The total gas flux and the apparent gas permeability are calculated and analyzed separately as a function of pore pressure. In addition, a diffusive-viscous gas flow model is proposed by coupling the adsorption-strain relationship to provide predictions for gas flux in realistic kerogen nanopores.

It is found that methane adsorption can induce a swelling volumetric strain up to 5.1% in the kerogen matrix, which narrows the 10 Å slit pore by 30% under the constant volume condition. The sorption-induced swelling dominates over the mechanical compression within 50 MPa. The decrease of the main flow path significantly reduces viscous gas flux in the confined environment. Compared with the rigid structure, the flexible kerogen slit pore results in less mass flux under the same pressure. This discrepancy is insignificant at low pressure but becomes more pronounced when pore pressure is high. For example, the relative reduction of mass flux under 50 MPa of gas pressure is 23%, 29%, 40%, 49%, and 64% for slit pores of size 40 Å, 30 Å, 20 Å, 15 Å, and 10 Å, respectively. Similar trends are also observed for the apparent gas permeability calculated from the total mass flux using Darcy's law. Moreover, the permeability ratio between the rigid and flexible slit pores declines hyperbolically with the increasing pore size and gradually approaches unity.

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Poster / 170

3D Microscale Flow Simulation of Newtonian and Shear Thinning Fluids in Sandstone and Carbonate Samples

Authors: Mehdi Amiri¹; Jafar Qajar^{None}; Ali Qaseminejad Raeini²

¹ *1Department of Petroleum Engineering, School of Chemical and Petroleum Engineering, Shiraz University, Shiraz, Iran*

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This study presents a series of 3D single-phase microscale simulations for flow of Newtonian and shear-thinning fluids through a sandstone and a carbonate samples over a range of flow velocities. Due to the requirements of multiple simulations and long computation times, the image size was chosen based on the representative elementary volume for porosity and permeability. Critical velocity was evaluated for both Newtonian and shear-thinning fluids to recognize when the flow was converted from Darcy to the non-Darcy regime. Approximately the same critical velocity was obtained

for both fluids. A lower critical velocity was found for the flow of the fluids through the carbonate samples compared to the sandstone samples. The calculated Forchheimer coefficients for the fluids indicated dependencies on the rock properties and also the Forchheimer coefficient for carbonate sample is larger than the sandstone sample. Furthermore, it was found that the shift factor that expresses the relationship between the porous medium and bulk viscosities was larger for the flow of shear-thinning fluids through the carbonate samples than those in the sandstone samples.

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Poster / 171

The Effect of Power Law Index on Shift Factor for Shear Thinning Fluids by 3D Microscale Flow Simulation

Authors: Mehdi Amiri^{None}; Jafar Qajar^{None}; Ali Qaseminejad Raeini¹

¹ *Research Associate*

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The flow of non-Newtonian fluids through porous media is of great importance for various applications, such as heavy oil recovery, polymer enhanced oil recovery, and liquid polymer molding. Understanding these processes, however, is a challenging task as the topology of the pore space results in a wide range of flow velocities and shear rates and consequently to variation of effective fluid viscosity in space and time. A common approach for the slow flow of a non-Newtonian fluid through a porous medium is to lump all non-Newtonian effects into a parameter called the porous medium viscosity. This parameter depends on the properties of both the fluid and the porous medium, including a shift factor that expresses the relationship between the porous medium and bulk viscosities. In this work, we investigate the effect of the power-law index (n) on the shift factor for the flow of shear-thinning fluids through rock samples with varying pore structure and heterogeneity. Direct simulations were performed on micro-computed tomography (μ -CT) images of several sandstones and carbonates using a non-Newtonian package based on OpenFOAM. It was found that for small values of n , the value of shift factor was very large, and with increasing the value of n , the shift factor decreased. In addition, for samples with low formation factors (samples with low complexity), the value of shift factor was obtained to be close to one for a wide range of n . However, for samples with large formation factors (sample with very high complexity), the value of shift factor was significantly larger, and the value of shift factor greatly increased for small values of n .

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Poster / 172

Characterisation and Comparison of Algal Biochar at Different Pyrolysis Temperatures

Author: Kamal Elyasi Gomari¹

Co-authors: David Hughes¹; Duncan Macquarrie²; Suranjana Bose²; Tabitha Petchey²; Tannaz Pak³; Thierry Tonon⁴

¹ School of Computing, Engineering & Digital Technologies, Teesside University, UK

² Green Chemistry Centre of Excellence, Department of Chemistry, University of York, UK.

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Algal biomass is a reasonable feedstock for the production of bio-energy and valuable bio-chemicals. Thermochemical techniques such as pyrolysis, liquefaction, and gasification are eminent approaches to produce biochar from the biomass in the absence of oxygen. Pyrolysis is proposed as an effective method compared to other techniques due to its operating state. Biochar is a porous, largely carbon-based material. Biochar from algal biomass has recently gained more attention in the application of supercapacitor, coal fuel, adsorbents, and catalysts. In this research, five brown algae (*Laminaria digitata*, *Saccharina latissima*, *Saccorhiza polyschides*, *Himanthalia elongata*, and pelagic *Sargassum*) have been converted to biochar at a wide range of temperatures (300-800°C). Chemical and physical properties of raw and algal biochars have been characterised using FT-IR, XRD, EDX, BET, and SEM. Then, a comparison between raw and algal biochars was conducted.

The results indicated that algal biochar yield is negatively correlated with temperature, where by increasing the temperature from 300 to 800°C, the yield of biochars decreased from 70% to 38%. The pH and electrical conductivity (EC) of algal biochars were high compared to the algal biomass. However, at high temperatures (600-800°C), the pH was constant for algal biochars. The EDX results showed that the most prevalent inorganic nutrients in algal biomass and biochar are K, Mg, Na, O, Ca, and Cl. Furthermore, the result of XRD, for both algal biomass and biochar, showed a crystalline structure of Sylvite/Halite at 28-29°. In respect to the FT-IR spectrum, three main functional groups, namely carbohydrates, proteins, and lipids were assigned in algal biomass, where the strong bond of C-O was detected at 110-1200 cm⁻¹. However, some of the functional groups disappeared by increasing the pyrolysis temperature. With respect to the BET analysis, there was a direct link between temperature and surface area. In fact, as temperature increased, the surface area also increased. SEM images confirmed that algal biomass was smooth without any pores. However, after the pyrolysis

process, several pores were created due to the volatilization of organic materials. Potential application of algal biochar in soil amendment for enhancing soil fertility, and reducing soil acidity is recommended.

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MS06-B / 173

The effect of surface tension and contact angle dynamics in averaged models for two-phase flow at the pore scale

Authors: Stephan B. Lunowa¹; Arjen Mascini²; Carina Bringedal^{None}; Tom Bultreys³; Veerle Cnudde³; Iuliu Sorin Pop⁴

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The mathematical models for the capillary-driven flow of immiscible fluids in porous media are typically assuming a static contact angle at the moving contact line. However, the dynamics of the fluid-fluid interface, particularly of the contact angle is an important feature. Here, we consider the flow of two fluids in a single pore. The geometry is idealized to a long, thin tube with slowly varying radius. The fluids are separated by a moving fluid-fluid interface, which is in contact with the pore wall. Its movement is driven by the fluid flow and surface tension. The contact line model incorporates Navier-slip boundary conditions and a dynamic and possibly hysteretic contact angle law.

Assuming a scale separation induced by a small aspect ratio of the typical radius to the length of the pore, we apply matched asymptotic expansions to derive effective models for the two-phase flow in the limit as this ratio approaches zero. These models form a system of differential algebraic equations in terms of the interface position and the total flux. The resulting model combines Darcy-type equations for the flow with a capillary pressure - saturation relationship involving dynamic effects. Numerical examples highlight the role and importance of such effects.

In the context of capillary rise in circular cylindrical tubes, the effective model extends the classical Lucas-Washburn model by incorporating a dynamic contact angle and slip. Since inertial effects can be relevant at early times, we further extend this model to account for inertia. To validate the

different models, their solutions are compared to experimental data. In contrast to the classical Lucas–Washburn model, the numerical results obtained using the models with dynamic contact angle are matching well with the experimental data, with respect to both the rise height and the contact angle, even at early times.

Finally, an outlook to ongoing work covers the upscaling from pore scale to Darcy scale. To this end, we include the effective model as pore-throat model in a dynamic pore-network simulation. Averaging over the pore network then yields the macro-scale behaviour including the effect of surface tension and contact angle dynamics.

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- S. B. Lunowa, A. Mascini, C. Bringedal, T. Bultreys, V. Cnudde, I. S. Pop, *Dynamic effects during the capillary rise of fluids in cylindrical tubes*, UHasselt CMAT Preprint UP-21-07. www.uhasselt.be/Documents/CMAT/Preprints

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S. B. Lunowa, A. Mascini, C. Bringedal, T. Bultreys, V. Cnudde, I. S. Pop, *Dynamic effects during the capillary rise of fluids in cylindrical tubes*, UHasselt CMAT preprint UP-21-07. www.uhasselt.be/Documents/CMAT/Preprints/2021/UP2

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MS09 / 174

A Geometry-based Throat Shape Correction of Pore Network Models

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Co-authors: Martin Lautenschläger²; Julius Weinmiller³; Timo Danner¹; Arnulf Latz⁴

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Pore network models (PNM) are a simplified but powerful tool for fluid flow simulation in porous media. In contrast to other computational methods, e.g. the lattice Boltzmann method (LBM), where complex transport equations are solved with high structural resolution, PNM uses a strongly simplified basis. The realistic pore space is often approximated as a network of spherical pores connected by cylindrical throats with constant diameters in which simple algebraic equations are solved. Thus, PNM is computationally extremely efficient. Compared to LBM simulations, the computational time is many orders of magnitude smaller. For typical porous media applications, it can be reduced from days to minutes. This, however, comes at the cost of physical insight, and is sometimes too simplistic, especially for microporous structures where the shapes of pores and throats strongly deviate from spheres and cylinders, respectively.

To reduce or overcome this issue, in the present work, we developed an improved PNM that takes the structural deviations into account. The underlying Purcell physics, which assume constricting throats, are corrected based on a physically motivated geometrical shape factor that depends on the ratio of the inscribed and equivalent throat diameter. Using the new PNM, pressure-saturation curves are determined and compared to LBM simulations. The electrolyte filling of porous battery components is utilized as a use case. The model is adjusted to data determined from the cathode side. It is shown that thereby the filling behavior of the structurally different anode side can be predicted accurately.

Electrolyte filling is just one example for a broad variety of setups involving porous media percolation. It is used here to show that PNM captures the main characteristics of two-phase fluid flow inside porous media. Due to its efficiency, the PNM is extremely useful to determine relevant parameter spaces for certain structures. It can give first indications to determine which detailed simulations with more accurate and realistic models or methods can be conducted. As next steps, further investigation for more generic porous media applications will be considered to validate the new model for a broad variety of macro- and microporous media.

Acknowledgement: This work has been funded by European Union's Horizon 2020 research and innovation program within the research project DEFACTO under grant agreement N° 875247.

Keywords: pore network models, Lattice Boltzmann method, porous media.

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MS01 / 175

3D Visualization of hydrogen storage in sandstones at reservoir conditions

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Hydrogen energy is poised to play a pivotal role in the global efforts to achieve net-zero targets and the planned transition from traditional fossil fuels to clean energy sources. While there has been increasing interest in the use of green hydrogen, the massive amount needed for future demand would require new storage facilities. Underground storage of hydrogen, e.g., in saline aquifers and depleted gas reservoirs, can provide a viable solution for short-term to long-term storage to meet the fluctuations in energy demand; however, it poses unique challenges due to hydrogen's distinctive physical and chemical properties. It is imperative to understand the different interactions and displacement mechanisms that would occur at the pore-scale when hydrogen is injected, stored, and then produced from rocks at reservoir conditions. In this study, we use X-ray micro-tomography to investigate the fundamentals of pore-scale fluid displacement processes during cyclic injection of hydrogen in an initially brine saturated Bentheimer sandstone sample at high pressure and temperature conditions. These imaging experiments allow us to visualize the flow patterns and rock-fluid interactions at the pore-scale, providing an initial indication about the trapping mechanisms and storage efficiency. We will extend this research further by performing time-resolved synchrotron X-ray imaging experiments, which will provide additional insights into the dynamics of pore-scale processes during underground hydrogen storage.

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MS17 / 176

A directed network feature for thermal anisotropy of granular materials

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In shallow geothermal engineering, thermal anisotropy of the ground leads to different heat transfer performances of horizontal and vertical ground heat exchanges systems even within the same site. Microstructure determines the anisotropy nature of the effective thermal conductivity in granular materials. However, existing microstructural parameters such as porosity, average coordination

number can neither characterise the anisotropy of the granular materials nor the thermal anisotropy. In the present work, sphere packings with some inherent structural anisotropy were generated and they were represented by directed thermal networks in which each node corresponds to a particle and each directed edge indicates the local heat transfer path via a thermal resistance. Complex network theory was applied to the thermal networks to find the shortest preferential end-to-end heat transfer path for each paired nodes at the hot and cold ends of a sample. Based on the shortest heat transfer paths, a new sample-scale feature named “*directed network thermal resistance*” was introduced to account for particle connectivity, interparticle contact orientation and contact quality simultaneously. After calculating the effective thermal conductivity of lattice and randomly distributed sphere packings in different directions, it is found that *directed network thermal resistance* correlates with thermal anisotropy well.

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MS09 / 177

Can we trust computers to analyse pore-scale images?

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Micro-CT imaging and pore-scale modelling have developed rapidly over the last decade by bridging the disciplines of geology, reservoir engineering, image processing, and computational fluid dynamics. They have provided new pathways for understating complex transport phenomena in underground geological formations and other porous media. However, there are several steps in this framework that are time-consuming and of user bias. Machine learning and Convolutional Neural Networks (CNN) as a part of the broader field of Artificial Intelligence (AI) can be integrated into the framework of pore-scale modelling and imaging. The trade-off between sample size and image resolution as well as the expensive computational cost associated with numerical simulations of fluid flow in the pore spaces can be addressed by the use of CNNs. We will show how we can recreate porous media images at a super-resolution and use them for exploring porous media transport phenomena. We also demonstrate the reliability and accuracy of CNNs for the determination of rock properties on images of porous media. Challenges and opportunities for the development of machine learning approaches in porous media applications will be discussed.

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MS18 / 178

Transport and retention of nanoparticles in natural porous media- Effect of pore structure and geometry.

Authors: Raoul Djou Fopa¹; Carlo Bianco²; Nathaly Lopes Archilha³; Tannaz Pak¹

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The understanding of the transport of nanoparticles (NP's) in saturated porous media is key during nanoremediation technology. There is a gap in knowledge regarding the processes occurring at the pore scale for a successful nanoremediation technique to be applied at larger scales (Pak et al., 2020). NP (e.g., zero-valent iron) transport mechanism at the pore scale is studied in a non-destructive way using X-ray computed micro-tomography (X-ray micro-CT) (Pak et al., 2019).

In this study, the effect of grain composition and size (fine sand, coarse sand, carbonate, and a mixed sample of carbonate and sand) on the mobility and deposition of NP's is reported. The porous materials were filled in small columns that were initially saturated with water, the injection of NP suspension followed with a post flush stage to remove the mobile particles. Lastly, X-ray micro-CT imaging is performed. 3D micro-CT data of these four columns is used in this study. All tomographic data are at 4.52 μm resolution.

The images obtained consisted of three phases (grains, pores and NP's) which were qualitatively studied using the free and commercially available software ImageJ and Avizo respectively. The images were filtered to remove any noise present, segmented (to identify the phases present) using several algorithms such as simple threshold, Weka and watershed segmentation. Pore network modelling and labelling analysis for the visualization of the pores geometry and to extract some other useful information aimed at understanding the relationship between the topologic and geometric properties of the porous media (Pak et al., 2018).

The objective of this work is to understand the effect of NP's injection on the structural and geometric properties of the pores and to identify the NP's transport mechanism at the pore scale.

Given the success in the characterisation of these natural rocks using μCT , we foresee these data as a teaching and research resource (Pak et al., 2019). The outcome of this experiment shows that, the structure of the porous media remains unchanged while the geometry of the pore system changes after NP injection. Pore clogging is noticed with a left shift of the pore and throats channel length size distribution due to decreasing absolute permeability (Hosseini et al., 2013; Pak et al., 2020). The porosity reduces with an increase in the geometric tortuosity due to NP injection. The work brings out the relationship between the size of the porous media, NP deposition and its effect on the permeability reduction. The amount of nanoparticle deposition in sand increases with reduction in grain size. NP saturation in the pore space follows the trend; fine sand (11.47) > coarse sand (8.80) > mix sand (8.44) > carbonate (6.15). Also, it is seen that permeability reduction increases with reduction in

grain size; fine sand (24.21) > coarse sand (18.76) > mix sand (16.45) > carbonate (11.71). The accurate quantification of the evolving trends among geometric, hydraulic and mechanical rock properties is important as it contributes to a sustainable exploration and utilisation of the geological subsurface.

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Poster / 179

Performance evaluation on temporary plugging of magnetic responsive hydrogel in hydraulic fracturing of hydrocarbon reservoirs

Authors: Mingliang Luo¹; Xiaodong Si¹; Yige Huang¹

¹ *China University of Petroleum(East China)*

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Hydraulic fracturing is a key technology for the efficient development of unconventional reservoirs (such as shale and tight sand reservoirs). Formation pressure depletion and fracture closure due to the development of oil and gas reservoirs cause low production. Thus, it is necessary to implement stimulation measures, such as refracturing or layered fracturing. However, fracturing fluid leakage into the original formation fractures results in substantial damage and pollution to the formation and may reduce production. A temporary plugging fracturing technology is often used and gel is widely used as a temporary plugging agent (TPA) to block the original fractures in near-well areas and to reduce the damage of the working fluid to the original layer. However, gel is mainly cross-linked by polymer or vegetable gum, and its bearing strength, cross-linking time and gel-breaking performance are difficult to control accurately. The emergence of magnetorheological (MR) materials provides a new basis for improving the performance of temporary plugging gels. Magnetorheological gel (MRG) is a new type of MR material, which, as a smart fluid, responds to stimulation by an external magnetic field and quickly adjusts and adapts to the corresponding treatment. The unique magnetorheological characteristics of MRG, which can be transformed from a flowable to a solid

state under the influence of an external magnetic field, renders its application in temporary plugging fracturing potentially useful.

In this study, we designed a magnetic responsive hydrogel, also known as magnetorheological gel (MRG), based on a carbonyl iron particle@polyacrylamide (CIP@PAM) composite and a water-soluble PAM matrix to use as a temporary plugging agent (TPA) in the hydraulic fracturing of unconventional hydrocarbon reservoirs. The CIP@PAM composite was characterized by Fourier transform infrared spectrometry (FT-IR), scanning electron microscopy (SEM), laser particle size analysis (LPSA) and vibrating sample magnetometry (VSM). The results show that a thin and uniform PAM layer was successfully coated on the surface of the CIPs, which plays a key role in enhancing the antioxidant capacity of the CIPs. Meanwhile, the CIP@PAM composite possesses a high saturation magnetization (148.83 emu/g). MRG as a TPA has a high gel strength and magnetorheological effect under a magnetic field intensity of 1 T, providing a breakthrough pressure up to 38.13 MPa at room temperature and great potential in temporary plugging for hydraulic fracturing.

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Poster / 180

Improved micro-continuum approach for pore scale simulation of capillary dominated flow with lower spurious velocities

Authors: Zhiying Liu^{None}; XU QIANGHUI^{None}; YANG JUNYU^{None}; SHI LIN^{None}

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Multiphase reactive flow in porous media is fundamental in many areas of subsurface science and engineering, such as mineral dissolution by acidic injection and hydrate decomposition. Pore scale simulation is an effective method to deeply investigate the mechanism of reactive mass transfer in porous media. Soulain presented a micro-continuum approach to simulate reactive flow at pore scale in the presence of multiple fluid phases. The micro-continuum approach avoids mesh generation and dynamic update for complex geometry of porous media. However, large spurious velocities in simulation of capillary dominated flow can cause adversely affect the prediction of concentration distribution and reaction rate. In this paper, the accuracy of the surface tension force calculation is improved by modifying gradient and curvature near the wall, and implementing the local mesh refinement, the Sharp Surface Force (SSF) model and the Piecewise Linear Interface Calculation (PLIC) algorithm. The improved method is validated for various multiphase flow scenarios for Capillary numbers of 10^{-3} - 10^{-4} . In the test case of flow in a capillary channel, the spurious velocities at gas-liquid interface and near the solid wall are compared to demonstrate that the maximum spurious velocity is near solid wall, which is mainly affected by the accuracy of gradient and curvature near the wall. The porous media cases show that the spurious velocities of the improved method can reduce at least one magnitude. The impacts of maximum time step and mesh resolution are also verified.

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MS20 / 181

A porous media flow model for simulating flow of non-Newtonian bone cement inside a deformable vertebra in the context of vertebroplasty

Authors: Zubin Trivedi¹; Dominic Gehweiler²; Arndt Wagner¹; Boyko Gueorguiev-Rüegg³; Tim Ricken¹; Oliver Röhrle¹

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Vertebroplasty is a medical procedure in which a “bone cement” is injected into the porous interior of a damaged or fractured vertebra in order to restore its structural strength. While the procedure is fairly successful and provides near-instant relief, sometimes the bone cement might leak out of the vertebra resulting into complications like pulmonary embolism, paralysis, etc. To mitigate the risk of cement leakage, simulations could serve as a useful tool for practitioners to decide the best operating parameters for each patient. However, in order to simulate the procedure, there are many aspects that need to be modelled, e.g. the interior porous geometry, the non-Newtonian behaviour of the bone cement, the curing phenomenon, the displacement of the present bone marrow, etc.

In this work, we use the Theory of Porous Media as the modelling framework, since it is essentially a porous media flow process. Upon this framework, suitable constitutive models are used for the non-Newtonian rheology of the bone cement and the bone marrow, e.g. the Carreau-Yesuda model, to which additionally upscaling is applied using Cannella model and the average viscosity model. The solid deformation problem is solved using the Finite Element approach, while the discretization for the flow problem is carried out using the Box-discretization technique, essentially resulting in a mixed Finite Element - Finite Volume discretization. Furthermore, experiments are carried out in order to characterize the non-Newtonian and curing behaviour of the bone cement. A benchmark injection experiment using aluminium foam is employed in order to validate the simulation results using experimental data. This is then used for trial and comparison of various constitutive models in order to choose the most suitable for this application. This whole modelling setup can be further upgraded to include thermal interactions for studying the temperature, or even to include fractures, possibilities for which will be presented in the outlook.

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MS04 / 182

Multidirectional gel swelling and drying: a linear-elastic-nonlinear-swelling theory for hydrogels

Authors: Joseph Webber¹; Grae Worster¹; Merlin Etzold²

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Super-absorbent polymers can form gels with polymer fractions less than 1% by volume when placed in water, with the water molecules being adsorbed by the hydrophilic polymer to form an elastic material known as a hydrogel. This water is not fixed in place: the polymer scaffold creates a porous structure through which it can flow to drive swelling and shrinking. Existing studies of the behaviour of these two-phase materials extend ideas of poro-elasticity, coupling the interstitial flow with a constitutive relation to describe the deformation stresses on the gel, or use a microscopic chemical understanding of water-polymer interactions to derive and then minimise an energy density, finding both steady and transient swelling states. In our work, we have derived both a constitutive relation and a dynamic model, expressed as a system of differential equations, which allow for nonlinearity in the swelling strains but linearise the deviatoric elastic response of the gel, in effect treating hydrogels as linear-elastic, instantaneously incompressible, materials. For one-dimensional problems, such as a gel sphere swelling in water with properties varying only in the radial direction, the swelling state can be described fully by the polymer fraction, which also determines the size of the sphere given the constraint of polymer conservation. However, in higher-dimensional problems, the polymer fraction alone cannot describe the gel, because there can be differential swelling in different directions. In such cases, we derive an equation for the displacement field for the gel, namely a modified biharmonic equation forced by the polymer-fraction field, a direct analogue of the biharmonic equation for the displacement field used in linear elasto-statics. Relying solely on the founding assumption of small deviatoric strains, we can determine the shape and composition of a gel as it swells or dries. As an illustration of the utility of this approach, we consider the problem of a cylinder with its base immersed in water while evaporating to the surrounding air. In this situation, there is both radial shrinkage and shrinkage along the axis of the cylinder, with the top of the cylinder drying to a greater extent than the base, as water is drawn up and evaporated away. Experiments have shown that the cylinder becomes concave on its top surface and convex at its base, and both of these phenomena can be described using this displacement formulation, providing further evidence of its ability to solve these more complicated problems. Furthermore, our modelling assumptions result in a description of the gel which agrees with a Lagrangian description of the drying of a cylinder as a series of stacked elastic plates which curve upwards to accommodate greater

shrinkage at the top of the cylinder, providing a physically intuitive understanding of the curvature that forms.

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Poster / 184

Optimization of operational parameters for geological hydrogen storage in a saline aquifer - Sothern North Sea Case Study

Author: Saeed Harati¹

Co-authors: Tannaz Pak¹; Sina Rezaei-Gomari¹; Firdovsi Gasanzade²

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Hydrogen has a critical role in meeting the UK's commitment to achieve net zero emissions by 2050. The transition towards net zero has been estimated to require 250-460TWh of hydrogen, making up 20-35% of the UK's final energy consumption in 2050. To facilitate hydrogen supply at the required scale, subsurface hydrogen storage in porous geological formations is essential. In the context of geological gas storage, a number of favourable structures (i.e., disused hydrocarbon reservoirs and saline aquifers) have been identified and studied in the Southern North Sea basin so far, particularly, as suitable candidates for storage of CO₂ or natural gas. These structures are strategically located in close proximity to the UK's east coast main industrial clusters, Humberside and Teesside, where the required infrastructure for hydrogen production and transportation within the energy grid can be achieved.

In this study, a cyclic hydrogen storage scenario is developed in a salt induced dome structure within the Bunter Sandstone Formation of the Bacton Group located in the UK sector of the Southern North Sea. The geological model consists of 603,394 active cells which covers an area of 25 km². The formation reservoir quality is quite good with high net to gross ratio (>80%), average porosity of 22%, and average permeability of approximately 200 mD, top sealed with multiple thick and laterally extensive impermeable formations. The site for this study is selected based on future considerations such as strategic location, potential storage capacity, and storage integrity. For hydrogen storage studies, the multiphase-multicomponent reservoir simulator Eclipse (Schlumberger) is used to evaluate storage capacity and deliverability, hydrogen injection/production rates, and pressure response at each cycle. A hypothetical scenario for hydrogen storage demand based on actual seasonal energy shortages for domestic heating in the Midlands (central region of England) is used to put the outcomes of the simulations into a real-world perspective. This enables us to select optimised operation

parameters for subsurface hydrogen storage in order to meet the possible future hydrogen demands within this region.

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Poster / 186

Micro experimental study on residual oil of marine carbonate rocks during water flooding based on CT scanning

Author: Wenlong Jing^{None}

Co-authors: Aifen Li¹; Lei Zhang²; Hai Sun¹; Jun Yao¹

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At present, carbonate reservoirs mainly rely on primary and secondary oil recovery. However, the complex pore structure leads to large production decline in the early stage of depletion development, and the distribution of oil and water in the reservoir is very uneven in the process of water injection. The key to solve these series of problems is to clarify the micro occurrence characteristics and laws of residual oil in carbonate reservoir. In this study, the natural cores of marine carbonate reservoir were used to carry out water flooding experiment based on CT scanning. We obtained the CT scanning results of oil saturated cores and cores after water flooding 3, 5, 10 and 20 PV (pore volumes), and established digital cores. According to the difference of gray value, the oil and water in pores were extracted respectively. The pore network models were then established, and the relevant parameters of pore structure, residual oil shape factor and Euler number were calculated. The distribution of remaining oil in cores at different displacement stages was described qualitatively and quantitatively. It is found that the oil saturation decreases with the water flooding. After injection of 20PV of water, all oil with a radius greater than 20 μm is basically displaced, and there is only a small amount of residual oil with a radius of 3 μm ~ 10 μm . In the process of water flooding, the main distribution type of remaining oil is isolated droplet. The remaining oil of other types is less, and the proportion remains basically unchanged with the water flooding.

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MS06-B / 187

Study on Flow Mechanism and oil Displacement Mechanism of Microcapsule Polymer in Porous Media

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Polymer microcapsules refer to microsphere particles with a core-shell structure using polymer as the core. Microcapsule Polymer is a new type of oil-displacing reagent that is suitable for deep profile control which has broad application prospects in enhancing oil recovery. However, microcapsule polymer has obvious time-varying characteristics and its flow mechanism and oil displacement mechanism also need to be further clarified. Therefore, we use microfluidic technology to study its flow mechanism and oil displacement mechanism.

We built a microfluidic experiment platform, which is composed of syringe pumps, micro-injectors, high-speed cameras, microscopes, pressure sensors, Polydimethylsiloxane (PDMS) chips and micro-etched glass chips. We firstly use a syringe pump to inject the aged microcapsule polymer into a single constricted channel PDMS chip. Then, we use a microscope and a high-speed camera to observe and collect images of the microcapsules flowing and use a sophisticated pressure sensor to record pressure data. Subsequently, we choose a complex network of micro-etched glass chips for oil-displacement experiments.

In this study, the micro-resistance factor is defined as the ratio of the inlet pressure for flow of microcapsules to that of only water. The experimental results show that with the increase of aging time, the microcapsules gradually become larger which can expand up to 20 times and the viscosity of the reagent will gradually increase to 20mPa·s. Microcapsules can undergo surface adhesion, throat blockage and elastic deformation inside the single-channel chip. The resistance factor remains around 1 when microcapsules flowing in the channel. While if the throat is blocked, the resistance factor will rise to a larger value. There are two patterns of blockage, single microcapsule blockage and multiple microcapsules blockage. The former pattern causes the resistance factor to rise sharply, while the latter blockage pattern makes the resistance factor rise slowly. But the blockage pattern of multiple microcapsules tends to produce a higher resistance factor. In the observed image, the microcapsules passing through the throat are all elastically deformed. The results of micro-etched glass experiments show that the microcapsules converge into clusters in the pores, which will preferentially block large channels, change the direction of fluid flow, and further displace oil that is not affected during water flooding.

This study firstly explains the relationship between the size of the microcapsules and the aging time and the flow mechanism of the microcapsules in porous media, then gives a further detailed description of the process of how to drive oil. This study provides important value for the promotion and application of new microcapsule polymer.

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MS08 / 188

Evidence of anomalous transport controls on long-term variability in stream water chemistry

Authors: Marco Dentz¹; Erwin Zehe²; James Kirchner³; Brian Berkowitz⁴

¹ IDAEA-CSIC

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⁴ Weizmann Institute of Science

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We investigate the occurrence of anomalous (non-Fickian) transport in three neighboring hydrological catchments, at kilometer-length spatial scales and over a 36-year period. Using spectral analysis, we show that the fluctuation scaling of long-term time series measurements of a natural passive tracer (chloride), for rainfall and runoff, show evidence of a broad, power-law distribution of residence times in the catchments. This behavior can be described by a continuous time random walk (CTRW) formulation, which is based on an α -stable (non-normal) distribution of transition times. Our CTRW analysis reveals two distinct scaling behaviors of the chloride concentration at the catchment outlet: the travel time distributions scale as $\sim t^{-1+\beta}$ over relatively short times, and as $\sim t^{-1-\beta}$ over relatively long times, where $0 < \beta < 1$. Notably, the short time scaling coincides with a gamma distribution, which has been identified previously in the literature as a statistical description of travel time distributions. Overall, anomalous transport is seen as a clear “fingerprint” of the wide range of temporal contributions characterizing tracer retention and release through the domain, despite the long time scales and transport distances over which homogenization might be expected to occur.

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MS03 / 189

on the deformation of porous medium by pressurized flow**Authors:** Arnold Bachrach¹; Yaniv Edery¹¹ *Technion***Corresponding Authors:** yanivedery@technion.ac.il, arnoldbachrach@gmail.com

Fluid injections into the underground occurs in many industrial processes as hydraulic fracturing for oil and gas recovery, wastewater disposal, enhanced geothermal energy systems (EGS) and Carbon storage technologies. Often, the increase in pore pressure due to the fluid injections lead to the activation of a preexisting underground shear fractures (named faults), forming unanticipated local earthquakes.

While studying the mechanism of injection induced earthquakes, the rock deformation due to the fluid injection is unknown. Understanding the rock deformation coupling with the pressure change, requires detailed experiments linking the global and local deformation with the pressure change during flow, which ultimately influence the earthquake triggering.

In this study we present a novel experiment on transparent plastic rocks, that offers a detailed analysis of the artificial rocks' deformation due to pressurized flow. In these experiments, we inject a fluid through the artificial rocks and analyze the internal deformation by capturing the displacement of fluorescent microspheres embedded in the artificial rock structure. Our analysis allows a straightforward correlation between the deformation of rocks, the pressure change and the fluid flow. The study points a similarity between the material deformation due to internal pressure induced by the fluid injection and material deformation due to an external pulling.

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Poster / 190

Pore-Scale Modelling of Hydrogen Transport in Porous Media

Authors: Shaobin Cai¹; Yongfei Yang¹; Quan Xie²

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Hydrogen energy has enormous potential for playing an important role as a clean fuel in energy transition. We have studied hydrogen transport in a sandstone porous media pre-saturated with brine at pore scale. Volume of fluid method was used to study the transport of hydrogen in sandstone porous media under different wetting conditions. The main purpose of this study is to determine the effect of sandstone wettability on hydrogen transport process. Based on the hydrogen-brine-quartz contact angle data measured by Stefan et al. under different conditions, the fluids properties of this study were determined and the contact angle hysteresis were considered. Then, based on these parameters, we simulated the hydrogen storage and extraction processes during underground hydrogen storage, and the distribution, transport behavior and storage/extraction efficiency of hydrogen in porous media under different wetting conditions were investigated comprehensively. The results have showed that sandstone ensures safe storage of hydrogen in underground porous media. However, under the hydrophilic condition and extremely low capillary number ($CA < 90^\circ$, $Ca < 10^{-5}$), hydrogen clusters stored in sandstone with saturated brine cannot be mobilized efficiently, and extraction of hydrogen by injecting brine will result in significant high residual hydrogen saturation. The critical capillary number for mobilizing trapping hydrogen should be kept above the 10^{-5} - 10^{-4} to ensure the successful extraction of hydrogen. The extraction efficiency of hydrogen can be improved by injecting some gas with stronger wettability to the wall, such as nitrogen. Therefore, study suggested that hydrogen storage in sandstone porous media can ensure the safe storage of hydrogen. However, how to effectively reduce the residual hydrogen saturation during hydrogen extraction is the key to the effective implementation of this measure.

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MS06-B / 191

Effect of nanoparticles on the water-soluble polymers flow in porous media

Authors: Mohsen Mirzaie Yegane¹; Fatemeh Hashemi²; Frank Vercauteren³; Nicole Meulendijks³; Ridha Gharbi⁴; Pouyan Boukany²; Pacelli Zitha²

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The addition of a small amount of water-soluble polymers (e.g. polyacrylamides and polyethylene glycol) to water can significantly affect the rheological response of aqueous solutions. These aqueous polymeric solutions have frequently been used to control the flow response of working solutions in several porous media applications, including chemical enhanced oil recovery. However, polymer chains are susceptible to degradation in high ionic strength (I) mediums which hinder their successful implementation and performance. Hybrid mixtures of hydrophobically modified polyacrylamide (HMPAM) with hydrophobic silica nanoparticles (NPs) appeared as an alternative approach to achieve enhanced stability and high viscosity in mediums having extremely high ionic strength ($I > 3800$ mM).

The utilized silica nanoparticles (with an average size of 7 nm) were modified by grafting an organic ligand (gamma-glycidoxypropyltrimethoxysilane) onto its surface to ensure the colloidal stability at high ionic strength. The rheological response of the hybrids at various concentrations of HMPAM and NPs was studied to investigate the synergic effects. Core-flood experiments were performed by injection of either HMPAM solution, NPs suspension, or an HMPAM–NPs hybrid at superficial velocities of 1 and 10 ft/day to assess their retention and injectivity.

The colloidal stability of NPs was successfully explained by an extended DLVO theory. Hybridization of HMPAM with NPs resulted in a higher viscosity at high ionic strength and elevated temperature ($T = 70$ degree Celsius). Viscosity improvement was more noticeable when the concentration of HMPAM was in the semi-dilute regime and the concentration of NPs was higher than a critical threshold where the viscosity increased roughly by a factor of 1.5. The underlying mechanisms are discussed by rheological measurements. The rheological data suggest the role of NPs in inter-chain associations of HMPAM chains through hydrophobic–hydrophobic interactions leading to increase hydrodynamic radius and therefore viscosity of the hybrids.

It was observed that the flow of HMPAM and NPs in the same solution in porous media has the following benefits: (a) the HMPAM–NPs hybrid has a higher flow resistance as compared to the injection of HMPAM alone (b) the HMPAM–NPs hybrid prevents filtration of the NPs in the inlet while the injection of NPs alone results in significant filtration in the inlet and (c) the co-injection of HMPAM and NPs also decreases the retention of both HMPAM and NPs as compared to when they are injected individually.

This study provides insights on the interaction of polymer molecules and nanoparticles in hybrid systems for enhancing stability and improving the viscosity opening a pathway for developing other polymer-based systems at harsh conditions for porous media applications.

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MS01 / 192

Trapping dynamics during geological carbon storage: Synchrotron time-lapse imaging of pore-scale capillary trapping events over the centimetre-scale in a heterogenous sandstone.

Author: Catrin Harris¹

Co-authors: Ann Muggeridge²; Sam Krevor; Samuel Jackson³

¹ *Student*

² *Imperial College London*

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A major challenge for geological carbon storage is increasing confidence in storage security. The ability to model and predict trapping in complex geological systems is essential to minimise risks and ensure the permanence of geological carbon storage. Capillary trapping is a key mechanism shown to improve storage security by immobilising a significant proportion of the CO₂ plume [1]. Current models predicting field-scale CO₂ movement and trapping at several sites around the world do not fully capture the impact of heterogeneity on upscaled flow physics and trapping dynamics [2]. The aim of this work is to understand the effect of natural geological heterogeneities on the transient dynamics of the CO₂ plume, and how CO₂ is trapped dynamically in heterogenous sandstone aquifers.

State of the art synchrotron experiments at the Australian synchrotron (ANSTO) have been carried out, achieving combined spatial and temporal resolution not possible with traditional lab-based techniques [3]. Pore-scale trapping mechanisms were captured with a field of view over the continuum core scale (5cm), allowing us to investigate how larger scale capillary heterogeneity trapping processes are impacted by pore-scale events. Experimental observations resolving trapping over many pores, representative of the large-scale process, are crucial for model validation, development and ultimately storage predictions [2].

The time resolution achieved at ANSTO allowed us to capture unsteady state displacements, the prevailing conditions at most storage sites [2,4]. Unlike typical lab-based experiments which only capture steady state due to resolution constraints [3,5,6]. The core was imaged in 7 minutes, at a resolution of 20 microns, capturing pore-scale displacements dynamically. We observed the frontal advance and subsequent imbibition proceeding until the residual saturation was reached, gaining an understanding into pore-scale displacements and trapping dynamics. Both drainage and imbibition displacements were captured in a heterogenous Bentheimer sandstone core, representative of typical saline aquifer storage sites [7]. To date, there have been no direct observations of transient trapping in sandstones with realistic layered rock heterogeneities, features ubiquitous across proposed and operational storage sites worldwide. To evaluate the rate dependency of trapping, experiments over 2 different rates are compared to explore potential trapping within a range of carbon sequestration projects.

Geological heterogeneities impact the timescale and distribution of capillary trapping [6]. We observe the transient interaction of the fluids with an oblique layered heterogeneity –witnessing in real time how the non-wetting phase builds up behind the barrier, and eventually breaks through once the entry pressure is overcome. We see how heterogeneity impacts upstream pore-filling events, and subsequent imbibition, allowing us to quantify the path to residual trapping, and therefore, crucially, dynamic models. Natural heterogenous capillary pressure barriers trap the non-wetting phase at saturations greater than expected from pore-scale residual trapping processes alone, potentially providing greater CO₂ storage capacity. Furthermore, injection rate impacts capillary trapping with lower rates of brine imbibition resulting in a greater proportion of capillary heterogeneity trapping, supporting numerical simulations [7]. The results from this synchrotron campaign demonstrate the potential impact of heterogeneity on the dynamics of capillary trapping within CO₂ storage sites.

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References:

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Poster / 193

Experimental Investigation of Relative Permeability Curves in Oil/water Transition Zone of Tight Sandstone Reservoir

Author: Min Ma¹

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The oil/water transition zone contains a significant portion of original oil in place (OIP) especially for those tight sandstone formations with rather small pore diameter and high capillary pressure. As the buoyancy balanced with the capillary force, the water saturation changes from 1.0 at the free water level to the irreducible water saturation at the top of the transition zone. Accordingly, both oil and water are mobile in the transition zone. A better understanding of the mechanism of how oil and water flow in the transition zone depends on the relative permeability data. However, traditional single relative permeability curve cannot provide enough information. Considering the characteristic of the transition zone, the impact of initial water saturation on the oil/water relative permeability curves need to be solved.

To solve the question above, a laboratory study was conducted to measure a set of oil/water relative permeability curves with different starting water saturation on reservoir core plugs from Changqing oilfield in China at the underground condition. The experiments take brine as the aqueous phase and silicone oil as the oleic phase. For the time consuming of the steady method, the unsteady method is cindered. The core samples were first saturated at residual water saturation to measure the bounding oil/water relative permeability curve. Then, the core samples were saturated at different initial water saturation to simulate different initial conditions in the transition zone and measured different scanning oil/water permeability curves. For the data processing, the JBN method is applied with a modification considering the capillary force. Finally, the impact of initial water saturation on the oil/water relative permeabilities were analyzed.

The experimental results revealed that the oil/water relative permeability curves with different initial water saturation vary differently. For the water is the wetting phase, the residual oil saturation reduces as the initial water saturation increases. The reason is that as the water saturation increasing, the wetting phase tends to occupy smaller throats and pore walls in the formation, leaving larger pores for the oil phase, which makes the oil phase displaced easily. The permeability curves gradually move towards right, and the movable water area narrows with increasing starting water saturation. Both the bounding relative permeability curves and scanning permeability curves have nearly the same shape.

The relative permeability data provide essential information for accurately simulating the production performance of the transition zone. However, the conventional reservoir simulation does not consider the initial water saturation factor into account and resulted deviation in simulation and actual field performance in oil/water transition zone. In conclusion, a set of oil/water relative permeability curves has essential impact on the field performance predictions for reservoir transition zone.

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Poster / 195

Novel Fabrication of Microfluidic Devices with Mixed Wettability

Author: Abdullah AlOmier¹

Co-authors: Antonia Sugar²; Dongkyu Cha³; Subhash C. Ayirala³; Hussein Hoteit¹

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1. Objectives/Scope: Microfluidics is an emerging technology that has gained attention by the industry for its capabilities to investigate and visualize fundamental recovery mechanisms at the pore scale in a microdevice, mimicking, to some extent, the actual rock pore-network. While current technologies are capable of building micromodels that are either water-wet or oil-wet, a technique to achieve a representative mixed-wet property is still unreached. In this work, we introduce a novel method to build microfluidic systems with selective wettability, oil-wet and water-wet, mimicking an actual mixed-wet rock.

2. **Methods, Procedures, Process:** The design of the microfluidic devices replicates the actual pore-network of an oil-bearing reservoir rock. The flow pattern was obtained through the digitalization of a thin section image from a core. A silicon substrate served as a foundation for the photolithography process optimization and to forge the workflow for wettability alteration. Deep reactive ion etching technique was used for silicon patterning and building the microfluidics device substrate imitating a pore-network structure with pore-throats ranging from 1 μm to 60 μm . The resulted micromodel substrate serves as a two-dimensional proxy, where we remove the inherent complexity of the three-dimensional porous network in rocks, which facilitates narrowing into the mechanisms that occur at pore-scale.
3. **Results, Observation, Conclusions:** We developed a fabrication workflow for silicon-based microfluidic devices with selective wettability. The selection of silicon-based microfluidic devices lies in the favorable compatibility of silicon for oil and gas applications, including high temperature and pressure and the affinity for crude oils and organic solvents usage. A selective wettability control mask and calcite coating using Atomic Layer Deposition technique (ALD) were used for surface wetting properties alteration. The calcite-coated regions of the microdevice substrate shift the localized wetting state of the silicon towards hydrophobic, while in the mask-protected areas, the wettability remains unchanged. Surface measurements, including X-Ray Diffraction (XRD) and Scanning Electron Microscopy (FIB-SEM) Imaging, were performed to evaluate the calcite film composition and morphology. The fabrication workflow resulted in a microfluidics device, also referred to as a "Reservoir-on-a-Chip", with controlled mixed-wet properties. Furthermore, we performed flow experiments to investigate fluid injectivity and connectivity of the microdevice. Variable temperatures between 23oC and 90oC were used for the flow experiments to ensure the microchip can withstand reservoir-like conditions.
4. **Novel/Additive Information:** This work presents a novel technique for fabricating microfluidic devices with mixed wettability for the first time. We used a control mask and calcite coating with Atomic Layer Deposition to alter the hydrophilic surface of the silicon device and generate hydrophobic surface in selected regions. Tuning the wetting state of the microdevices to mimic the mixed-wet characteristics of reservoir rocks, such as carbonates and shales, can enhance the understanding of fundamental fluid behaviors and interaction between the water-oil-rock phases.

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MS09 / 197

Extraction of three-dimensional pore network and corner network with pores of high aspect ratios

Authors: Ninghua Zhan^{None}; Rui Wu¹; Evangelos Tsotsas^{None}; Abdolreza Kharaghani²

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² *Otto von Guericke University*

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The Euclidean distance map which is widely employed in thinning, transformation, expanding and locating of extraction algorithms cannot describe the porous media with pores of high aspect ratios, since the hierarchy of the void voxels cannot be distinguished clearly by the Euclidean distance map. To address this issue, we propose a pore network extraction method based on the concept of the omnidirectional Euclidean distance, which is a set of Euclidean distances from a void voxel to all the accessible solid boundary voxels. Besides, the corner structure of porous media also plays an important role in the simulation of mass transfer flow. The existing models lack the extraction of corner network of real porous media. In this model, we propose an appropriate method to extract the corner network of porous media and couple it with the pore network of the main space. The proposed pore network extraction method is validated by comparing the pore network modeling results, in terms of the single-phase flow and the quasi-static two-phase drainage, against the direct numerical simulation results and the experimental data. The proposed pore network extraction method not only preserves the topological and morphological properties of the void spaces in porous media but also is robust and insensitive to the image noise.

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MS14 / 198

Potential geological sequestration of CO₂ in Kazakhstan

Authors: Aibar Kamashev¹; Yerlan Amanbek²

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CO₂ storage in subsurface is one of ways to mitigate the CO₂ emissions in many places including Kazakhstan. To achieve the goals to achieve the 25% emission reduction strategy by 2030 according to Paris agreement in 2016, Kazakhstan may require additional actions to be performed. CO₂ sequestration is one of the possible solutions in the reduction of CO₂ emission.

In this work, we explore the possibility of CO₂ storage in the region of the Precaspian basin using the compositional reservoir simulation flow model. We propose the potential place of the CO₂ storage and provide the amount of stored CO₂ based on the reservoir simulation model of Precaspian basin. We also present CO₂ plume migration in the post-injection period.

Moreover, we study the effect of parameters that can be essential in the modeling of CO₂ storage

evaluation in a potential subsurface of Kazakhstan.

We conducted uncertainty and sensitivity analysis by incorporating machine learning algorithms and reservoir simulation tool by varying model parameters and finally received 3 probability cases P10, P50, and P90 for the amount of trapped CO₂.

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MS01 / 199

Impact of compression on the properties of the fuel cell diffusion layer

Authors: Asma SHARIF^{None}; Manuel MARCOUX¹; Marc Prat^{None}

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A fuel cell (FC) directly converts chemical energy from the oxidation-reduction reaction during which a transfer of electrons takes place between two chemical species into electrical energy. The powering off FC is supplied by continuous injection of hydrogen at the anode, and oxygen at the cathode. Continuous electrical energy is then available at the battery terminals. We will only focus on Proton Exchange Membrane Fuel Cells (PEMFC). FCs are expensive to remove and have a too low lifespan. Thus, reducing their cost and increasing their lifespan has become a challenge for many manufacturers. It was shown that the battery life depends on the degradation of the gas diffusion layer (GDL). In order to have a better understanding of the aging of GDL we simulated it mechanically using a compression bench to study its impact on the diffusion of water vapor through the GDL as well as the impact on its internal structure with the pore size distribution complementing with a visualization of GDL before and after aging with a scanning electron microscope (SEM).

We use a mechanical compression bench to simulate the mechanical aging of GDLs. The bench allows us to apply cyclic compression over several days to our GDLs in order to compare the properties of our GDLs before and after aging. GDL, due to its high porosity, is the element of the battery that is the most sensitive to mechanical stresses which will impact its performance. Studies have shown that GDL have an atypical mechanical behavior as the relationship between stress and strain is not linear.

The SEM serves us as the first visual comparison tool of our GDLs before and after aging. It allows us to confirm that the GDLs are indeed impacted by the compression cycles undergone as can be seen in image 1.

A dynamic vapor sorption device (DVS) which allows the measurement of sorption isotherms, is used to characterize gas transfer in the GDL. The objective of the measurements with the DVS is to allow the determination of the coefficient of diffusion of water vapor through the GDL. We carried out these tests on new GDLs and old GDLs in order to determine if the mechanical degradation of the GDL had an impact on the diffusion through the GDL. For our tests we used a Payne cell to determine the diffusion coefficient of a membrane through 1D diffusion. The diffusion coefficient is then determined using the slope of the evolution of the mass versus time at the beginning of the process.

There is a decrease in the diffusion coefficient following the aging by mechanical compression of the GDL.

The charge / discharge cycles undergone by the FC were simulated using a mechanical compression bench which allowed us to demonstrate that the GDL is indeed impacted by the compressions initially thanks to the observation with the SEM and then thanks to the determination of the diffusion coefficient using the DVS which also varies at the end of a week of compression on our GDL.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 200

Film-to-pore filling transition during water adsorption in nanoporous media

Author: Abdullah Cihan¹

Co-authors: Tetsu Tokunaga¹; Jens Birkholzer¹

¹ Lawrence Berkeley National Laboratory

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Multiphase fluid behavior in nanoporous materials is of interest for various science and engineering applications, including geoscience applications, chemical and material engineering, and biological sciences. In the context of geoscience applications, nanoporous rocks have considerable importance as low-permeability seals for geologic carbon sequestration or nuclear waste disposal and as source rocks for hydrocarbon fluids. Improved knowledge of the fundamental interactions of fluids with nanoporous rocks would have significant energy, water and environmental benefits. When the pore sizes approach nanoscales, the impact of the molecular interaction forces between fluids and solids becomes increasingly important. These forces can alter macroscopic fluid phase behavior and control transport. In this work, we have conducted theoretical and computational investigations to understand the processes controlling adsorption, condensation and imbibition in nanoporous media. Our theoretical model, based on the square-gradient classical density functional theory, explicitly includes the relevant interaction forces among fluids and solids in nanoporous media. We will present applications of the model at pore-scale and macroscopic-scale to predict the impacts of water-pore wall attractive forces on multiphase water behavior and transport in nanoporous media.

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MS07 / 201

Numerical modelling the hydromechanical behavior of undrained triaxial tests on saturated concrete

Author: Jinzhou Bai¹

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¹ Univ. Lille, CNRS, UMR 9013-LaMcube-Laboratoire de Mécanique, Multiphysique, Multi-échelle

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Concrete structures constitute a large portion of civil engineering constructions, such as building, hydroelectric dams and bridges, etc. Due to the relatively small permeability of concrete, the cores of these structures could remain quasi-saturated during most of their lifetime even though their facings dry very quickly. A heterogenetic distribution of free water content is then observed. Numerous research exhibit mechanical behaviour of concrete depends strongly on the free water content. During the lifetime of these structures, they may be subjected to some accidental or intentional extreme loadings, such as ballistic impact, earthquake, vehicle shocking or explosion. As a result, concrete

is subjected to very high triaxial compression. Moreover, the duration of these extreme loadings is quite short, the interstitial water in concrete cannot escape quickly due to the low permeability of concrete. In order to evaluate the vulnerability of concrete infrastructure subjected to near-field detonations or impacts, it is necessary to understand the undrained triaxial behaviour of concrete with the presence of free water.

By using the poromechanical approach, an elastoplastic model is adopted to describe mechanical behaviour of concrete. The model's parameters are identified by using one hydrostatic compression test and one triaxial compression test. Finally, a series of triaxial compression tests under a wide range of confining pressure (from 0 to 650 MPa) are simulated. The comparison of numerical results exhibit that an important increase of pore pressure and volumetric stiffness is observed when the confining pressure increases. The numerical predictions and discussions can help engineers to enhance their understandings on the influence of interstitial pore pressure on structural vulnerability of concrete structures subjected to near-field detonations or impacts.

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MS06-B / 202

Assessing uncertainties and identifiability of foam displacement models employing different objective functions for parameter estimation

Author: Bernardo Rocha¹

Co-authors: Andres Valdez²; Grigori Chapiro¹; RODRIGO Weber dos SANTOS³

¹ *Universidade Federal de Juiz de Fora*

² *PhD candidate in computational modeling*

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Foam injection in porous media is often used to control the gas fingering in multi-phase flow. Mathematical models of foam dynamics involve non-newtonian formulations. To numerically simulate these complex phenomena, experimental data is gathered and used to estimate the parameter values of models via optimization techniques. The present work improves this procedure by introducing a new objective function based on the mobility reduction factor and does not require further experimental observations other than those usually obtained in core-flooding experiments. We show that the new objective function generates better calibrated models with high fidelity, low uncertainties and alleviates parameter non-identifiability issues.

Acknowledgements: The current work was conducted in association with the R&D project ANP n° 20715-9, “Modelagem matemática e computacional de injeção de espuma usada em recuperação avançada de petróleo” (UFJF/Shell Brazil/ANP). Shell Brazil funds it in accordance with ANP’s R&D regulations under the Research, Development, and Innovation Investment Commitment. This project is carried out in partnership with Petrobras.

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Poster / 204

Experiment and model of multi-scale dynamic diffusivity and permeability for gas(CH₄/He) flow in micro-nano pores in series connection of coal

Author: zhiqiang Li¹

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Abstract: Coal is a porous medium that contains multi-scale pores with a pore aperture from millimeter level to nanometer level. The pore aperture differential can reach one million orders of magnitude, which causes the multi-scale characteristics in space and time for coal permeability and significantly influences gas drainage. However, the current experiment and theory of steady-state permeability cannot reflect the multi-scale characteristics. A cylindrical coal sample with a height of 100 mm and diameter of 50 mm is used to conduct the unsteady diffusion-seepage experiment with and without stress loading using methane and helium. Meantime, the steady method is adopted to conduct the experiment with the same stress loading for comparison. The experimental results show that, the apparent diffusion coefficient of a cylindrical coal sample attenuates with time. This apparent diffusion coefficient shows two different multi-scale characteristics in time, one is the smooth dynamic attenuation and the other is the dynamic attenuation in a two-stage step. A dynamic model for the apparent diffusion coefficient is proposed, and it can accurately describe the complete unsteady flow process of gas in a cylindrical coal sample. The geometrical and mathematical models of the multi-scale pores in series are proposed. Then, the multi-scale structure of pore in series is validated by the mercury injection experiment. After that, the multi-scale permeability model is mathematically proved. Based on Knudsen number, the continuous flow, slip flow, transition flow and molecule free flow are identified and introduced with the multi-scale pore aperture to build a multi-scale permeability model that reflects the effect of the effective stress and gas flow regime. The mechanism of the multi-scale seepage is that the pore aperture and the number of pores in series connection determine multi-scale permeability. The multi-scale effect is far larger than the effect

of the effective stress. The gas outflow firstly starts from the outside fractures, and then the inside small pores and finally the nano pores. With time goes on, the gradual increase in the number of pores in series connection leads to the gradual reduce in the equivalent pore aperture, which causes the equivalent pore aperture to get close to the minimum pore aperture. Therefore, the equivalent permeability quickly decreases with time, which is a reflection of the multi-scale pore space in coal. In coal, gas flows through the multi-scale pores with different flow regimes, and the coal permeability decreases by a million orders of magnitude from millidarcy level to nanodarcy level. The new experimental observation and modelling of the multi-scale permeability are different from the previous experiments and theory of seepage and diffusion, which provides an experimental solution for the research of the multi-scale seepage. The diffusion coefficient and permeability are apparently unified, and the distinguishment in micro-level and combination in macro-level of the multi-scale permeability are realized. The research results are significant for the dynamic measurement and theory description of the ultra-low permeability of coal, the explanation of the fast reduction in coalbed methane production and the assessment on gas drainage.

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MS15 / 205

Image-based physics-constraint workflow for multi-phase flow simulation in heterogeneous media

Authors: Jingyan Zhang¹; Bicheng Yan²; Yuhe Wang³

¹ *Texas A&M University College Station*

² *King Abdullah University of Science and Technology*

³ *China University of Petroleum (Huadong)*

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The prediction of multi-phase flow in heterogeneous porous media traditionally relies on physics-based numerical simulation with high computational costs. Due to the intrinsic heterogeneity of porous media and the non-linearity of the governing partial differential equations (PDEs), high fidelity simulation models can lead to solving expensive large-scale system of equations, which can be unmanageable given the computational infrastructure at one's disposal. Therefore, developing techniques to honor the trade-offs between efficiency and accuracy has always attracted attention from researchers. Apart from traditional numerical techniques, deep learning has come into sight in recent years and there have been a lot of studies on the ability of neural networks in solving nonlinear differential equations and model reductions. Moreover, compared to traditional fully connected neural networks, image-based neural networks such as convolutional neural networks (CNN) usually

have sparser connectivity, which benefits training efficiency, especially under circumstances with high dimensional data. This sheds lights on the possibility of maintaining fidelity in fluid dynamics with lower computational costs. The objective of this work is to investigate efficient image-based deep learning techniques for approximating the dynamics of multi-phase flow.

By breaking down the coupled governing nonlinear PDEs into pressure and saturation equations, we describe a hybrid workflow in predicting the evolution of pressure and saturation as multi-phase fluids flow in heterogeneous porous media. As opposed to an expensive implicit pressure solver, we construct image-based neural networks to capture spatial and temporal patterns. The surrogate model takes inputs including images of permeability field, production information, and the initial fluid status, and predicts pressure fields at different time steps. Physics-constraint is introduced as loss penalty to impose the match of network output with inherent physics in fluid dynamics. The predicted pressure fields are further fed into an efficient explicit numerical solver for saturation calculation. As a result, the workflow brings decent accuracy but reduces the associated computational cost. The performance and effectiveness of the aforementioned workflow will be discussed by numerical examples. Our experiments show that, by training image-based networks with physics-based loss functions, the evolution of fluid dynamics can be predicted accurately and with certain temporal stability maintained. The results also suggest that the proposed hybrid deep learning numerical workflow is capable of providing accurate approximation for solutions in nonlinear multi-phase flow problems with considerable efficiency.

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MS04 / 206

μCT investigation of liquefaction mechanisms at the pore scale

Author: Nicolaine Agofack¹

Co-authors: Haili Long-Sanouiller²; Pierre Cerasi¹

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We investigated in this work liquefaction of an outcrop, the Saltwash South (SWS) poorly consolidated sandstone, due to exposure to different solutions including fresh water, KCl- and NaCl-rich solutions. This sample is composed of 84% quartz, 5% feldspar and rock fragments, around 11% clay. Its porosity is around 30%, its density 1.8 g/cm³. It also has a Young's modulus of 0.3 GPa and an unconfined strength of 1.9 MPa [1, 2]. The exposure experiments included total immersion of samples

in the above-mentioned solutions and micro-Computer Tomography (μ CT) scans after drop-by-drop fluid exposure. The results show that the SWS sandstone collapses within only few seconds when totally immersed into a fresh water or NaCl-rich solution (Figure 1). The disintegration process is held back when 5 wt% or more KCl is present in fresh water or in NaCl-solution (see Figure 2). Adding few percentages (up to 2%) of KCl into a 3.5% NaCl solution shows an interesting result: it slows down the disintegration process from less than a minute after immersion to 5 minutes before total collapse. The microstructure changes due to these exposures at pore level have been captured by analysing the μ CT images. Another procedure was drop-by-drop fluid exposure on the sample's top surface, using a syringe and a paper filter (Figure 3).

Investigation at pore scale with μ CT was performed on 7 mm diameter and 15 mm length samples. The procedure consisted in first scanning the sample dry, then repeatedly add fluid drops on the sample's top face and perform fast scanning. Figure 4 and Figure 5 show the resulting disintegration process for fresh water. The sample collapses from the top part while the bottom part remains intact. In Figure 5, it can be seen that the water leads to an expansion of the total volume and is followed by sample collapsing. The change was slow enough to be captured by μ CT scanning. Although this work focussed on the collapsing of SWS sandstone, it suggests a methodology to study quick clay activation. This is done through the proxy of a larger-grain sandstone, in order to understand the pore-scale details of how liquefaction starts, develops and spreads in the volume studied. Loss of strength can be seen as similar between SWS and quick clay, with local swelling of clay cement at the matrix grain contacts.

References:

1. Cerasi, P. and L.E. Walle, Investigation of Potential Loss of Injectivity and Formation Integrity Due to Pressure Cycling. *Energy Procedia*, 2016. 86: p. 420-431.
2. Pradhan, S., et al., Fracturing tests on reservoir rocks: Analysis of AE events and radial strain evolution, in *48th US Rock Mechanics / Geomechanics Symposium*. 2017: Minneapolis, MN, USA.

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1. Cerasi, P. and L.E. Walle, Investigation of Potential Loss of Injectivity and Formation Integrity Due to Pressure Cycling. *Energy Procedia*, 2016. 86: p. 420-431.
2. Pradhan, S., et al., Fracturing tests on reservoir rocks: Analysis of AE events and radial strain evolution, in *48th US Rock Mechanics / Geomechanics Symposium*. 2017: Minneapolis, MN, USA.

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Time Block A (09:00-12:00 CET)

Participation:

Online

Impact of nano-porous coatings on rates of coupled dissolution-precipitation reactions

Author: Simon Emmanuel¹

¹ *The Hebrew University of Jerusalem*

Corresponding Author: simon.emmanuel@mail.huji.ac.il

During fluid-rock interaction, nano-porous coatings can build up on mineral surfaces. Such coatings often form as result of coupled dissolution-precipitation reactions and are thought to impede reaction rates. While this effect is widely recognized, a complete mechanistic description of the way coatings impact mineral reaction rates has not yet been developed. In this study, we present a boundary layer model that predicts the rates of coupled primary mineral dissolution and secondary phase formation in the presence of a nano-porous coating. Our simulations show that as the thickness of the coating increases, reaction rates can drop by orders of magnitude. The magnitude of the effect is determined by the porosity and tortuosity of the layer, as well as a complex interplay between the rate constants in the reaction rate equations. In contrast to natural mineral grains in soils and rocks, minerals used in laboratory dissolution experiments are usually coating-free, and our results suggest that this difference could account for the much slower dissolution rates that are measured under field conditions.

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Time Block B (14:00-17:00 CET)

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Online

MS08 / 208

Pollutant dispersion in heterogeneous porous media: On the impact of the heterogeneity of the exchange rate and permeability field in Mobile-Immobile transport simulations

Authors: laurent talon¹; emma ollivier-triquet²; Marco Dentz³; Daniela Bauer²

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Transport in the subsurface is strongly characterized by the heterogeneity of the porous medium. As the subsurface is strongly influenced by human activity, obtaining an accurate description of mass

transport in such media remains a crucial task. Tracer transport in porous media has been extensively treated in the literature. However, considering the many pollutants in industry and agriculture that enter the subsurface further research is ongoing. In addition, for many pollutants (nuclear waste, microplastics, pharmaceuticals, etc.), contamination remains critical at very low concentrations and cannot be ignored. Here, heavy tailing is a major issue particularly in water remediation. Further understanding of the coupling between transport, diffusion, and exchange kinetics (due to stagnant zones or adsorption), including tailing effects, remains a crucial task in the actual environmental context. Dynamics of spreading and the temporal spatial extension of the pollutants but also the time to reach a critical location (e.g. aquifer, well) strongly depend on the underlying heterogeneity of the permeability field. Moreover, in the case of solute retention, transport is also strongly impacted by local exchange kinetics that depend on the local aquifer properties. Consequently, exchange (retention) times are expected to be spatially heterogeneous.

In this work, we simulate transport in a two-dimensional heterogeneous medium under spatially varying permeability and mobile-immobile mass transfer parameters. Equations are solved using a Lattice-Boltzmann TRT algorithm. We assume the following relation between the local permeability K and the local retention time $1/\tau$: $1/\tau \approx K^\gamma$.

Taking into account this relation, we investigate the impact of the Damköhler number (Da , ratio of the retention and convection time scales), the disorder of the permeability field and the value of the exponent of the coupling function (γ) on the spatial evolution of the concentration field and the breakthrough curve. We show that, depending on the parameters (Da , γ , etc.), we can observe normal or anomalous dispersion, which are characterized by power-law tails of solute breakthrough curves and non-linear evolution of the spatial variance of the solute distribution. These behaviors are upscaled using a continuous time random walk approach based on a spatial Markov model for particle velocities that couples advective-dispersive transport and heterogeneous mass transfer through a compound Poisson process. The model can be parameterized by the distributions of permeabilities and exchange parameters.

Coupling between the heterogeneous permeability field and the local mass transfer properties can strongly influence transport and explain the experimentally observed non-Gaussian behavior.

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MS10 / 209

Imaging fluid transfers in pores and pore changes through dynamic NMR relaxometry

Author: Benjamin Maillat¹

Co-authors: Rahima Sidi-Boulenouar²; Philippe Coussot³

¹ *Laboratoire Navier*

² *UGE*

³ Univ. Paris-Est

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Magnetic Resonance Imaging (MRI) is well known to be a powerful non-destructive means to get local information on the spatial distribution of water in porous media. However, it does not easily provide quantitative information on the pore size distribution, the pore filling, and the evolution of these characteristics in time, i.e. the dynamics of the structure and the process. Here we show that this type of information can be obtained in a straightforward way through an original approach, namely “dynamic NMR relaxometry”.

Data from a standard NMR (Nuclear Magnetic Resonance) sequence are analyzed with the help of a Contin treatment (basically a Laplace transform), which provides the distribution of relaxation times in the samples, i.e. the probability density function to have each relaxation time value. This information is critical as the NMR relaxation time is related to the pore size and liquid filling of the pore, all aspects which may be quantified through the Brownstein and Tarr model. The originality of our approach is to quantitatively analyze the evolution in time (dynamics) of this distribution during transfers in porous media such as drying, imbibition, diffusion, swelling, etc. We then get a straightforward quantification of a variety of possible phenomena such as:

- progressive homogeneous or inhomogeneous emptying of pores
- isotropic or differential shrinkage of the pores
- possible development of liquid films along the pore walls
- transfers between bound and free water

In association with independent MRI measurements such data allow to get a complete view of the transfers and changes of porous media. We show examples from our recent works on wood [1-2], cement, cellulose [3], model compressible biporous materials [4], composite systems, etc.

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References:

- [1] H. Penvern, M. Zhou, B. Maillet, D. Courtier-Murias, M. Scheel, J. Perrin, T. Weitkamp, S. Bardet, S. Caré, P. Coussot, How bound water regulates wood drying, *Phys. Rev. Applied*, 14, 054051 (2020)
- [2] D.M. Nguyen, S. Caré, D. Courtier-Murias, M. Zhou, P. Coussot, Mechanisms of softwood imbibition inferred from Magnetic Resonance Imaging, *Holzforschung*, 75, 225-236 (2021)
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 211

Microporosity-permeability relationship for complex South East Asia carbonate reservoir

Author: Wen Pin Yong^{None}

Co-authors: Sebastian Geiger ; Hannah Menke ; Kamaljit Singh ; Julien Maes

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The porosity and permeability relationships in carbonate reservoirs are complicated and do not have an easily derivable upscaling functions due to the complex multi-scale pore systems and diagenetic history during the formation of the reservoir. This paper aims to share a proof-of-concept microporosity study in the Central Luconia carbonate fields, Malaysia that is based on 2D and 3D imaging techniques. This study analyses the relationship between microporosity and permeability for Miocene carbonate samples using 2D thin section and 3D Computed Tomography (CT) scan images. First, the heterogeneity of our carbonate samples is examined using Routine Core Analysis (RCA) porosity permeability results, micro-CT images and Scanning Electron Microscope (SEM) images. Then, the amount and size of the microporosity is quantified by Mercury Injection Capillary Pressure (MICP) laboratory analyses and Winland equation by observing pore throat size with less than 10 μm . The amount of microporosity and the contribution of microporosity towards permeability are then analysed analytically based on 2D digital image analysis (DIA) and 3D digital core analysis (DCA). Based on the findings, Central Luconia carbonate samples contain significant amount of microporosity, ranging from 15 to 83% of the total measured porosity. The porosity-permeability matching accuracy decreases with increasing amount of microporosity in the samples. In addition, we have extended the microporosity-permeability relationship from 2D to 3D using the Darcy-Brinkman-Stokes (DBS) model with different structural attributes and pore features.

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MS03 / 212

Efficient Solvers based on Hybrid High Order (HHO) methods for flow simulations in fractured rocks.

Authors: Alexandre Ern¹; Florent Hédin²; Géraldine Pichot³; Nicolas Pignet⁴

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In many subsurface applications (water resources, geothermal applications, oil/gas extraction, nuclear waste disposal), fractures play a major role as they are preferential flow paths. Fractures appear

at all scales, from the centimeter to the kilometer. This wide range of scales spread over large computational domains requires efficient and robust numerical methods, capable of managing networks with millions of fractures. In this presentation, we investigate the computational performance of hybrid high-order methods [Di Pietro, et al., 2014; Cicuttin, et al., 2018] applied to flow simulations in extremely large discrete fracture networks (over one million of fractures). We study the choice of basis functions, the trade-off between increasing the polynomial order and refining the mesh, and how to take advantage of polygonal cells to reduce the number of degrees of freedom [Ern, et al., 2021].

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References:

D. Di Pietro, A. Ern and S. Lemaire, An arbitrary-order and compact-stencil discretization of diffusion on general meshes based on local reconstruction operators, *Comput. Methods Appl. Math.*, 14(4), 461-472, 2014.

M. Cicuttin, D. A. Di Pietro and A. Ern, Implementation of Discontinuous Skeletal methods on arbitrary-dimensional, polytopal meshes using generic programming, *J. Comput. Appl. Math.*, 344, pp. 852–874, 2018.

Alexandre Ern, Florent Hédin, Géraldine Pichot, Nicolas Pignet. Hybrid high-order methods for flow simulations in extremely large discrete fracture networks, Preprint, <https://hal.inria.fr/hal-03480570>, 2021.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

Poster / 213

Effect of pore structure characteristics on imbibition recovery of shale with different fabric facies

Author: Qinghao Sun¹

Co-authors: Yuliang Su¹; Jilong Xu ; Wendong Wang¹; Xincheng Guo ; Guanqun Li ; Tianyu Zhang

¹ *China University of Petroleum (East China)*

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Shale oil reservoir has different fabric facies (lamellar, thin lamellar, massive, etc.) rock based on lamina development degree and longitudinal superposition relationship of different lithology. Laboratory tests show that the spontaneous imbibition recovery rate of shale with different fabric facies is different, and the difference of pore structure is the main reason. In this paper, spontaneous imbibition experiment of shale based on nuclear magnetic resonance (NMR) technology is carried out. The difference of pore structure of shale with different fabric facies and its influence on imbibition are comprehensively compared, and the imbibition transport mechanism of shale oil in pores with different sizes is studied.

The cores used in this study are two kinds of fabric facies rock from continental shale oil reservoirs in China, which are lamellar (single lamina thickness 1mm-1cm) and massive (single lamina thickness > 50 cm). Firstly, the samples were tested by scanning electron microscopy (SEM), high-pressure mercury intrusion and low-temperature nitrogen adsorption (LTNA). It is difficult to characterize nano-micropores in high-pressure mercury intrusion test. However, the pore size distribution of shale can be characterized by LTNA and NMR. With the help of NMR and high precision electronic balance, the slick water spontaneous imbibition experiment of shale core was carried out. The imbibition recovery of shale oil in different pore sizes was calculated according to the measured NMR T2 spectrum and core weight variation.

SEM showed that the development degree of inorganic pore: lamellar > Massive, organic matter content and organic pore development degree: massive > lamellar. The average pore size of lamellar shale (20.30nm) is larger than that of massive shale (9.96nm) by LTNA test. The pore size distribution of lamellar shale (69.00% mesopores, 30.11% macropores, 0.89% micropores) is different from that of massive shale (83.26% mesoporous, 15.37% macroporous, 1.37% microporous). The experimental results show that the imbibition recovery rate of lamellar shale (25.60%) is significantly higher than that of massive shale (17.74%). Compared with the shale oil recovery rate in the pore of massive shale, the rate of micropores in lamellar shale is higher (37.12% vs. 6.63%), the rate of mesopore is higher (35.24% vs. 14.80%), and the rate of macropore is lower (2.65% vs. 34.63%). The difference in shale oil recovery of micropores is due to the difference in micro-wettability, that caused by the rich inorganic micropores in lamellar shale and organic micropores in massive shale. The low recovery rate of macropores in lamellar shale is due to the fact that the large pores mainly act as migration channels during spontaneous imbibition, and most of the oil is retained in the large pores after the imbibition process is balanced.

The major contribution is to gain insight on the pore structure difference of shale with different fabric facies, and hence reveal the cause of the imbibition recovery difference among different fabric facies shale. The outcomes are of great interest for the field operators to optimize the designs of well stimulation best for their reservoirs.

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MS15 / 214

Upscaling investigations of dissolution using machine learning and GeoChemFoam

Author: Hannah Menke¹

Co-authors: Sebastian Geiger ; Julien Maes ¹

¹ Heriot-Watt University

Corresponding Authors: j.maes@hw.ac.uk, h.menke@hw.ac.uk, s.geiger@hw.ac.uk

The current conceptual model of mineral dissolution in porous media is comprised of three dissolution patterns (wormhole, compact, and uniform) - or regimes - that develop depending on the relative dominance of flow, molecular diffusion and reaction rate during dissolution. Here, we examine the evolution of pore structure during acid injection using our new fast numerical simulator GeoChemFoam on two synthetic pore spaces of increasing complexity. We examine the boundaries between regimes using transverse dispersion and agglomerative hierarchical clustering and prove the existence of a fourth regime called channelling, where already existing fast flow pathways are preferentially widened by dissolution. Channelling occurs in cases where the distribution in pore throat size results in orders of magnitude differences between transverse, longitudinal dispersion and flow rate for different flow pathways. This focusing of dissolution along only dominant flow paths induces an immediate order of magnitude change in permeability with a comparatively small change in porosity, resulting in a different porosity-permeability relationship than has been previously seen. These new dynamic porosity-permeability relationships are then used to train a machine learning model for predicting permeability change with porosity with local flow and reactive conditions. This model is then bootstrapped to GeoChemFoam's Darcy-Brinkman solver and used to predict dissolution at the Darcy scale. The results are then compared to both traditional upscaling techniques and a full pore-scale simulation. Our results highlight the importance of including pore-scale information in upscaled domains. This work demonstrates that our current conceptual model of dissolution regimes must be modified to include channelling for accurate predictions of dissolution in applications such as geologic carbon storage and geothermal energy production and is the first step in upscaling dissolution for accurate Darcy scale prediction.

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Participation:

In person

MS23 / 216

Bifurcating-Paths: the relation between preferential flow bifurcations, void, and tortuosity on the Darcy scale.

Authors: yaniv edery¹; Dagan Avioz²

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Darcy scale transport in porous media ranges between Fickian and non-Fickian according to the medium conductivity layout, which ranges between homogenous and heterogeneous. Yet, evidence shows that preferential flows that funnel and bypass even areas with high conductivity occur in heterogeneous and homogenous cases. We model the Darcy scale transport using a 2D conductivity field ranging from homogenous to heterogeneous and find that these preferential flow bifurcate,

leaving voids where particles do not invade while forming a tortuous path. The fraction of bifurcations decreases downflow and reaches an asymptotical value, which scales as a power-law with the heterogeneity level. We show that the same power-law scaling holds for the void fraction, tortuosity, and fractal dimension analysis. We conclude that the scaling with the heterogeneity is the dominant feature in the preferential flow geometry, which will lead to variations in weighting times for the transport and eventually to anomalous transport.

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MS08 / 217

Feedback mechanisms between precipitation and dissolution reactions across randomly heterogeneous conductivity fields

Authors: yaniv edery¹; Martin Stolar¹; Giovanni Porta²; Alberto Guadagnini²

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Our study investigates interplays between dissolution, precipitation, and transport processes taking place across randomly heterogeneous conductivity domains and the ensuing spatial distribution of preferential pathways. We do so by relying on a collection of computational analyses of reactive transport performed in two-dimensional systems where the (natural) logarithm of conductivity is characterized by various degrees of spatial heterogeneity. Our results document that precipitation and dissolution jointly take place in the system, the latter mainly occurring along preferential flow-paths associated with the conductivity field, the former being observed at locations close to and clearly separated from these. High conductivity values associated with the preferential flowpaths tend to further increase in time, giving rise to a self-sustained feedback between transport and reaction processes. The clear separation between regions where dissolution or precipitation takes place is imprinted onto the sample distributions of conductivity which tend to become visibly left skewed with time (with the appearance of a bimodal behavior at some times). The link between conductivity changes and reaction-driven processes promotes the emergence of non-Fickian effective transport features. The latter can be captured through a continuous time random walk model where solute travel times are approximated with a truncated power law probability distribution. The parameters of such a model shift towards values associated with increasingly high non-Fickian effective transport behavior as time progresses.

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<https://doi.org/10.5194/hess-25-5905-2021>

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MS09 / 218

Pore scale modelling of stress-dependent permeability and tortuosity of hydrate bearing sediment based on high resolution synchrotron x-ray computed tomography imaging

Authors: Li Rui¹; Yingfang Zhou^{None}; Wenbo Zhan²; Jianhui Yang³

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Gas hydrate contains abundant methane and is expected to be a promising energy supply to mitigate the influence of climate change in the future, in addition, it is also relevant to geological hazards. Permeability governs the gas production rate when extracting gas from hydrate deposits, which is a stress-dependent factor that varies while depressurizing the hydrate deposit. Probing the relation between permeability characteristics and effective stress is thus critical for better planning the gas production in hydrate reservoirs. However, the study of stress-dependent permeability of hydrate-bearing sediments is rare due to restricted access to in-situ hydrate-bearing cores and the sensitivity to pressure and temperature disturbance of hydrate-bearing cores.

In this work, we constructed a set of hydrate-bearing rock models with a wide hydrate saturation range based on high-resolution synchrotron x-ray computed tomography imaging. We then adopted the Finite Element Method to investigate the deformation of these hydrate-bearing rock models under different effective pressures. The deformed pore space was then used as input for direct single phase flow using a Lattice-Boltzmann method.

The proposed simulation approach was first validated using capillary tube models (see Figure 1). The porosity and permeability results demonstrate that the deformation-flow coupling workflow proposed in this work is valid (see Figures 2 and 3). The simulation in realistic hydrate bearing sediments extracted from high resolution synchrotron x-ray computed tomography imaging were performed under various hydrate saturation to understand the effect of effective stress on permeability and tortuosity of the hydrate-bearing rock.

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Poster / 219

Development of a salt-impregnated SAPO-34 porous matrix with graphene oxide for water sorption applications

Authors: Samar Abd Elwadood¹; Ludovic Dumeé²; Yasser Al Wahedi³; Ali Al Alili⁴; Georgios Karanikolos²

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Composites “Salt Inside Porous Matrix” (CSPMs) are promising materials for atmospheric water adsorption/generation. In this work, CSPMs were synthesized by impregnating porous SAPO-34 with hygroscopic salts (LiCl and/or CaCl₂), and further functionalized with incorporation of graphene oxide (GO). The physicochemical, morphological, and textural properties of the resulting hybrids were determined, and their water adsorption performance was evaluated.

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Participation:

In person

MS22 / 220

Fabrication, Characterization, and Testing of Architected 3D Graphene Foams

Author: Somayya E. Taher¹

Co-authors: Juveiriah M. Ashraf²; Kin Liao¹; Rashid K. Abu Al-Rub³

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Three-dimensional (3D) porous structures fabricated from a 2D material such as graphene have recently attracted huge attention owing to the outstanding electro-mechanical and thermal properties of various types of 2D materials. The interest has expanded to integrate the 2D materials into 3D printed structures to form an architected multifunctional foam. Several studies have focused on fabricating 3D porous structures from 2D materials using different techniques. Most of the existing fabrication techniques are often time-consuming and require specialized equipment. In this work, a practical and scalable self-assembly hydrothermal-assisted dip-coating technique has been employed to fabricate architected graphene foams. The graphene is coated on a 3D printed polymeric scaffold that takes the topology of the mathematically-known triply periodic minimal surfaces (TPMS). Then, the initial scaffold is removed by thermal etching to produce the freestanding graphene foam. Three different TPMS topologies (Gyroid, IWP, and Diamond) have been used in fabricating graphene foams. Different characterization techniques such as x-ray diffraction (XRD) and Raman spectroscopy were utilized to verify the presence of graphene. Scanning electron microscopy (SEM) and micro-computed tomography (Micro-CT) scans were used to visualize the internal pore structure and study the difference in pore size between the original TPMS structure and the 3D graphene foam. A series of tests were performed to measure the multifunctional (electrical, thermal, mechanical) properties of the TPMS-based graphene foams. The graphene foam based on TPMS structure shows an excellent specific stiffness value of 32.04 kPa cm³ mg⁻¹ for a sample with low density of 69.6 mg cm⁻³. The specific thermal and electrical conductivity values were recorded to be 0.025 W cm² K⁻¹ mg⁻¹ and 1.077 S cm² mg⁻¹, respectively. The unique structure and its multifunctional properties show that these lightweight 3D graphene foams (3DGF) can be used in various applications including heat sinks, energy storage, and sensors.

Keywords—Graphene Foams; Triply Periodic Minimal Surfaces; Self-assembly; Dip-coating; 3D Printing; Multifunctional Properties.

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In person

MS02 / 221

Explicit spatial modeling at the pore scale unravels the interplay of soil organic carbon storage and structure dynamics

Authors: Nadja Ray¹; Simon Zech²; Steffen Schweizer³; Franziska Bucka³; Ingrid Kögel-Knabner³; Alexander Prechtel⁴

¹ *Friedrich-Alexander Universität Erlangen-Nürnberg*

² *Friedrich-Alexander University Erlangen-Nürnberg (FAU)*

³ *TUM*

⁴ *Mathematics Department, University of Erlangen-Nürnberg*

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Key functions of soils, such as their contribution to the carbon cycle are significantly influenced by structures down to the microaggregate scale (< 250 μm). Although advanced imaging techniques now allow snapshots even down to the nanoscale, the mutual interdependence of the turnover of particulate organic matter and dynamic restructuring of soil aggregates is not completely understood yet. In this study, we take advantage of a process-based mechanistic model which is spatially and temporally explicit. Based on the cellular automaton framework presented in [1, 2, 3], it allows to investigate disaggregation and re-formation of the soil microstructure taking into account inert primary particles, interacting minerals, water stable solid building units, and organic matter. Likewise the input of fresh particulate organic matter can be integrated into the modeling approach. Its decomposition and the related dynamics of glueing agents is captured by means of (partial) differential equations. With the help of this modeling approach we contribute in particular to the understanding of a structural priming effect, where the increased input of POM stimulated the mineralization of old POM [4].

[4] Simon Zech, Steffen A. Schweizer, Franziska B. Bucka, Nadja Ray, Ingrid Kögel-Knabner, Alexander Prechtel. "Explicit spatial modeling at the pore scale unravels the interplay of soil organic carbon storage and structure dynamics." in preparation 2022.

[3] S. Zech, T. Ritschel, N. Ray, K. U. Totsche, A. Prechtel. "How water connectivity and substrate supply shape the turnover of organic matter – Insights from simulations at the scale of microaggregates." *Geoderma* 405, 2022.

[2] A. Rupp, K.-U. Totsche, A. Prechtel, and N. Ray. "Discrete-continuum multiphase model for structure formation in soils including electrostatic effects." *Frontiers in Environmental Sciences* 6(86), 2018.

[1] N. Ray, A. Rupp, and A. Prechtel. "Discrete-continuum multiscale model for transport, biofilm development and solid restructuring in porous media." *Advances in Water Resources* 107, 2017.

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Poster / 222**Production and characterization of porous sludge-derived biochar as a sustainable solution for the water industry****Author:** Andre Frota¹**Co-authors:** Naiara Oliveira²; Mona Lisa Oliveira³; Thiago Xavier⁴; Erdin Ibraim⁵; Odair Ferreira²; José Capelo Neto²; Tannaz Pak⁶¹ *Federal University of Ceara*² *Federal University of Ceará*³ *State University of Ceará*⁴ *Federal University of Espírito Santo*⁵ *University of Bristol*⁶ *Teesside University***Corresponding Authors:** t.pak@tees.ac.uk, thiago.p.xavier@ufes.br, opferreira@fisica.ufc.br, andremadson@alu.ufc.br, erdin.ibraim@bristol.ac.uk, naiara@fisica.ufc.br, capelo@ufc.br, mona.lisa@uece.br

It is known that conventional coagulation/flocculation, sedimentation, and filtration techniques are partially efficient in removing extracellular-soluble cyanotoxins and compounds in water; therefore, advanced water treatment methods are often used instead. Conventional methods of remediating persistent pollutants from aqueous and gaseous phases mainly employ chemical precipitation, ion exchange, adsorption (using activated carbon), and membrane separation processes, among others. These methods are costly and often generate considerable amounts of chemical residues, which have no economic value. A key concern regarding the direct discharge from water treatment waste residuals to water bodies is the potential toxicity of iron and aluminum –chemicals normally used as primary coagulants in the flocculation–sedimentation stage (Sotero-Santos et al., 2005).

Pyrolysis is a mature heat treatment method in bio-energy production, solid waste management, and preparation of carbon-based materials (Li & Jiang, 2017). Due to the advantages of pyrolysis, this study proposes a new technique based on the use of drinking water treatment sludge as a feedstock for the manufacture of porous biochar and its application in the treatment of contaminated waters (Chen et al., 2021; Zheng et al., 2021). The choice of sludge as a feedstock material was due to its availability in large quantities, attractive characteristics for resource recovery, also, because under current Brazilian legislation, it is considered an environmental liability. The starting material was pyrolyzed via slow pyrolysis at 450 °C and 600 °C in a bench-scale pyrolysis unit. We also investigated the characterization of the porous biochar. Different techniques were used to characterize the samples: proximate analysis, Fourier-transform infrared spectroscopy (FT-IR), Raman spectroscopy, X-Ray diffraction analysis (XRD), zeta potential, adsorption-desorption isotherms, thermogravimetric analysis (TGA/DTG), and scanning electron microscopy (SEM).

The biochar produced from sludge at different pyrolysis temperatures was tested as sorbents for the improvement of natural eutrophic water quality in jar tests to simulate a conventional coagulation/flocculation process. The present study was designed with the major objectives: to characterize the composition and structural properties of the biochar, explore and compare the adsorption behaviors of the tested biochar, and discuss how these properties can influence their application in water treatment. The results may shed light on the management and use of waste materials, such as water treatment sludge, and be valuable for developing porous biochar as low-cost sustainable adsorbents in natural waters and water treatment systems.

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Chen, W., Zhao, B., Guo, Y., Guo, Y., Zheng, Z., Pak, T., & Li, G. (2021). Effect of hydrothermal pretreatment on pyrolyzed sludge biochars for tetracycline adsorption. *Journal of Environmental Chemical Engineering*, 9(6), 106557. <https://doi.org/10.1016/j.jece.2021.106557>

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Sotero-Santos, R. B., Rocha, O., & Povinelli, J. (2005). Evaluation of water treatment sludges toxicity using the *Daphnia* bioassay. *Water Research*, 39(16), 3909–3917. <https://doi.org/10.1016/j.watres.2005.06.030>

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Time Block C (18:00-21:00 CET)

Participation:

Online

Poster / 224

Impact of Novel Nano-particle Solutions on Foam Stability, Wettability Reversal and Interfacial Tension Reduction

Authors: Mohammad Rezaee¹; Seyed Mojtaba Hosseini-Nasab²; Jalal Fahimpour³; Mohammad Sharifi³

¹ *Amirkabir University of Technology, Department of Petroleum Engineering*

² *School of Chemical, Oil and Gas Engineering*

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One of the most important methods for increasing the oil recovery of petroleum reservoirs is gas injection. However, it will not result in good oil recovery in many cases due to a low volumetric sweep efficiency. Foam flooding emerged as a promising solution for improving gas flooding. Still, there are significant concerns regarding the use of foam due to its un-stability in reservoir conditions and the vicinity of crude oil.

For a foam flooding process to be successful, high-performance foaming agents must be selected to produce stable foam. One of these agents could be the use of nanoparticles. In this paper, we have attempted to create foam by making a low-cost nanoparticle, which can be obtained from an industrial waste called fly ash, and addressing its impact on the crucial parameters of the foam EOR process. In the current study, fly ash nanoparticles were first obtained using a specific procedure, and then it was used with a surfactant solution to form foam. Foam performance at bulk volume was evaluated, and results showed that a small amount of fly ash nanoparticle could significantly increase the foam stability in the presence of a cationic surfactant. Foam agents also changed the surface wettability from completely oil-wet to water-wet. Furthermore, it has been observed that fly ash nanoparticles can reduce the IFT between the oil and water phase. In addition to bulk stability tests, flooding tests showed that the nano-stabilized foam could increase the ultimate oil recovery in quasi-two-dimensional (2D) porous media tests.

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Poster / 225

Imaging and chemical analysis of ureteral stent encrustation and incrustation

Authors: Tal Amitay-Rosen¹; Ishai Dror²; Yaniv Shilo³; Brian Berkowitz²

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³ *Kaplan Medical Center*

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Ureteral stents are effective in alleviating flow disruptions in the urinary tract, whether due to ureteral stones or either intrinsic or extrinsic ureteral obstruction. Stents are also used following various endourological and surgical procedures that can affect the ureter, to promote urine flow until edema decreases and incisions heal. However, significant stent encrustation and incrustation can occur, which may interfere with stent functioning and/or removal. The goal of this work was to quantify stent encrustation and incrustation, mapping depositions along the entire length of representative, intact stents. This information was used to identify possible correlations between encrustation and incrustation, and to examine potential stent lumen obstruction resulting from incrustation. Micro-computed tomography (micro-CT) was used to non-invasively image encrustation (stent external wall) and incrustation (stent lumen). Subsequently, x-ray diffractometry (XRD) and scanning electron microscopy–energy dispersive x-ray spectroscopy (SEM-EDS) enabled analysis of samples of encrusted and incrustated material collected from the distal, proximal and mid-ureteral stent regions, to characterize the mineral structure and chemical content of the deposits. The micro-CT analysis shows, most significantly, that extensive *incrustation* can occur along any region of a stent, even when there is only incidental or minor *encrustation* along the entire length of the (exterior) stent wall. Analysis of mineral structure and chemical content demonstrates the occurrence of broad variations among individual stents. Deposits can consist of crystalline deposits (e.g., CaCO₃) and/or amorphous, non-crystalline, organic and/or inorganic constituents. A clinical implication of our findings is as follows: given that the degree of incrustation cannot be predicted or determined in advance, and in the absence of any other correlating clinical data, the practice of inserting a guidewire into the stent to facilitate its direction to the kidney may result in inadvertent delivery of large amounts of depositional material into the upper urinary tract. Such deposits may act as nucleation material for future kidney stones. Moreover, deposits containing significant amounts of organic/biological constituents may lead to contamination of the urinary tract and potentially to bacteremia under high renal pressures.

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Poster / 226

Evaluation of saturation of tight sandstones using dielectric logs: Ordos Basin, China

Authors: Peiqiang Zhao¹; Zhiqiang Mao¹; Gaoren Li²; Haopeng Guo²

¹ *China University of Petroleum, Beijing*

² *PetroChina Changqing Oilfield Company*

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Due to shallow mud invasion in unconventional reservoirs such as tight sandstone, shale, the dielectric dispersion logs have advantage in the saturation evaluation of unconventional reservoirs. Dielectric dispersion logs had been applied in the evaluation of unconventional reservoirs in North America with good results. A large number of unconventional reservoirs are found in the basins in China that are a huge source of oil production. However, the applicability of dielectric dispersion logs in those basins are rarely studied. Ordos Basin is one of the largest petroliferous basins in China. In this paper, we mainly investigate the applicability of interpretation models for dielectric logs in the tight sandstone of the Yanchang Formation of Triassic. The conventional sandstone of Yan'an Formation of Jurassic is taken as comparative example. This study could help identify for the oil and water layers in the Ordos Basin.

Firstly, the core samples were drilled from the two formations are measured with the dielectric dispersion in laboratory to get the permittivity of the matrix. The samples are measured with two states that are dry and saturating salty water. The matrix permittivity of conventional sandstone are calculated as 4.5 while the tight sandstone is high at about 6.2. Then, we applied these values to investigate the interpretation models in the real formations. The commonly used Complex Refractive Index (CRIM), Stroud-Milton-De (SMD) and shaly sandstone (SHSD) model are selected. In the conventional sandstone, the CRIM model used for permittivity and conductivity measured at 1GHz and SMD model is used for permittivity and conductivity in 20MHz-500MHz frequency band. In tight sandstone, the CRIM and SHSD models are used to construct the misfit function due to that the shale content is higher. Next, the particle swarm optimization (PSO) algorithm is used to optimize the objective functions, and examples are constructed to test the algorithm. Finally, the method is applied to the target reservoir to obtain saturation, tortuosity index of water phase, salinity of flushing zone.

The results show that the relative error between the synthetic log response and the measured log is less than 20% in the two formations, indicating that the combination of the interpretation models

are rational and effective. Furthermore, the calculated oil saturation is in good agreement with the core analysis and oil test data, which verifies the accuracy of the proposed method.

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Online

MS09 / 227

Absolute permeability of glass bead packs: the first principles agreement between experiment and pore-scale simulations

Authors: Siarhei Khirevich¹; Maxim Yutkin¹; Tadeusz Patzek¹

¹ *King Abdullah University of Science and Technology*

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We prepare two porous samples and estimate their permeabilities using experiment and simulation. After comparing experimental and simulated permeabilities, we have identified a major flaw affecting many permeability measurements with out-of-sample pressure port placement.

Each sample is composed of densely packed 500-micron glass beads obtained from different manufacturers. A special care is taken to minimize the scatter in measured permeability values, typical of standard permeability experiments. Measured permeability values are ~1% stable when varying flow rate 4-fold and fluid viscosity 2.5-fold.

Each sample is scanned in three dimensions (3D) using X-ray computed tomography (CT) for a wide range of discretization resolutions, from 3 to 65 voxels per average bead diameter. Detailed analysis of the CT scanning settings and image processing routines allowed to obtain 3D sample images free from contrast loss and CT artifacts. Hereafter, gray-scale CT images were binarized (segmented) using global segmentation threshold. For each sample, the threshold value was obtained from independently measured porosity. Such a segmentation approach avoided operator-dependency for the resulting images.

The segmented 3D images of the pore space were used to simulate Stokes flow with the two-relaxation-times lattice Boltzmann method. After performing resolution study and using extrapolation (doi:10.1063/1.5042229), we obtained ~0.1% accurate, resolution-independent permeability values. Stable experimental values and accurate simulated values demonstrated ~1% discrepancy, which is well within inaccuracies of the employed experimental equipment.

After obtaining accurate experiment–simulation agreement, we design a simple model system with out-of-sample pressure ports placement. This model system suggests the existence of a major flaw

in permeability measurements, including industry standards. The flaw also affected our own permeability measurements. More details will be available in the accompanying manuscript [1] and during presentation.

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[1] Correct estimation of permeability using experiment and simulation. S. Khirevich, M. Yutkin, T. Patzek. Submitted.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS02 / 228

Dynamic changes in gas concentration in the sap of plants reiterate the enigma of plant water transport under negative pressure

Authors: Luciano Pereira¹; Steven Jansen¹; Marcela Trevenzoli Miranda²; Vinicius Sacramento Pacheco³; Lucian Kaack^{None}; Gabriel Silva Pires³; Xinyi Guan¹; Eduardo Caruso Machado²; H. Jochen Schenk⁴; Rafael Vasconcelos Ribeiro³

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Despite a long research history, we do not fully understand why plants are able to transport sap under negative pressure without constant interruption by microbubbles. The hydraulic transport system of plants is composed of macroporous conduits, which are interconnected by mesoporous cell walls in the xylem tissue. Moreover, the concentration of dissolved gas in xylem sap is traditionally assumed to follow Henry's law. Here, we investigated to what extent xylem sap of well-watered Citrus plants includes dissolved gas, and which parameters affect gas solubility. Direct measurements of the gas concentration in the aqueous phase of xylem were obtained by extracting gas from plants under varying air temperature and xylem water potentials, and then compared to data based on a gas diffusion model. Our results indicated that gas concentrations in xylem ranged by at least 5% compared to the expected solubility in water, and was higher when water potential decreased during transpiration. The modelled gas concentration in xylem sap based on Henry's law for an anisobaric situation did not explain the measurements, including daily changes in gas concentrations. Instead, our data revealed dynamic changes in dissolved gas concentration in xylem and gas oversolubility in confined liquids, with a possible role of xylem sap surfactants for acting as diffusion barriers.

The capacity of plants to transport sap with high amounts of dissolved gas could provide conduits an important buffering characteristic to prevent hydraulic failure through bubble nucleation under varying internal pressure and temperature. Therefore, dynamic changes in dissolved gas provide novel evidence to answer the longstanding question of how plants can transport xylem sap under negative pressure.

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MS13 / 229

Effect of osmosis on spontaneous imbibition of fracturing fluid in shale oil formation

Author: Qinghao Sun¹

Co-authors: Wendong Wang¹; Xincheng Guo ; Yuliang Su¹; Jilong Xu ; Guanqun Li ; Hao Sun

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The traditional theory of spontaneous imbibition is fluid displacement caused by capillary force. However, the imbibition of fracturing fluid in shale reservoir is not only related to capillary force, but also affected by osmotic pressure. Shale pores are in micro/nano scale and have high clay content. Clay is mainly distributed on the pore wall, and can act as a semi-permeable membrane when the fracturing fluid is imbibed, thus causing water molecule osmotic transport, that is, water molecule migration from low salinity fracturing fluid to high salinity formation water. For the spontaneous imbibition of fracturing fluid during well shut-in after fracturing, people often pay attention to the effect of capillary force. In addition, the existing imbibition experiments considering osmosis are multifaceted shale gas formations. Therefore, the osmosis on spontaneous imbibition of fracturing fluid in shale oil formation needs to be further studied.

The cores used in this study are shale from continental shale oil reservoirs in China, and their petrophysical properties (porosity 5%, permeability 0.002mD) are basically the same. By means of nuclear magnetic resonance (NMR) technology and high precision electronic balance measurement, spontaneous imbibition experiment of fracturing fluid with different salinities was carried out on the core. The shale oil used in the experiment contains 10% water, which is saturated by the core and forms bound water to simulate the oil-water two-phase environment in the core matrix. Fracturing fluid and bound water have different salinity. Different osmotic pressure can be formed by changing the salinity of fracturing fluid. The imbibition recovery rate of shale oil can be calculated according to the NMR T2 spectrum measured in the imbibition experiment, and the imbibition fracturing fluid content can be calculated based on the change of core weight during the experiment.

When the high salinity fracturing fluid (18 wt.% $\text{MnCl}_2 \cdot 4\text{H}_2\text{O}$) was imbibed, the core weight first increased, then decreased, then increased again, and finally stabilized. This kind of imbibition can be divided into four stages: initial imbibition stage, drainage stage, secondary imbibition stage and stationary stage. The drainage stage indicates that the core is dewatering and dominated by osmosis, while the initial and secondary imbibition stages are dominated by capillarity. The imbibition of high salinity fracturing fluid (20 wt.% KCl) appears the same phenomenon when the salt ion type is changed. For low salinity fracturing fluids (2.4 wt.% KCl), there was no core dewatering phenomenon, but a significant increase in shale oil imbibition recovery. This is because when the fracturing fluid salinity is lower than the bound water, the great salinity difference between the fracturing fluid and the bound water will form a strong osmotic pressure, driving the fracturing fluid to move deeper into the core matrix.

The major contribution is to prove that capillarity and osmosis are important imbibition mechanisms in shale oil reservoirs, distinguish the imbibition stage dominated by osmosis or capillarity, and reveal the influence law of osmotic pressure on shale oil imbibition recovery under different salinities.

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MS07 / 230

Development and experimental validation of lattice Boltzmann method-based simulator for vapor transport in air over a moist soil layer

Author: Jakub Klinkovský¹

Co-authors: Radek Fučík²; Andrew Trautz³; Tissa Illangasekare

¹ *Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University in Prague*

² *Czech Technical University in Prague*

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We present an efficient computational approach for simulating component transport within single-phase free flow over a soil. A numerical model based on this approach is validated using controlled experiments in a climate-controlled low-speed wind tunnel. The wind tunnel is interfaced with a soil tank to study problems of heat and mass flux across the land-atmospheric interface. The developed modeling approach is based on a combination of the lattice Boltzmann method (LBM) formulated for a weakly compressible fluid flow and the mixed-hybrid finite element method (MHFEM) for solving

constituent transport. Both those methods individually, as well as when coupled, are implemented entirely on a GPU accelerator in order to utilize its computational power and avoid the hardware limitations caused by slow communication between the GPU and CPU over the PCI-E bus. We describe the mathematical details behind the computational method, focusing primarily on the coupling mechanisms. The performance of the solver is demonstrated using modern high-performance supercomputers. Flow and transport simulation results are validated and compared herein with experimentally obtained velocity and relative humidity data based on measurements made above the soil surface over which water evaporates under steady air flow conditions. Model robustness and flexibility is demonstrated by introducing rectangular bluff-bodies to the flow in several different experimental scenarios.

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MS07 / 232

Numerical Analysis of a Mixed Finite Element Approximation a Model of Biofilm Growth in Porous Media

Authors: Azhar Alhammali¹; Malgorzata Peszynska²; Choah Shin³

¹ *Imam Abdulrahman Bin Faisal University*

² *Oregon State University*

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We consider a coupled system of advection-diffusion-reaction PDEs modeling biofilm growth and nutrient consumption in porous media. One of the PDEs is subject to a constraint on the biomass density, so it can be formulated as a parabolic variational inequality (PVI). Moreover, the model is coupled to a heterogeneous Brinkman model of flow of an ambient fluid flowing within and outside the biofilm. We approximate the model using a mixed finite element method. We conduct realistic simulations in complex pore-scale geometries. We study the solvability of the associated PVI and derive a rigorous error estimate of the fully implicit approximation of the biofilm-nutrient model. We compare the results with our previous work where the Galerkin finite element method is used.

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MS06-B / 233

Comprehensive Study of Fluid-Fluid Displacement in Mixed-Wet Porous Media

Authors: Ashkan Irannezhad¹; Bauyrzhan Primkulov²; Ruben Juanes²; Benzhong Zhao³

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Fluid-fluid displacement in porous media occurs in many natural and engineering processes such as water infiltration into soil, geological carbon dioxide storage, and enhanced oil recovery. It has long been recognized that wettability plays an important role in the displacement process. For instance, the displacement pattern of a viscous ambient fluid by a less viscous invading fluid becomes more compact as the invading fluid becomes more wetting to the porous medium. Thanks to decades of research, we now have a fairly good understanding of fluid-fluid displacement in porous media with uniform wettabilities. In contrast, our knowledge of fluid-fluid displacement in porous media with heterogeneous wettabilities (i.e., mixed-wet) is much less complete, even though mixed-wet conditions are common in many subsurface processes.

Here, we study the fluid-fluid displacement pattern in porous media with spatially heterogeneous wettabilities. Experimentally, we perform constant-rate displacement of a viscous ambient fluid by a less viscous invading fluid in microfluidic flow cells patterned with vertical posts. Our microfluidic flow cells are made of a UV-sensitive photo-curable polymer whose surface energy can be locally tuned by exposure to high-energy UV light. These microfluidic flow cells let us achieve clusters of posts that are distinctly more wetting to the invading fluid than the rest of the flow cell. We image the experiment at high resolution, providing simultaneous visualization of both the physics of wetting at the pore scale and the impact of wetting on the macroscopic displacement pattern. These experiments show the preferential filling of the mixed-wet pores when the hydrophilic post is weakly hydrophilic, whereas the invading fluid fully saturates the hydrophilic clusters when the hydrophilic post is more strongly hydrophilic. Numerically, we study the quasi-static evolution of a meniscus through a mixed-wet pore throat and simulate the experiments by using a novel pore network model. We achieve excellent agreement between the pore network model results and the experiments. Finally, we apply the pore network model to explore the impact of cluster size, correlation and distribution, and wettability contrast on the displacement pattern. Our work presents a fascinating and complex phase diagram of fluid-fluid displacement in mixed-wet porous media.

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MS11 / 234

Wettability alteration in thiolene-based polymers: surface characterization and advanced fabrication techniques

Authors: Mahtab Masouminia¹; Benzhong Zhao¹

¹ *McMaster University*

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Fluid-fluid displacement in porous media plays a significant role in many industrial applications, including geologic carbon dioxide sequestration, enhanced oil recovery, and fuel cells. Microfluidics systems are powerful tools to study fluid-fluid displacement in well-controlled geometries. Recently, the thiolene-based polymer called NOA81 emerged as an ideal material in the fabrication of microfluidic devices, since it combines the versatility of conventional soft photolithography and a wide range of achievable wettability conditions. Specifically, the wettability of NOA81 can be continuously tuned by exposing it to high-energy UV light (Levaché et al., 2012, Zhao et al., 2016, Odier et al., 2017). Despite its growing popularity, the exact physical and chemical mechanisms behind the wettability alteration have not been fully characterized.

Here, we apply a suite of different characterization techniques, including X-ray photoelectron spectroscopy (XPS), zeta potential measurements, and atomic force microscopy (AFM) to investigate the impact of high-energy UV on the chemical and physical properties of NOA81 film. We find that high-energy UV exposure increases the ratio of oxygen to carbon (O/C) and polar functional groups of the polymer film, which enhances the surface energy and hydrophilicity. The zeta potential measurements demonstrate that the alteration of surface chemical composition leads to a more negative surface charge. In addition to changes in the surface chemistry, our AFM measurements show that high-energy UV exposure reduces the roughness of the NOA81 surface. Lastly, we advance the state-of-the-art of NOA81 based microfluidic systems by creating i) a 2D surface with a wettability gradient (Fig. 1A) and ii) a 3D column packed with NOA81 beads with controlled wettability (Fig. 1B).

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MS03 / 235

Governing Forces in Fractured Reservoirs: A Data-Driven Sensitivity Analysis

Authors: Zhen Zhang^{None}; Xupeng He^{None}**Co-authors:** Marwah AlSinan¹; Hyung Kwak¹; Hussein Hoteit²¹ Saudi Aramco² Merchant logo King Abdullah University of Science and Technology**Corresponding Authors:** zhen.zhang.1@kaust.edu.sa, marwa.sinan@aramco.com, xupeng.he@kaust.edu.sa, hyung.kwak@aramco.com, hussen.hoteit@kaust.edu.sa

In recent years, research to understand recovery mechanisms in fractured porous media has become more common. Specifically, recovery in fractured rock is governed by three forces: viscous force, gravitational force, and capillary force. This study provides a review and numerical simulation to capture the effect of the combined forces that determines the oil recovery in fractured porous media. Also, we extend our discussion to include an upscaling method for field-scale applications.

We capture these governing forces through numerical simulation with a finite volume scheme and unstructured grid. The fractures are modeled with the Discrete Fracture Model (DFM) approach. We conducted a series of oil-water and oil-gas flow simulation scenarios by varying permeability contrast, viscosity contrast, density contrast, capillary contrast, injection rate, fracture opening (aperture), fracture orientation, and fracture network. Then, we developed a ternary diagram to classify several recovery mechanisms based on the percentage of working forces. Also, we developed a new upscaling method for field-scale application. We conducted a comprehensive literature review to compare our results with existing theories in the literature. For verification, we matched the published experimental data and assigned the results to existing technology, such as conventional water injection and injection in the weak water-wet reservoir, ... etc. Finally, this method will help our understanding of the dominant recovery mechanisms in fractured porous media.

From the simulation results, we observed that permeability contrast, viscosity contrast, and injection rate control the viscous force in the reservoir. Also, fracture aperture has a significant impact on viscous forces since it is related to permeability via the cubic law. The capillary contrast between fracture and matrix governs the water-oil interface position in fracture-matrix connection. When capillary forces dominate over viscous forces, it can slow down the water breakthrough and increase oil gain, which is known as imbibition. However, when gravitational forces increase, they will negatively impact capillary forces. As a result, oil recovery will be mainly driven by viscous forces. Also, since the ratio of competing forces varies at different positions in the reservoir, we introduced a new upscaling technique to assess the dominant recovery mechanism at certain areas of interest in a reservoir.

This work aims to improve the understanding of several possible recovery mechanisms scenarios in fractured porous media based on the fundamental forces acting in a reservoir. Also, we present an upscaling technique of these mechanisms for field-scale application.

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MS12 / 237

Study on the distribution characteristics of in-situ stress of Chang 7 reservoir in Ordos Basin

Authors: Hou bing¹; Zuo luo²; Kou xiaoxuan¹; Zhang yu¹; Zhuang li³

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In the Ordos Basin, the Chang 7 shale oil reservoir in northern Shaanxi is superimposed with multiple lithologies in the longitudinal direction. There are differences in the interlayer stress of the thin sand-shale-shale interbeds. The internal stresses in small layers are changeable, resulting in high hydraulic fractures and short extension distances. The effective reconstruction volume did not meet expectations. Based on the Kessel in-situ stress test to test the in-situ stress of key layers, finely interpret the in-situ stress logging results of a single well to obtain the distribution of longitudinal multi-interbed and different lithological in-situ stress, aiming at the characteristics of the 3 small reservoirs in the Chang 7 member of the Xin'anbian area in northern Shaanxi. Based on the geological, structural, and sedimentary characteristics of the block, a three-dimensional in-situ stress regional model of complex lithological reservoirs based on fine geological bodies was established, which simulated the distribution of in-situ stress in the sand-soil-shale interbedded lithology region, and mastered the geological stress. The difference between horizontal and vertical stress field space. The calculation results show that the overall three-dimensional stress of the block is $\sigma_V > \sigma_H > \sigma_h$, the maximum principal stress range between layers in the longitudinal direction is 35~58 MPa, the minimum principal stress range is 28~54 MPa, and the horizontal stress difference range is 6~8 MPa, the stress value of the sandstone in the lateral upper layer is greater than the stress value of the shale and the stress value of the mudstone. Through the analysis of the in-situ stress distribution of the different interlayer depth and bedding lithology, it provides parameter guidance for the fracture height design of the complex lithological reservoir layer of the Chang 7 member in northern Shaanxi, Ordos Basin.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

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Online

MS01 / 238

Understanding induced seismicity for a safe use of porous media to reach carbon neutrality: the case of the Underground Gas Storage of Castor, Spain

Author: Víctor Vilarrasa¹

Co-authors: Silvia De Simone²; Jesus Carrera¹; Antonio Villaseñor¹

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The use of the subsurface for low-carbon energy-related activities, such as geothermal energy, geologic carbon storage and underground energy storage, will intensify during the transition towards a carbon-neutral society. Such intensification requires managing induced seismicity to avoid the cancellation of projects like the Underground Gas Storage (UGS) project of Castor, Spain, which implied a cost of 4.73 billion euros of public money. Castor has been the case with the largest induced earthquakes among the more than 640 UGS facilities around the world, with three earthquakes with magnitude around 4. The typically assumed triggering mechanism of pore pressure buildup was not the cause of the induced seismicity at Castor because the focal depth is located several kilometers below the storage formation and because the earthquakes were induced 20 days after the stop of injection, when pore pressure buildup had already attenuated. Instead, we have found that buoyancy of the gas, which has a permanent effect, aseismically destabilized the Amposta fault, which bounds the storage formation. The progressive accumulation of aseismic slip at the Amposta fault caused an increasing stress transfer that eventually destabilized a critically stressed fault located in the crystalline basement. Then, several patches of this deep fault were reactivated due to shear slip stress transfer and slip-driven pore pressure changes, inducing the sequence of felt earthquakes. We conclude that a thorough characterization of the site would have avoided the large earthquakes because a detailed analysis of the initially performed surveys would have served to highlight the high risk of inducing seismicity at Castor.

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Vilarrasa, V., De Simone, S., Carrera, J. and Villaseñor, A., 2021. Unravelling the causes of the seismicity induced by underground gas storage at Castor, Spain. *Geophysical Research Letters*, 48, e2020GL092038

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Participation:

Online

MS23 / 240

Characterising flow and transport in fractured geological media: 20 years later

Author: Sebastian Geiger^{None}

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In 2002, Brian published his seminal review paper that concisely and elegantly summarises the key challenges and advancements in the characterisation of flow and transport processes in fractured geological formations [1]. 20 years later, much progress has been made but many of the challenges that Brian outlined still remain, most notably how to model flow and transport processes effectively, efficiently, and robustly in practical applications where we need to represent fracture networks that “do not possess any homogenization scale, so that, strictly speaking (at least in mathematical terms), a representative elementary volume (REV) cannot be defined.”

This presentation, inspired by Brian’s many contributions in the field, will review some of the recent ideas and concepts that allow us to design improved hierarchical fracture models that represent multi-scale fracture networks in reservoir models, as well as the interactions between fractures and rock matrix, with greater accuracy while keeping computational challenges at bay. Furthermore, the emergence of machine learning to decipher flow behaviours in fractured geological formations and link them to the key characteristics of the fracture network will be discussed.

The endeavour to continue improving our understanding of flow and transport processes in fractured geological formations is instrumental to providing our society with secure and affordable access to energy (e.g. geothermal) and freshwater resources as well as to sequestering waste products such as CO₂ and radioactive waste securely in the subsurface - key points that Brian has made 20 years ago.

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MS09 / 241

Modelling liquid transport in PEM fuel cells: The effects of compressive stress

Author: Yanyao Bao¹

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The performance of polymer electrolyte membrane fuel cells (PEMFCs) is greatly influenced by the residual water content generated during the cell operation, and a comprehensive understanding of water management is critical for elevating the efficiency of PEMFCs [1]. The liquid accumulation at the interfacial gaps between PEMFC components account for a substantial part for water flooding which impedes subsequent electrochemical reaction of hydrogen and oxygen [2]. In this study, the liquid transport and accumulation at the interfacial region of micro-porous layer (MPL) and catalyst layer (CL) of PEMFC is investigated numerically. The contacting membrane layers are featured with surface roughness and pore size distribution that are comparable to real MPL and CL properties. Different levels of compressive stress derived from fuel cell assembly pressure are applied on the MPL/CL components resulting in different interfacial morphology, and the corresponding influences on the liquid accumulation at the interface as well as within MPL/CL components is analysed. The effects of compression on the pore size distribution are further incorporated to reflect the change of MPL/CL pore structure. The wettability of MPL/CL material is adjusted to simulate the contact angle variation resulted from different working temperature during the start-up phase of cell operation. Finally, the liquid transport and accumulation at the MPL/CL interface are compared with available experimental observations, and a numerical framework is proposed for optimising compressive stress that best facilitates the water management. This study provides a parametric assessment on identifying the appropriate compressive stress for cell assembling and design of PEMFCs.

Keywords: PEMFC; contact mechanics; surface roughness; pore size distribution; lattice Boltzmann method.

References

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MS07 / 242

Coupled flow in porous media with thin inclusions: preconditioning based on rational approximations of the fractional interface operators

Author: Svetozar Margenov¹

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Flow in porous media with inclusions is a determining processes within natural and artificial materials [6]. One important feature of thin inclusions is that they represent fractures. In fractured formations, the equations are strongly coupled, so the accurate and robust numerical methods are of great importance.

Flow in fractured porous media is a typical example of non-local process, thus naturally connected with fractional diffusion. Here we use some recent advances in numerical methods for fractional diffusion problems [2]. It may be surprising that the matrix-vector multiplication is a more difficult task than solving systems with \mathbb{A}^α .

The presented results are in the spirit of multiphysics or multiscale problems which involve coupling at interfaces that are manifolds of lower dimensions, thus giving rise to interface conditions formulated in fractional Sobolev spaces [1]. Aimed at large-scale applications we focus on the iterative solution of the arising linear systems. Two examples are considered.

E1: Let $\Omega = \Omega_S \cup \Omega_D \subset \mathbb{R}^2$, $\Omega_S \cap \Omega_D = \emptyset$. The exchange through the interface Γ between a Stokes flow in Ω_S and a Darcy flow in Ω_D is modeled. The preconditioner $C_{D-S} = \text{Diag}(-\Delta + D\mathcal{T}_t^T\mathcal{T}_t, K^{-1}(-\nabla\nabla \cdot + \mathcal{I}), \mathcal{I}, K\mathcal{I}, \mathcal{T}_t$ is a tangential trace operator, provides an optimal condition number estimate.

E2: Let $\Omega \subset \mathbb{R}^3$ be a bounded domain, while Γ represents a 1D manifold inside Ω . The trace coupled problem is studied. We consider the preconditioner $C_{3-1} = \text{Diag}(-\Delta + I, -\Delta + I, -\Delta^{-0.14})$. The choice of fractional power is analyzed in [KLMZ-21], observing that $\alpha \in [-0.145, -0.1]$ yields bounded condition numbers. The additional stability analysis has led to the preferred value $\alpha = -0.14$.

The question is how to implement the nonlocal blocks of C_{D-S} and C_{3-1} . Until recently, this was an open problem in the case of general geometry of Γ . In 2019, multigrid methods for discrete fractional Sobolev spaces were proposed in [1]. The constructed smoother involves $(\nu + 1) \times (\nu + 1)$ blocks $\mathbb{A}_{\ell,\nu}^{-\alpha}$, $\alpha \in (-1, 1)$, where ν is the graph-degree of the mesh node ℓ .

As an alternative, we propose to use the best uniform rational approximation (BURA) of $\mathbb{A}^{-\alpha}$, $\alpha \in (0, 1)$. As correctly noted in [1], a disadvantage of the method introduced in 2018 in [4] is that its accuracy depends on the condition number of \mathbb{A} . This drawback was completely overcome in [3]. Thus, the currently used BURA method is defined as $\mathbb{A}^{-\alpha} \approx \lambda_{1,h}^{-\alpha} r_{\alpha,k}(\lambda_{1,h}\mathbb{A}^{-1})$, $r_{\alpha,k}$ is the best uniform rational approximation of degree k of z^α on $[0, 1]$. In the case of negative degree $\alpha \in (-1, 0)$, the approximation $\mathbb{A}^{-\alpha} \approx \lambda_{1,h}^{-\beta} r_{\beta,k}(\lambda_{1,h}\mathbb{A}^{-1})$, $\beta = 1 + \alpha \in (0, 1)$, is applied.

The obtained results show that presumably small degrees of BURA (say, $k = 2, 3, 4$) are enough to get a relative condition number which is competitive to the multigrid preconditioner. Among the advantages of the BURA based preconditioners are that: (i) the condition number estimates are independent of the geometry of the interface Γ ; (ii) the new approach is applicable to coupled PDEs defined on domains and interfaces with different dimensionality; (iii) no regularity assumptions are required.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS10 / 243

Enhancement of in-situ terahertz liquid front tracking technique in porous media using a novel experimental setup and associated analysis tool

Author: Jongmin Lee¹

Co-authors: Daniel J. Goodwin²; Ranjit M. Dhenge²; Gabriele Bano²; Axel Zeitler¹

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Terahertz pulsed imaging (TPI) technology can be used to track a liquid front in-situ during the imbibition of porous media such as pharmaceutical tablets and ceramic catalyst supports [1,2]. The method can resolve relatively fast transport phenomena with a time resolution of less than 100 ms. It can also be used as a non-contact and non-invasive quality inspection method to estimate the porosities of dry samples [3] with potential applications, in particular, in the pharmaceutical industry.

One of the applications of interest is the investigation of the correlation between the liquid uptake kinetics in pharmaceutical solid dosage forms and the resultant disintegration process. In the previously used experimental setups, the imbibition process commenced by bringing water in contact with the bottom surface of the sample using a flow cell. Given the design of the flow cell the deaggregated agglomerates largely remained within a certain boundary from the tablet matrix and liquid ingress was restricted to the bottom surface and not from the sides, which may affect the kinetics of the liquid uptake compared to the typical disintegration process in dissolution medium where aggregates can freely erode in all directions during liquid ingress into the tablet matrix.

In this study, we present a novel experimental setup for in-situ terahertz liquid tracking in pharmaceutical tablets. This setup adopts a bespoke sample holder that exposes over half of the tablet surface to the liquid medium. The new method exposes the tablet samples to its sides as well as its bottom face so that radial as well as axial liquid transport can take place thus removing some of

the constraints in the experimental boundary conditions. We also introduce a novel terahertz signal analysis tool that compares terahertz time-domain signals each other after applying a digital signal filter to identify and extract the subtle traces of the water front in the tablet which allows us for the first time, without the need for any hardware modifications, to investigate liquid transport in tablets up to 5.5 mm thick, compared to measurements that were previously limited to roughly half the thickness.

The observations of this study for complex formulations of drug products suggest two-phase kinetics with a linear function for the predominant phase whereas prior research on less complex formulations was able to rationalise the liquid transport using a single power-law function based on the concept of Darcy flow in porous media. The aim of our future research will be to explore the complexity of typical pharmaceutical tablet formulations on the liquid transport and particle swelling processes that result in the disintegration of the dosage form and to model the process based on physical understanding in order to develop predictive capabilities to aid rational dosage form and process design.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 244

The influence of Wettability and flow rates on two-phase fluid displacement in porous media: Pore scale experimental visualization and numerical simulations

Author: Peixing Xu¹

Co-authors: nong kang ; Congjiao Xie ; Shuangmei Zou

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Multiphase flow in porous media widely exists in many natural and industrial processes, such as enhanced oil/gas recovery, geological CO₂ sequestration,. Wettability is one of the key factors that affects multiphase flow in porous media. In this study, by means of high-resolution imaging in microfluidic flow cells patterned with random pore network, we performed displacement processes

that occur during water flooding by using a microfluidic approach under controlled wettability conditions and recorded how wettability and flow rates influences the resulting displacement patterns. We further use the LBM method to numerically investigate the influence of wettability and flow rates on two-phase flow under various ranges of flowrates and wettability conditions. By using LBM simulation, the speed model adopts the D2Q9 model, and the collision item adopts the LBGK model. The pseudopotential model (Shan-Chen model) is used to describe the interaction force between particles. The boundary conditions are as consistent as possible with the experimental conditions. The entrance and exit adopt the Zou-He boundary, and the pore-solid interface adopts a half-step rebound impermeable boundary. Then numerical simulations by using Lattice Boltzmann Method (LBM) are firstly verified based on same experimental conditions and then extend to a wide range of flow rates and wettability conditions. Simulated results show LBM simulations are in good agreement with the experimental results. With the invading fluid being more wetting to the medium, fluid interface area is increased with slow displacement front velocity. Thus, the trapping of non-wetting and the breakthrough time of invading fluid are suppressed, resulting higher displacement efficiency. In addition, increased flow rate makes fluid invasion stable for all contact angles, indicating that the impact of wettability on the fluid invasion processes becomes negligible. Our work extends the classic phase diagram, explores the controls of wettability and flow rate on the displacement pattern at pore scale and provide a fundamental understanding on macroscopic multiphase flow behaviors.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS09 / 246

Efficient permeability prediction of real digital rock based on Darcy's law

Authors: Qinzhuo Liao¹; Jun Li²; Gang Lei³; Weiqing Chen²; Xu Liu²; Shirish Patil²

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² *King Fahd University of Petroleum and Minerals*

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Permeability of digital rock can be predicted by the pore-scale simulations based on the Navier-Stokes equation for rock characterization. Besides the complicated pore geometry, the main challenge is the large number of spatial grids/voxels needed to make the digital rock representative. The computational cost can thus be very high, even using the efficient Lattice Boltzmann method that has almost linear scalability for parallel computation. In this study, a novel method is proposed to simplify the 3D pore-scale simulation to multiple decoupled 2D ones based on the Navier-Stokes equation. Each 2D simulation provides the velocity distribution over a slice. The obtained velocity at each voxel is then used to assign a local permeability distribution on the corresponding slice. The interaction between neighboring slices neglected in the simplification is then modeled by constructing the 3D local permeability distribution using the 2D ones, from which the effective block permeability of the original 3D digital rock can be computed via solving the Darcy equation. By this decoupled simulation approach, the expensive simulation based on the Navier-Stokes equation is conducted only on 2D domains, and the final 3D simulation of Darcy equation using the finite difference method is very cheap. A large number of 3D digital rocks of both sandstone and carbonate are tested using the proposed approach and the computed permeabilities are all in good agreement with those of direct 3D pore-scale simulations of using the Lattice Boltzmann method. The computational cost is found to be significantly (about an order of magnitude) reduced. The proposed method will be useful for assessing large-scale digital rocks, where the cost of direct 3D pore-scale simulation becomes prohibitive, if not impossible.

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Time Block A (09:00-12:00 CET)

Participation:

Online

MS02 / 247

Modeling evaporation from leaves

Author: Sina Ackermann¹

Co-author: Rainer Helmig¹

¹ *University of Stuttgart*

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Current predictions with respect to the global climate suggest that severe weather events will occur more often and more intense than in recent years. One example for such extreme events are heat waves, which have a significant impact on agriculture and daily life in urban areas. With evaporative cooling, plants can help to reduce the heat in big cities during such periods.

In the scope of our project, we model leaves as porous media to describe the process of evapotranspiration. The rate of evaporation depends on the leaf structure, flow and transport processes within the leaf, as well as environmental conditions such as solar radiation and wind speed. To capture the respective effects on different spatial scales, we model an individual leaf on both the pore-scale and the REV-scale. In a first step, we apply a pore-network model [1] to discretely describe the leaf structure. Especially challenging is the accurate representation of the small openings on the lower surface (stomata), which regulate the gas exchange between the leaf and the atmosphere [2]. In a second step, we use the information obtained with the pore-network model to parameterize an REV-scale model such that larger computational domains can be handled.

Collaborations with experimental scientists yield the required data to adapt the simulation to realistic scenarios. By comparing simulation results with measured data, we aim at improving the accuracy of our model.

So far, only the gas exchange between leaf and atmosphere is considered. Under certain conditions, liquid drops form on the stomata and influence the exchange processes. In the future, we will extend our model to take these drops into account.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS21 / 248

The role of birefringent strands on the stability of viscoelastic flows through porous media

Authors: Omar Mokhtari¹; Jean-Claude Latché²; Michel Quintard³; Yohan Davit³

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² *Institut de Radioprotection et de Sûreté Nucléaire (IRSN), France*

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We consider the flow of dilute polymer solution through model porous media consisting of an array of cylinders. Our recent results (Mokhtari et al. 2022) demonstrate that birefringent strands are key in understanding viscoelastic effects in such systems. These strands act as a distribution of tangential forces that reduce the velocity in their vicinity and induce a complete reorganization of the flow on large scales within porous structures.

While being simple, arrays of cylinders have proven useful in capturing many important mechanisms inherent to viscoelastic flows past obstacles and have recently attracted a lot of attention (Walkama et al. 2020; Haward et al. 2021). Walkama et al. (2020) showed that introducing disorder in a staggered geometry locally reduces polymer stretching and enhances flow stability with a delay in transition to chaos. Haward et al. (2021) showed a very different arrangement of the strands in staggered and aligned geometries and demonstrated instead that stagnation points control this transition, independently from the disorder. This raises the question of the role of the strands in the transition to chaos: Could it thus be that birefringent strands also control the transition to chaos in porous structures?

Here we use numerical simulations to study the role of the birefringent strands on the flow stability through crystalline structures of cylinders. Our approach combines a recently developed numerical scheme for viscoelastic models of dilute polymer solutions (Mokhtari et al. 2021) with high performance computing. We find that the strands yield an angle between the direction of the imposed pressure gradient and the average flow, favouring certain flow directions. This causes a hysteresis of the flow angle and multistability, which may be fundamental to understand experimental results and transition to chaos.

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Haward, S. J., Hopkins, C. C. & Shen, A. Q. 2021 Stagnation points control chaotic fluctuations in viscoelastic porous media flow. *Proceedings of the National Academy of Sciences* 118 (38).

Mokhtari, O., Latché, J.-C., Quintard, M. & Davit, Y., 2022 Birefringent strands drive the flow of viscoelastic fluids through porous media (in preparation).

Mokhtari, O., Davit, Y., Latché, J.-C. & Quintard, M. 2021 A staggered projection scheme for viscoelastic flows. <https://hal.archives-ouvertes.fr/hal-03400727>

Walkama, D. M., Waisbord, N. & Guasto, J. S. 2020 Disorder suppresses chaos in viscoelastic flows. *Physical Review Letters* 124 (16), 164501.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

Poster / 249

Complex Fluids –Thin Porous Materials Interactions revealed via Electrical Impedance Spectroscopy (EIS)

Authors: Nicolae Tomozeiu¹; Hélder Marques Salvador²; Hamid Mansouri²¹ *R&D Canon Production Printing*² *R&D, Canon Production Printing***Corresponding Authors:** helder.marquessalvador@cpp.canon, nicolae.tomozeiu@cpp.canon, hamid.mansouri@cpp.canon

A brief introduction of the EIS technique, precedes the presentation of the two experimental setups, with planar and respectively cylindrical electrodes. Home made devices have been employed to study material properties (e.g. dielectric constants) of complex materials as well as physical phenomena as water evaporation of aqueous mixtures, complex liquid transport into porous paper, latex film formation. Each experimental setup was dedicated to a specific process; regarding the dielectric constant measurements, this was possible to be made with both setups and a comparison of the outputs is made.

EIS was used for:

- i) water evaporation from liquid mixtures;
- ii) liquid penetration into porous paper considering the same liquid and different papers (e.g. thickness), as well the same paper and various liquids;
- iii) latex film formation –revealing the structure of the solid formed film, have been tackled via the EIS method.

The dynamics of the physical processes (e.g. evaporation rate, liquid absorption rate, phases in latex film formation) have been studied having time as a parameter. Theoretical models and computational simulations were used to analyze the experimental data and to improve our understanding.

The EIS results have been confirmed by HRSEM measurements on post-mortem samples. We consider the EIS as a valuable tool in these studies; however besides its advantages, we will discuss the limitations of the method, too.

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Time Block A (09:00-12:00 CET)

Participation:

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MS11 / 250

Flow-direction dependence of upscaled capillary pressure-saturation curve

Author: Javad Shokri¹

Co-authors: Omar Emmanuel Godinez Brizuela²; Hamidreza Erfani³; Yongqiang Chen¹; Masoud Babaei¹; Brian Berkowitz⁴; Vahid Niasar¹

¹ *University of Manchester*

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Immiscible two-phase flow is widely present in natural and synthetic processes. The flow behaviour of two fluids is governed by constitutive relations, relative permeability and capillary pressure. These empirical relations are often influenced by the dynamic of the process and the characteristics of porous media such as heterogeneity. The effect of the non-equilibrium condition on the capillary pressure-saturation behaviour has been investigated and shown that the dynamic capillary pressure is different from the one measure under the equilibrium condition. Moreover, recent studies showed that the presence of micro-heterogeneity in porous media changed the trend and the extent of the capillary pressure-saturation compared to the background porous medium. Although, the magnitude and the trend of the capillary pressure-saturation curves remained almost unchanged irrespective of the direction of the fluid flow in these studies.

The present work investigates the effect of heterogeneity interface on saturation distribution and capillary pressure-saturation behaviour in a micromodel study. The micro model is made up of two sections called fine and coarse sections. Microfluidic experiments and optical imaging and analyses were used to calculate capillary pressure and saturation of fluids. Drainage experiments were conducted at four different flow rates with a wide range of capillary numbers in both directions (i.e. fine to coarse and coarse to fine). The saturation of each phase was measured using image analysis. Moreover, the capillary pressure at the pore scale was calculated by estimating the curvature of each fluid-fluid interface. Then using the fluid-fluid interfacial surface area, the averaged capillary pressure in the coarse section, fine section and the entire micromodel, was calculated.

Results show that the averaged dynamic capillary pressure-saturation curve with the presence of a heterogeneity interface does not follow the monotonic shape of the conventional capillary pressure curve, measured under equilibrium conditions. Moreover, the results demonstrate a non-monotonic relationship between the remaining wetting phase saturation and the capillary number. It is mainly due to the competition between the capillary and viscous forces during the transition from capillary fingering to viscous fingering regime. The results reveal that considering the flow direction with respect to the heterogeneity interface, can lead to a better prediction of the upscaled capillary pressure-saturation relation and the remaining wetting phase saturation.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 251

3D reactive transport modeling of laboratory-scale CO₂ injection in limestone leading to wormhole formation

Authors: Atefeh Vafaie¹; Jordi Cama²; Josep M Soler²

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Carbon capture and storage in deep saline aquifers is a promising approach to mitigate global warming as a first-rate challenge of the world today. The injected CO₂ dissolves in brine, making it acidified and promoting geochemical interactions with the rock. Such interactions likely alter CO₂ trapping and transport mechanisms, which are directly linked with the carbon mitigation capacity of this technology. In this study, we combine laboratory experiments with 3D reactive transport simulations to better understand geochemical controls on the evolution of carbonate rock structure. A 28-day percolation experiment was conducted on a Pont Du Gard limestone specimen (a cylindrical core of 2.5 cm in diameter and 4.4 cm long) with CO₂-saturated water at an injection pressure and temperature of 100 bar and 60°C, respectively, replicating subsurface conditions. We integrate fluid chemistry analyses, X-ray imaging, porosity, and permeability measurements to assess the temporal evolution of rock structure, porosity, and permeability in the altering specimen throughout the injection. The employed monitoring procedures consistently point to a porosity enhancement of 9.6% and permeability increase of 3 orders of magnitude. X-ray images depict that the porosity enhancement coincides with the formation of a large wormhole inside the specimen, most likely developed in response to the specimen's natural heterogeneity. A three-dimensional permeability map was built using imaging data to capture the effect of rock heterogeneity on the dynamics of wormhole formation and the evolution of the fluid flow. Preliminary modeling results show that our model can reproduce the total dissolved mineral mass and porosity enhancement of the reacted specimen with high accuracy (2-5% error). The porosity-permeability relationship and mineral surface area are found to impact model predictions. Thus, we calibrate the model against these parameters to precisely track wormhole evolution inside the specimen (i.e., structure and orientation). Sensitivity analyses conducted using the calibrated model reveal the dependency of the dissolution patterns on the injection flow rate to a large extent. Combined experimental and simulation results provide insights into wormhole formation and evolution that will be important during field injection.

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Time Block B (14:00-17:00 CET)

Participation:

Online

MS11 / 252

Salt crystallization at a hydrophobic-hydrophilic interface in quasi 2D layered porous material.

Authors: Rozeline Wijnhorst¹; Leo Pel²; Noushine Shahidzadeh¹

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Corresponding Authors: n.shahidzadeh@uva.nl, l.pel@tue.nl, r.j.wijnhorst@uva.nl

Understanding the ability of salts to crystallize at the interface between two porous media with different material properties is of paramount importance to understand the decay mechanisms involving salt crystallization in composite materials. This problem is that is very relevant to art conservation practice and civil engineering problems.

Over the past decades, much has been learned about the effects of salt crystallization within a single type of porous material and on its surface. In order to uncover the more complex but realistic situation of layered porous materials, the European JPI-CRYSTINART project was initiated in 2020. We present our results on salt crystallization on the presence of an interface between hydrophilic and hydrophobic porous media during evaporation of aqueous salt solutions. For this purpose, we designed artificial 2D single layered porous media for studying the fundamentals of crystallization at the interface of two porous materials with different wettability properties at the microscale. The hydrophobic layer is created by a targeted silanization of only the top few layers of a porous medium consisting of sintered microscopic glass beads. Our manufacturing method is also a versatile tool for creating monomodal or multimodal pore size 2D porous media and allows to quantitatively study multiphase flows using different microscopy techniques. These data can subsequently serve to implement numerical models that can be extended to the 3D situation where visualization is experimentally difficult.

In the experiments, the drying kinetics and dynamics of salt precipitation (NaCl) are investigated in real-time by simultaneously using optical microscopy with automated image analysis and mass change registration during evaporation. The drying regimes identified during the evaporation of the composite material are shown to be different than the drying behaviour of a purely hydrophilic or hydrophobic porous medium. In the early stages of evaporation, a drying front penetrates into the sample into the hydrophobic upper layer without any salt precipitation. Subsequently, the air progressively penetrates into the sample via the formation of steady or transient continuous air networks in the larger pores resulting in a rather homogeneous drying of the hydrophilic region up to the interface region. Consequently, the precipitation of large crystals starts on the hydrophilic side close to the interface region; this can be viewed as subflorescence. Subsequently, the salt is observed surprisingly to slowly creep, as tiny crystals into the hydrophobic region; We show that such dynamics of crystallization with a gradient of crystal size results in the interruption of the complete drying of the whole material and to entrapped liquid pockets within the hydrophilic region.

The existence of an interface within a layered composite porous material with different wettability properties plays a major role in both the drying and crystallization dynamics of a salt solution. Understanding these principles could help to understand the materials dynamic due to crystallization of salts at the interface and propose alternative solution to prevent salt damage. As crystallization at the interface region is a major issue in the delamination and damage of ceramics, tiles and mural paintings, this is an important observation.

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References:

Shahidzadeh-Bonn, N., Azouni, A., & Coussot, P. (2007). Effect of wetting properties on the kinetics of drying of porous media. *Journal of physics: condensed matter*, 19(11), 112101.
Lieberink, R. W., Naillon, A., Bonn, D., Prat, M., & Shahidzadeh, N. (2018). Single layer porous media with entrapped minerals for microscale studies of multiphase flow. *Lab on a Chip*, 18(7), 1094-1104.
Qazi, M. J., Salim, H., Doorman, C. A. W., Jambon-Puillet, E., & Shahidzadeh, N. (2019). Salt creeping as a self-amplifying crystallization process. *Science advances*, 5(12), eaax1853.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS23 / 256

Structure induced vortices control anomalous dispersion in porous media

Authors: Ankur Bordoloi¹; David Scheidweiler¹; Marco Dentz²; Marco Abbarchi³; Mohammed Bouabdellaoui³; Pietro de Anna¹

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Natural porous systems, such as soil, membranes, and biological tissues comprise disordered structures characterized by dead-end pores connected to a network of percolating channels. The release and dispersion of particles, solutes, and microorganisms from such features is key for a broad range of environmental and medical applications including soil remediation, drug delivery and filtration. Yet, the role of microscopic structure and flow for the dispersion of particles and solutes in such disordered systems has been only poorly understood, in part due to the stagnant and opaque nature of these microscopic systems. Here, we use a microfluidic model system that features a pore structure characterized by dead-ends to determine how particles are transported, retained and dispersed. We observe strong tailing of arrival time distributions at the outlet of the medium characterized by power-law decay with an exponent of 2/3. Using numerical simulations and an analytical model, we link this behavior to particles initially located within dead-end pores, and explain the tailing exponent with a hopping and rolling mechanism along the streamlines inside vortices within dead-end pores. These dynamics are quantified by a stochastic model that predicts the full evolution of arrival times. Our results demonstrate how microscopic flow structures can impact macroscopic particle transport.

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Participation:

Online

MS11 / 257

Novel Pore Scale Visualization during CO₂ Injection into CH₄ Hydrate Saturated Porous Media

Author: Jyoti Shanker Pandey¹

Co-authors: Ørjan Strand²; Nicolas von Solms³; Geir Ersland⁴; Stian Almenningen⁵

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CO₂ capture in sediments through CO₂-rich gas injection into methane gas hydrate reservoir is a recently proposed technology for methane recovery and simultaneously storing CO₂ in deposits. CO₂ capture and storage in CH₄ hydrate formations located at low-temperature, high-pressure conditions, is an attractive proposition as technical and economic costs are lower and it is safer option to store as hydrates, since it offer confined storage, presence of elevated pore pressure, very low CO₂ leakage rates and long-term storage potential. The current literature lacks visualization studies that could improve our understanding of fluid migration and hydrate rearrangement during CO₂ injection into CH₄ hydrate. This experimental study is the first to provide pore-scale visualization (using high-pressure micromodel) when CO₂ is injected into CH₄ hydrates. Our study shows that the CO₂ richness in the invading liquid phase controls the CO₂ injectivity and the redistribution of the hydrates. The CO₂ content in the liquid phase is controlled by the CO₂ injection scheme. The resulting CH₄/CO₂ mixed hydrates were stepwise depressurized to visualize the hydrate reformation below the CH₄ hydrate phase that would improve the recovery of CH₄ while reforming the CO₂ hydrate, thus keeping the hydrate mass intact. This research would help improve our understanding of an effective CO₂ injection scheme for improved CH₄ recovery and CO₂ storage.

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Participation:

Online

MS09 / 259

An improved network extraction algorithm by tracking size variation of throats

Author: Yang Liu^{None}

Co-authors: Wenbo Gong ; Moran Wang

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Pore-network model is a pore-scale modeling method, in which the complex pore space is represented by idealized geometries [1]. With the advantage of high computation efficiency and easy up-scaling, pore-network model has been widely used to simulate immiscible fluid displacement, reactive transport, phase change and heat transfer, and gas-water transport in proton exchange membrane. Pore-network model has become a powerful tool for simulation of millions of pores which is computationally unacceptable for direct numerical simulation.

Network construction, local transport rules, and calculation of transport properties constitute the main parts of pore-network models. In network construction, the void space is simplified into pore bodies and pore throats that are endowed with different local transport rules. This step is the foundation to simulate the physical and chemical behaviors of fluid in porous media. With the explosion in imaging capacity, researchers are highly motivated to extract pore-networks from the voxel-based representation of porous medium. Based on three-dimensional (3D) images, there are several types of algorithms for network construction, such as medial axis algorithm, maximal ball algorithm [2], grain-based algorithm, and watershed algorithm. Despite decades of efforts by many scholars, the lack of a specific definition for what constitutes pores and throats in void space remains a challenge. The ambiguous definition of pores and throats causes the inappropriate pore space segmentation, and further leads to inaccurate geometrical information. Some of this information impacts the simulation results significantly. For example, incorrect throat length causes great errors in permeability calculation in pore-network models.

In this study, we modify the SNOW algorithm [3] to distinguish pores and throats accurately. The throat voxels are determined by tracking size variation from the interface of two neighboring 'regions' to both sides. It obtains accurate descriptions of throats including throat length, shape variation, and throat volume. Compared with the experimental data or results of direct numerical simulations, the improved pore-networks predict more accurate permeability than that reported by other scholars.

Keywords: pore-network model; extraction method; watershed algorithm; pore-throat segmentation.

Reference

- [1] Fatt, I. (1956). The network model of porous media. Transactions of the AIME, 207(01), 144-181.
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- [3] Gostick, J. T. (2017). Versatile and efficient pore network extraction method using marker-based watershed segmentation. Physical Review E, 96(2), 023307.

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Participation:

Online

MS12 / 260

Multimodal geo-dynamic flow characterization in heterogeneous carbonate reservoir: An integrated approach linking static and dynamic behavior

Authors: Jiaheng Chen¹; Liping Yi¹; Liang Wei¹; Yongjun Wang¹; Chaozhong Ning¹

Co-author: Guangya Zhu¹

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Towards bioclastic limestone reservoirs, deposition and diagenesis are often inherently complicated, resulting in extremely strong reservoir heterogeneity, which significantly affect the flow mode and field development by waterflooding. A lot efforts have been put for the study of heterogeneity from the aspect of geology and reservoir separately. Geologists usually struggled on the impact of sedimentation and diagenesis on rock type while reservoir engineers focused on relative permeability features/classification from special core analysis. However, few papers investigate multimodal flows and their influence on development by integrating geological attributes and petrophysical properties while linking with dynamic behavior. This paper presents a multidisciplinary study about the geo-dynamic flow characterization of carbonate reservoir, their corresponding mechanism, application in simulation and potential impact on waterflooding.

For establishment of geo-dynamic analysis, an integrated iterative approach involving multiscale and multiphase adjustment was created. The method rather emphasizes on the interaction among rock formation environment, diagenetic mechanism and the association between rock and fluid. Image analysis alongside thin section description were used to qualitatively group samples of the same genetic origin. Rock types were then distinguished through incorporating geological controls during the pore evolution and petrophysical group into pore networks definition. This workflow differs from many studies by ensuring the dynamic parameters, including water-free coefficient, water-front saturation and shape factor of fraction flow, are involved to define the flow characterization of rock type. Multi-interactions and clustering analysis were finally conducted for consistency between geology and reservoir and the acquirement of geo-dynamic flow types. The above issues were addressed on a giant bioclastic limestone reservoir in Middle East.

Twelve subsurface geo-dynamic flow-types and four rock modes are summarized, and a set of seepage-pattern diagram is established. Results indicate that the heterogeneity and seepage are mainly controlled by depositional environment. The superior rock properties are usually associated with channel and shoal and the inferior rock properties are usually associated with shoal flank, lagoon and swamp. But the diversities among deposits, sedimentary process and diagenetic control usually lead

to a variety of reservoir modal types and seriously strikes the foundation flow. Consequently, superior rock properties are not always linked with higher oil displacement efficiency and the inferior rock properties are not with lower oil displacement efficiency. The outcome was applied in simulation and the output showed that compared with petrophysical-group based or facies-based flow type, the initial water cut compliance degree of well was increased from 60% to 80% and real production data matching degree of the reservoir is about 20% higher than the common method without geological parameters modified and simulation efficiency loss.

This study establishes a bridge between static and dynamic. Compared with the common method, multimodal geo-dynamic flow types are more representative with much higher accuracy, which are also beneficial for dynamic analysis in waterflooding and the forecasting issue of simulation. Furthermore, this paper can be extended to evaluate the waterflooding of other bioclastic limestone in Middle East.

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MS21 / 261

Elastic flow instabilities in 3D porous media

Authors: Christopher Browne¹; Richard Huang¹; Callie Zheng¹; Sujit Datta²

¹ Princeton University

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Corresponding Authors: cabrowne@princeton.edu, ssdatta@princeton.edu, cwzheng@princeton.edu, rbhuang@princeton.edu

Many energy, environmental, industrial, and microfluidic processes rely on the viscous flow of polymer solutions through porous media. In many cases, the macroscopic flow resistance abruptly increases above a threshold flow rate in a porous medium—but not in bulk solution. The reason why has been a puzzle for over half a century. Here, by directly visualizing the flow in a transparent three-dimensional (3D) porous medium, we demonstrate that this anomalous increase is due to the onset of an elastic instability in which the flow exhibits strong spatio-temporal fluctuations reminiscent of inertial turbulence, despite the vanishingly small Reynolds number. We find that the transition to unstable flow in each pore is continuous, arising due to the increased persistence of discrete bursts of instability above an onset flow rate; however, this onset value varies from pore to pore. Thus, unstable flow is spatially heterogeneous across the different pores of the medium, with unstable and laminar regions coexisting. Guided by these findings, we quantitatively establish that the energy dissipated by unstable pore-scale fluctuations generates the anomalous increase in flow resistance through the entire medium. Thus, by linking the onset of unstable flow at the pore scale to transport at the macroscale, our work yields generally-applicable guidelines for predicting and controlling polymer solution flows. As a demonstration of this principle, we demonstrate how

such elastic flow instabilities can be harnessed to homogenize flow and passive scalar transport in structurally heterogeneous porous media, beyond what is possible using traditional Newtonian fluids.

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References:

C. A. Browne and S. S. Datta, "Elastic turbulence generates anomalous flow resistance in porous media", *Science Advances*, 7, eabj2619 (2021). URL: <https://www.science.org/doi/10.1126/sciadv.abj2619>

Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

In person

MS13 / 263

Confined phase behavior of a CH₄-CO₂ binary system: molecular simulations, equation of state, and lattice Boltzmann method

Authors: Lingfu Liu¹; Carlos Nieto-Draghi²; Véronique Lachet³; Heidaryan Ehsan⁴; Saman Aryana¹

¹ *University of Wyoming*

² *IFP Energies nouvelles*

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Phase behavior of confined fluids may deviate significantly from that of the bulk fluid due to the fluid-walls interactions being a significant portion of all intermolecular interactions under confinement. There are recent advancements in understanding confined phase behavior of pure species, confined phase behavior of mixtures remains an understudied topic. In this work, we examine the confined phase behavior of a CH₄-CO₂ binary system by combining Monte Carlo (MC) simulations, equation of state (EOS), and the lattice Boltzmann method (LBM). First, the effects of confinement on density and phase distribution in nano-sized pores are established using Gibbs Ensemble Monte Carlo (GEMC) calculations, which produces precise results of liquid and vapor confined pressures and accounts for the modification of the phase change location. By comparing the Pxy diagrams of bulk and confined mixtures at a fixed temperature, it is observed that the Pxy diagrams shrink with reductions in pore size. Based on this observation, we extend a modified Peng-Robinson (PR) EOS that was originally developed for pure species to mixtures via a van der Waals-type mixing rule and by incorporating shifts in the critical point of CH₄-CO₂ mixtures. The resulting phase envelopes are in good agreement with the MC data. Finally, we incorporate this EOS in a multi-component LBM that uses a pseudopotential model to represent intermolecular forces. This work utilizes multiscale simulation techniques to shed light on the confined phase behavior of CH₄-CO₂ binary systems and to bridge the behavior of multi-component systems across scales.

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Online

MS05 / 264

A quantitative study of the effect of pore-scale heterogeneity on MICP in meter-long microfluidic porous media analogues

Author: Ariadni Elmaloglou¹

Co-authors: Dimitrios Terzis¹; Pietro De Anna²; Lyesse Laloui¹

¹ EPFL, Laboratory of Soil Mechanics, Lausanne, 1015, Switzerland

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Microbially-Induced Calcium Carbonate (CaCO₃) precipitation (MICP) has a great potential for soil improvement of granular soils as a more environmentally friendly alternative to traditional grouting technologies. The application of MICP in real geotechnical problems requires better engineering control of the spatiotemporal evolution of MICP. Moreover, the optimization of chemical reaction efficiency, which is defined as the percentage of injected calcium and urea that convert to calcite is necessary to avoid the waste of raw materials. In this study, we developed a setup to investigate the effect of pore-scale heterogeneity on the spatiotemporal evolution of MICP and the chemical reaction efficiency along distance from the injection point. Our novel setup combines meter long microfluidic devices of homogenous and heterogenous porous networks of same initial porosity, real-time video microscopy monitoring and pressure monitoring at the inlet and outlet. We applied the same MICP injection strategy to the two chips in triplicates; firstly, we introduced 6.7 pore volumes (PVs) of bacterial solution in the fully saturated chip with MilliQ water to achieve a uniform distribution in the whole chip. Subsequently, we introduced 6 PVs of calcifying solutions and monitored the evolution of bacterial concentration and crystal growth during the flow of the solution and 17h of no-flow conditions. A comprehensive algorithm was developed in Matlab to detect bacteria and crystals from time-lapse microscopy data at multiple positions along the meter-long trajectory. Thereby, we estimated crystal numbers and diameters and calculated the chemical reaction efficiency. We demonstrate that although the initial bacterial distribution was identical in the two chips prior to the injection of the calcium rich solutions, the average CaCO₃ mass growth rate was overall higher in the heterogeneous porous medium. We observed that the peak of the average chemical reaction efficiency over the three replicates of the heterogeneous porous medium was in the middle of the reactive trajectory. Moreover, the efficiency remained higher in the heterogeneous than the homogeneous pore network at the second half of the meter-long path. This can be attributed to the intrinsic property of the heterogeneous microfluidic to consist of zones of higher and lower velocity, with the zones of higher velocity directing the reactants further downstream in the reactive path, leading to the nucleation of higher number of crystals that created larger crystal aggregates. This trend was

different in the homogeneous microfluidic, where predominantly small single crystals were created which were not able to clog pore throats and attract more reactants, thus resulting in a lower efficiency. At the end of the injection of the calcification solution the permeability of the heterogeneous porous medium was decreased by 21.7%, while the reduction in the homogeneous porous medium was 5.7% lower.

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Participation:

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MS01 / 265

A Field-Data Based Numerical Investigation of Factors Controlling CO₂ Plume Migration in Storage Candidate Sites

Authors: Qi Shao¹; Maartje Boon²; AbdAllah Youssef³; Stephan Matthai¹; Sally Benson⁴

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Field-data-based numerical simulations of CO₂ injection and plume migration are carried out to investigate competing impacts of geo-heterogeneity, top-seal topography, and flow rate on the shape of the evolving injection plume and the ensuing CO₂ saturation distribution. The presented sensitivity analysis is performed on cylinder-shaped well-spot models, which capture property distributions and spatial correlations of the heterogeneous fluvio-deltaic sandstones in the Otway basin, Victoria, taking into account novel rate-dependent and heterogeneity-aware saturation functions derived from an analysis of thinly-bedded sandstone cores. To resolve the impact of this lithologic complexity, we use the Australian CO₂ Geo-Sequestration Simulator (ACGSS), a hybrid finite element –finite volume compositional simulator for space-time adaptive simulation.

Preliminary results indicate that the nested bedforms and other intermediate-scale geologic features determine plume spreading in models with a flat top-seal. Due to its high mobility, CO₂ displacement is unstable and confined to high-permeability streaks, leading to multi-layer plumes. Seal topography controls plume spreading in uneven models, where permeability heterogeneity still has a major impact on plume shape. Comparisons for different injection rates shows that high injection rates cause viscous and heterogeneity-induced fingering. Low injection rates lead to gravity override and buoyant rise of the plume. For closed lateral boundaries, the plume develops a more cylindrical compact shape than for constant pressure open boundaries. An asymptotic build-up of fluid pressure is

observed. Since CO₂ velocity in the nested heterogeneous rocks varies over many orders of magnitude, the novel anisotropic flow rate-dependent saturation functions operate between the capillary and viscous limits, creating significant differences in the shape of the evolving saturation front and the plume saturation as compared with standard saturation functions.

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Time Block A (09:00-12:00 CET)

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Online

Poster / 266

Numerical Investigations on the Dissolution Characteristics of CO₂ in Fractured Porous Media using Density Driven Modelling

Author: Manojkumar Gudala¹

Co-authors: Bicheng Yan²; Shuyu Sun³

¹ *Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal, 23955, Saudi Arabia*

² *King Abdullah University of Science and Technology*

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In the present work, numerical simulation experiments were performed to examine the influence of fractures on the flow of dissolved CO₂ plumes using the density driven (i.e., convective mixing) model. Porous media domain with a size of 500 m by 200 m (x-z plane) was used in the present work. The impacts of fracture aperture, fracture angle and fractures intersection on the movement of CO₂ plumes have been investigated comprehensively. Single fracture scenarios with varied inclined angles and multiple fractures with horizontal, vertical, and combination of these two were examined. We found that the fractures play a vital role by serving as superior flow pathways for water and CO₂ plumes. The distribution of CO₂-rich fingers is comparatively even at the top boundary of the computational domain without fractures, further it is extended into the fractured area. Porous media with fractures brings an active matrix-fracture mass transfer which results in rapid CO₂ dissolution. In the field-scale model, 200 fractures are randomly generated with aperture varying from 1 mm to 5 mm, and length from 5 m to 50 m. Our results demonstrate that high connectivity of fractures leads to enhancement in the dissolution of CO₂ in the water.

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MS06-B / 267

Coupling porous medium-free flow: Formation and evaporation of multiple droplets at the interface

Authors: Maziar Veyskarami¹; Rainer Helmig¹; Cynthia Michalkowski^{None}; Carina Bringedal^{None}

¹ *University of Stuttgart*

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Formation a droplet at the interface of a coupled porous medium-free flow system affects the behavior of the whole system by altering the interaction between the two domains. The droplet at the interface acts as an intermediary which not only handles the exchange between the free flow and the porous medium, but also stores mass and energy [1]. Furthermore, the droplet can experience a growth or a shrinkage in its size depending on the feed from the porous medium and the evaporation to the free flow. Such phenomena are of great importance in industrial applications such as water management in fuel cells and cooling systems and even in our daily life where the sweat droplets emerge on our skin. Thus, we developed a new concept to describe the droplet formation and accordingly derived a new set of coupling conditions for a coupled porous medium-free flow system which takes impact of multiple droplets on the whole system into account. Applying the new concept, we developed a model which is able to handle non-isothermal compositional coupled systems. The model consists of a pore network to model the porous medium [2], and Navier-Stokes equations to describe the free flow domain. Selected examples are used to discuss how the developed model enables us to capture the droplet formation and evaporation at the interface between the porous medium and the free flow.

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References:

[1] Ackermann, S., Bringedal, C., & Helmig, R. (2020). Multi-scale three-domain approach for coupling free flow and flow in porous media including droplet-related interface processes. *Journal of Computational Physics*, 109993.

[2] Weishaupt, K., Terzis, A., Zarikos, I., Yang, G., Flemisch, B., de Winter, D. A. M., & Helmig, R. (2020). A Hybrid-Dimensional Coupled Pore-Network/Free-Flow Model Including Pore-Scale Slip and Its Application to a Micromodel Experiment. *Transport in Porous Media*, 135(1), 243–270.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS16 / 268

Capillary imbibition and swelling of thin paper sheets

Authors: ruben nicasy^{None}; Henk Huinink¹; Ulrich hirn²; Carina Waldner²; Bart Erich¹; Olaf Adan¹

¹ *Eindhoven University of Technology*

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The imbibition process inside paper sheets is a complex process [1], where effects such as swelling, penetration and wetting determine the capillary uptake behavior. Understanding all these processes can give crucial information for optimizing printing inks and media. Measuring liquid penetration is still a challenging task. Most experimental techniques can measure either swelling or liquid uptake in ‘global’ manner without spatial information. Here we demonstrate that our previously introduced high-speed NMR imaging technique [2] can visualize coherently swelling and uptake inside printing paper with spatial resolution. A schematic representation of the set-up is shown in the figure (left). Liquid distributions during penetration of a microliter droplet are shown in the same figure (right). The technique was able to observe both swelling and penetration. At the beginning ($t = 0$), the paper sample lies between 0 and 90 μm . As time progresses, the fluid front can be observed to move inside the printing paper (black arrow), while the paper swells (red arrow). The corresponding swelling front (red) and penetration front (black) are depicted in the upper right figure. In this presentation we will discuss the capillary uptake as a function of systematic variations in the paper sheet properties: sizing [3] (degree of hydrophobicity) and calendaring [4] (compression of the fibers). It will be shown that the penetration rate will be largely influenced by the amount of sizing as also a retardation in the uptake behavior that was firstly observed in paper samples. On the other hand, calendaring influences the pore structure and swelling behavior during liquid uptake. Measuring the liquid profiles at this time and length scales can provide crucial information in understanding the uptake behavior inside complex swellable media by providing information of both swelling and penetration coherently.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS18 / 269

Evaluation of zero-valent iron nanoparticles (nZVI) injection tests in porous media using synchrotron X-ray computed microtomography

Authors: Daphne Silva Pino¹; Tannaz Pak²; Luiz Fernando de Lima Luz Junior³; Tiziana Tosco⁴; Reginaldo Bertolo⁵; Nathaly Lopes Archilha⁶

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² *Teesside University*

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This study aims to investigate the mobility and entrapment of zero-valent iron nanoparticles (nZVI) in porous media at a pore-scale, using synchrotron X-ray microtomography (µCT). As the dynamics of fluid flow in porous media is a fast process, benchtop CT scanners are unable to capture the details of this process, thus requiring high time resolution only made possible by synchrotron techniques [1-3].

Two sand-packed columns were analysed by µCT imaging. They were first saturated with water and subsequent injected with the nanoparticle suspension. A post water flushing was done to remove the mobile nanoparticles. Using an X-ray transparent flow cell allowed capturing a sequence of 3D images during the experiments. The column was imaged in three segments by moving the µCT stage in the vertical direction, helping to preserve image resolution whilst analysing a relatively large sample (1 cm tall, 0.29 cm diameter), and thus to investigate nanoparticle mobility along the entire column length at each experiment step. Each segment image has temporal resolution of 6 minutes, and spatial resolution of 1024³ voxels with 3.28 µm side.

Image processing includes filtering, segmentation and analysis regarding the degree of nZVI mobility in the different samples, and the calculation of flow properties (e.g. permeability) based on the images collected before and after nZVI injections. Some of the challenges encountered during segmentation were related to ring artifacts, particularly in the centre of the image, and to less concentrated portions of the nZVI suspension, which presented a similar texture and greyscale when compared to some of the sand grains.

Label analysis has shown that grain size distribution is quite similar between samples, despite one of the samples having a few bigger grains. Nonetheless, their total porosity is very similar, with high values compatible with unconsolidated sand (40 and 45%).

We were able to increase nZVI saturation on the second sample during the injection experiment, by increasing the injection rate (from 400 to 800 $\mu\text{L}/\text{min}$). As samples consisted of packed unconsolidated sand, some grains moved after nZVI injection. Despite differences in saturation, in both cases about half of the nanoparticles injected was mobile and was removed with the final water injection. The trapped nanoparticles are mainly observed to occupy the pore-throats, that is, the narrowest parts of the flow pathways.

The nZVI suspension is not miscible with the water phase, first occupying the larger pore-spaces. The images also show the formation of a water film covering some of the sand grains in presence of the nanoparticle suspension phase, making water the wetting phase. Nonetheless, this is not observed in all cases, which could be related to the irregular surface of grains –or even to image resolution.

This experiment shed light on the pore-scale mechanisms involved in nZVI entrapment in porous media. Future studies shall take advantage of the higher spatial and temporal resolution at the new beamline at Sirius, allowing the analysis of the nZVI suspension front during injection, observing the movement and trapping of the nanoparticles in nearly real time.

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References:

[1] Pak, T.; Luz, L. F. L.; Tosco, T. Costa, G. S. R.; Rosa, P. R. R.; Archilha, N. L. (2020). Pore-scale investigation of the use of reactive nanoparticles for in situ remediation of contaminated groundwater source. *Proceedings of the National Academy of Sciences* 117 (24), 13366-13373.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS06-B / 270

Foam Formation and Flow Diversion in Surfactant-Alternating-Gas Injection in Porous Media Micromodels

Author: Nicolle Lima¹

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¹ PUC-Rio

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Foam has the potential to significantly improve sweep efficiency in oil recovery, gas storage, and acidification processes. It can be used to solve problems caused by a thief zone or gravity override and in the remediation of contaminated sites. When foam is created in situ, it fills high permeability

areas and diverts displacing fluid towards trapped oil, lowering the relative permeability of gas and resulting in a more stable displacement front. The efficiency of these processes largely depends on the generation and stability of the foam films (lamellae) residing in the pores. The mobility of the injected gas is reduced when foam is formed; this reduction is attributed to the reduction of the gas phase relative permeability. The liquid films formed create resistance against the gas flow, impeding its free motion inside the porous media.

Surfactant-alternating-gas injection, also known as SAG, is an enhanced oil recovery method in which alternated slugs of surfactant solution and gas are injected into a reservoir. During SAG injection, foam is formed in the reservoir as the surfactant solution is drained by gas. SAG has several advantages over other methods, in addition to foam formation: it cannot completely block the porous medium, avoiding excessive injectivity reduction; it also helps to reduce corrosion in injection facilities by reducing contact between gas and water.

The goal of this research is to understand foam formation during gas injection in a microfluidic device completely saturated with oil. It focuses on its implications for oil displacement during SAG injection, considering different surfactant concentrations.

Image processing was used to visualize pore-scale displacement and correlate the evolution of foam formation during gas injection with pressure behavior for different flow conditions using a microfluidic setup consisting of a glass micromodel, a syringe pump, a pressure transducer, and a stereo microscope.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS22 / 271

THE EFFECT OF POROSITY AND PORE STRUCTURE ON THE ACCUMULATION OF PARTICLES INTO CELLULOSIC FIBROUS FILTERS

Authors: Antti Koponen¹; Jussi Virkajärvi²; Kimmo Heinonen²; Tuomas Turpeinen²

¹ VTT Technical Research Centre of Finland Ltd

² VTT

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Air filters are usually composed of fibres that are laid randomly and planarly by using some non-woven technology. Presently these filters are made mainly from plastic or glass fibres, but it would be environmentally important if one could replace them at least partly with cellulosic fibres. To overcome some problems of the traditional nonwoven technologies VTT has developed foam laying technologies that enable good fiber uniformity and the use of clearly higher fiber consistencies with wood fibers and mixes of staple and wood fibers than the traditional nonwoven techniques.

In this work we study the filtration properties of two industrial air filters and several generic test filters of different porosity that are made from a mixture of viscose fibres and softwood pulp by foam forming. The filtration efficiency of these filters is measured and the filters are loaded with fine test dust. The clean and dirty filters are imaged with X-ray microtomography. The 3D structure of the clean filters and the spatial distribution of the dust particles in the dirty filters are analyzed. Moreover, accumulation of particles is analyzed with flow simulations and the obtained spatial distributions of the particles are compared with the measured distributions.

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS11 / 272

Experimental basis and numerical modeling for a statistical characterization of multimodal spatial heterogeneity of nanoscale calcite dissolution rates

Authors: Chiara Recalcati^{None}; Martina Siena¹; Monica Riva¹; Alberto Guadagnini¹

¹ *Politecnico di Milano*

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Dissolution/precipitation of minerals are key reactions in various scenarios (e.g., contaminants transport in subsurface environments or sequestration of CO₂). Challenges in the assessment of the reaction kinetics arise from the high spatial heterogeneity characterizing precipitation/dissolution processes, typically resulting in a broad range of reaction rate values. High-resolution imaging of the mineral surface with techniques such as the Atomic Force Microscopy (AFM) enhance our ability to assess the mechanisms taking place at the nanoscale at the solid-fluid interface. Here, we rely on experimental results depicting highly heterogeneous patterns and couple these with kinetic Monte Carlo (kMC) numerical simulations to support the origin of such heterogeneous behavior to local inhomogeneities and defects in the crystal lattice. We then rely on a stochastic approach grounded on the use of Gaussian mixtures to view the spatial heterogeneity of reaction rates evaluated (a) from in situ and real-time AFM imaging of the topography of a calcite sample subject to dissolution at far-from-equilibrium conditions and (b) from kMC simulations. Experimental data and results from kMC simulations are clustered into categories with an imaging semantic segmentation technique, each cluster being associated with a component of the mixture. Analysis of the temporal behavior of the parameters associated with our mixture model leads to a quantitative appraisal of the dynamics of the mechanisms driving the reaction.

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Online

MS08 / 274

How does the presence of an oil phase influence the non-Fickian salt transport during low salinity waterflooding EOR?

Author: Arman Darvish Sarvestani¹

Co-authors: Behzad Rostami¹; Hassan Mahani²

¹ *University of Tehran*

² *Sharif University of Technology*

Corresponding Authors: hmahani@sharif.edu, arman7d@gmail.com, brostami@ut.ac.ir

Salt dispersion in a porous medium occurs due to salt concentration gradient. During low salinity waterflooding (LSWF) EOR, a reduced-salinity brine is injected to the porous media containing originally high-salinity brine. Brines with different salinities start mixing by dispersion mechanism and by the movement of the injected brine within the porous media, the salinity at the front of injected brine increases. Hence, the salinity profile of the injected brine differs from the step input evolving into a s-shape curve.

Modeling studies often use the dispersivity derived from single-phase experiments and neglect the presence of oil. In this paper, the salt dispersion during low salinity in the presence of oleic phase through sandpack tests was studied for the first time, to the best of our knowledge.

Sandpack, as a synthetic porous media, was used to perform flooding tests to investigate the effect of oil presence on salt dispersion. Sandpack flooding experiments, including two single phase tests and two two-phase tests were performed with different salinity differences to study the salt dispersivity in single-phase and two-phase conditions. In two-phase experiments, the sandpacks were first saturated with the high-saline brine. Next, a model oil like kerosene, as a non-reactive oleic phase, was injected to the sandpack to reach irreducible water saturation and initialize the core. Thereafter low salinity water was injected and the effluent brine salinity was analyzed to obtain breakthrough curves. Finally, salt dispersivity under two-phase conditions was estimated based on the advection-dispersion theory for non-Fickian dispersion using mobile-immobile model.

Salt dispersivity for a system with initial salinity of 100,000 ppm NaCl that was flooded with 2,000 ppm NaCl and injection rate of 0.2 ml/min (~4.5 ft/day) was 0.0069 ft. The dispersivity of the mentioned system in the presence of non-reactive oleic phase increased by 89% and reached 0.0131 ft. This means that the Peclet number reduces due to the presence of second phase. The same trend was observed for the salinity difference of 34,000 ppm. In a system with initial salinity of 40,000 ppm and injected salinity of 2,000 ppm, the dispersivity of single-phase and two-phase tests were 0.0050 ft and 0.0100, respectively and the dispersivity increased by 100%. In single phase tests, the whole cross-sectional area of the porous medium is accessible to the brine movement, and fluid velocity is less than that in two-phase condition. Presence of kerosene reduces the accessible area (and volume) for water fluid flow and increases the brine velocity. Hence, dispersivity is intensified due to the presence of the second phase and the increased interstitial velocity. Compared to single-phase results, salinity profiles under two-phase flow are wider and breakthrough of injected low-saline

brine occurs faster.

These findings highlight that the estimated dispersivity from single-phase experiments does not accurately reflect the real dispersivity values of LSWF at reservoir condition, and the estimated pore volumes of low-saline brine for injection may be under-estimated.

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Time Block C (18:00-21:00 CET)

Participation:

In person

MS09 / 275

Using In-situ Wettability Measurements to Reconstruct the Wet-ting Conditions of a Natural Rock

Author: Ruichang Guo¹

Co-authors: Cheng Chen²; Dustin Crandall³; Laura Dalton⁴; James McClure⁵; Hongsheng Wang⁵

¹ *Virginia Tech*

² *Stevens Institute of Technology*

³ *US Department of Energy - National Energy Technology Laboratory*

⁴ *U.S. Department of Energy National Energy Technology Laboratory*

⁵ *Virginia Tech*

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This study is to infer the wetting status of a realistic rock based on measured contact angles (CAs) in a Bentheimer sandstone after one drainage-imbibition cycle in a scCO₂ flooding experiment. Much research indicated that the wettability of natural rocks was heterogeneous. The heterogeneous wettability of natural rocks was usually assumed to be either mixed wettability or fractional wettability. In this study, a new fractional wettability model with wide-spectrum wettability will be proposed to represent the wetting status of a natural rock which assumes the wettability of rock surface is continuously distributed and covers a much larger range of wettability, measured as CA, in this study. Based on the measured CAs, a Kriging method will be used to reconstruct the wetting status of the Bentheimer sandstone used in the scCO₂ flooding experiment. To evaluate the reliability of the reconstructed wetting status, a hybrid CPU/GPU parallel computing accelerated LBM algorithm will be used to simulate the scCO₂ flooding process. The distribution of brine and scCO₂ will be compared. The flooding curve, relative permeability curve and capillary pressure curve of the rock sample with reconstructed wetting status will also be investigated. This new wettability model is expected to be closer to the actual wetting conditions of a given rock sample.

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References:

Guo, R. C., Dalton, L. E., Fan, M., McClure, J., Zeng, L., Crandall, D., & Chen, C. (2020). The role of the spatial heterogeneity and correlation length of surface wettability on two-phase flow in a CO₂-water-rock system. *Advances in Water Resources*, 146, 103763.

Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

Poster / 276

Heterogeneous nucleation and precipitation on solid surfaces: Experimental observation of calcium carbonate formation on primary and secondary substrates

Authors: Mohammad Nooraiepour¹; Mohammad Masoudi²; Nima Shokri³; Helge Hellevang⁴

¹ *University of Oslo (UiO)*

² *University of Oslo, Department of Geosciences*

³ *Hamburg University of Technology*

⁴ *University of Oslo*

Corresponding Authors: helghe@geo.uio.no, nima.shokri@tuhh.de, mohammad.nooraiepour@geo.uio.no, mohammad.masoudi@geo.uio.no

Mineral nucleation and growth are prime examples of (geo)chemical reactions giving rise to geometry evolution during reactive flow and transport in porous media. The precipitation reactions can reduce porosity, alter pore space connectivity and morphology, modify tortuosity, and deteriorate permeability. Therefore, change the fluid flow and solute transport. Additionally, precipitation reshapes the available surface area for growth, leading to changes in the system's reactivity, reaction progress, and reaction rates. As the probabilistic nucleation model highlights, it is necessary to delineate both amount and location of nucleation and precipitation events in the spatiotemporal domain for precise prediction of changes in transport properties. This work aims to improve the understanding of factors controlling crystal nucleation and growth rates, the impact of ambient and aqueous phase properties, and the substrate characteristics. To explore the effect of solute concentration, temperature, and experimental elapsed time on the surface coverage area and the number of precipitated crystals, we carried out a total of 27 mineral synthesis experiments on the surface of heterogeneous quartz-rich sandstone with a solution stoichiometry of close to 1 (Ca/CO₃ ≈ 1). The tests were performed at three temperatures (T = 20, 40, and 60°C) and three supersaturations (Ω = 15, 50, and 130x). The principal objective was to evaluate solid formation at different controlling conditions when the solid-liquid interface plays a key role. Effects of primary and secondary substrates and control imposed by preferential precipitation locations are identified and discussed. The results indicate that supersaturation and temperature imposed control on the amount, distribution pattern, and growth rate of crystals while the phenomenon still being probabilistic. Substrate characteristics governed the nucleation and crystal growth location and stochastic dynamics across time and space evolution. Moreover, substrate surface properties introduced preferential sites that

were occupied and covered with solids first. For reactive transport modeling, in addition to porous medium's geometry and aqueous phase properties, a stochastic nucleation and growth model is necessary to implement substrate surface properties and compute solute transport and fluid flow for different spatial and temporal locations distinctively.

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Country:

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References:

Nooraiepour, M., Masoudi, M., Shokri, N. & Hellevang, H. 2021. Probabilistic Nucleation and Crystal Growth in Porous Medium: New Insights from Calcium Carbonate Precipitation on Primary and Secondary Substrates. *ACS Omega*, 6 (42), 28072–28083. <https://doi.org/10.1021/acsomega.1c04147>.

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Masoudi, M., Fazeli, H., Miri, R., Hellevang, H. 2021. Pore Scale Modeling and Evaluation of Clogging Behavior of Salt Crystal Aggregates in CO₂-Rich Phase during Carbon Storage. *Int. J. Greenh. Gas Control*, 111, 103475. <https://doi.org/10.1016/j.ijggc.2021.103475>.

Hellevang, H., Wolff-Boenisch, D., Nooraiepour, M. 2019. Kinetic Control on the Distribution of Secondary Precipitates during CO₂-Basalt Interactions. In *E3S Web of Conferences*, Vol. 98. <https://doi.org/10.1051/e3sconf/20199801001>.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS03 / 277

Impacts of fractures on hydrodynamic trapping for CO₂ storage in deep saline aquifers

Authors: Yuhang Wang¹; Cornelis Vuik¹; Hadi Hajibeygi²

¹ *Delft University of Technology*

² *TU Delft*

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Natural or induced fractures are typically present in subsurface geological formations, which have received an increasing interest for geo-energy production and storage as well as for long-term carbon dioxide storage. Generally speaking, fracture networks have high-contrast properties compared to the neighbouring matrix. For instance, they may serve as highly conductive pathways which could potentially lead to the leakage of CO₂. This undermines the storage capacity. On the other hand, they may act as flow barriers, causing significant pressure and stress gradients. Nevertheless, despite their high sensitivities, impacts of fractures on the full-cycle storage process have not been fully understood. In this study, a numerical model is used to examine the role of fractures on the flow and transport of CO₂ plume in various conditions. A unified multiphysics framework is developed to

model the hydrodynamic trapping mechanisms in a robust manner. In particular, the projection-based embedded discrete fracture model is incorporated into the compositional framework to describe fractures with varying conductivities. We first apply this numerical model to an illustrative domain with a single fracture of different configurations, and then simulate such process in a complex fracture network which is representative of a field-scale fractured system. Findings from the test cases for single fracture geometries are also observed in the larger-domain with complex geometries. Results indicate that the fracture exhibits differing effects regarding the dissolution/residual trapping, and therefore, accurate characterization of fracture geometry and its conductivity is essential for evaluation of CO₂ storage in fractured formations.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS08 / 278

Impact of nanopores in clay on accessibility and connected porosity in sandstone samples

Authors: Md Fahim Salek¹; Fanqi Qin^{None}; Lauren Beckingham¹

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Imaging is a valuable tool to identify and characterize the spatial distribution of minerals in rock samples. Scanning electron microscope (SEM) can capture microscale features, and when equipped with energy dispersive spectroscopy (EDS), can be utilized to identify minerals; however, it is limited to only two-dimensional images. X-ray computed tomography (X-ray CT) can be used to capture pore-grain structure in 3D, although lab-scale X-ray CT instruments are limited in resolution. The 2D SEM and 3D X-ray CT images can be combined to get various mineral properties including, mineral volume fraction, accessibility, porosity, pore connectivity, mineral surface areas etc. and these can be utilized to conduct reactive transport simulation. However, the regular SEM and X-ray CT fails to capture the nanoscale pores in clays. In this study seven sandstone samples with varying amounts of clays are imaged using 2D SEM and 3D X-ray CT at Auburn University. Additionally, focused ion beam-scanning electron microscopy (FIB-SEM) images are captured on the clay-rich areas of the polished samples to understand the nanopore connectivity within clays. Mineral abundances are determined by counting mineral pixels of same the color in the segmented 2D images while mineral accessibilities are calculated by counting interfacial pixels between associated mineral and adjacent pore. Moreover, the 3D X-ray images are processed to determine the connected surface area. Three types of accessibility are considered: the first approach accounts for all the pore space, the second approach considers only the connected macropores and the third approach includes connected porosity considering nanopores in clays. Finally, reactive transport simulations is

carried out using the accessible mineral surface area calculated from the three approaches and the corresponding simulated evolution of minerals and reaction rates compared.

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Time Block C (18:00-21:00 CET)

Participation:

Online

MS15 / 279

The Method Of Solving incompressible Two-phase Seepage Equation In Porous Media By Deep Neural Networks

Author: JiangXia Han^{None}

Co-author: Liang Xue

Corresponding Authors: 2021310162@student.cup.edu.cn, xue_liang1983@163.com

Abstract: A method is proposed to solve incompressible two-phase seepage equation in porous media, based on the Physical-informed Neural Networks(PINN) combined with the Implicit Pressure Explicit Saturation method(IMPES method). Different from the conventional PINN model, this approach implicitly solves the pressure field and then explicitly solves the saturation field by combining the operator splitting technique of numerical calculation. The neural networks loss function is composed of spatial well-bottle pressure and production data matching, PDE residual, initial conditions, boundary conditions, and other measurable prior knowledge. By minimizing the loss function, the neural network parameters that not only fit the data but also adhere to the governing equation are obtained. This method provides a general, efficient, and robust methodology to solve the nonlinear flow equation with a source and sink term. The results show that this method can accurately solve the oil-water two-phase seepage equation. Compared with the numerical simulation method, the determination coefficients of the model pressure field and saturation field prediction can reach more than 0.95.

Keywords: Physics-Informed Neural Networks, Surrogate Modeling, Reservoir Numerical Simulation

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Time Block A (09:00-12:00 CET)

Participation:

Online

MS08 / 281

Effect of the connectivity of alluvial aquifers on groundwater flow and solute transport**Authors:** anthony beaudoin¹; Alejandro Boschan²; ivan Colecchio²¹ *Université de Poitiers*² *Grupo de Medios Porosos, Facultad de Ingeniería, UBA***Corresponding Authors:** aboschfi@gmail.com, anthony.beaudoin@univ-poitiers.fr, colecchio.ivan@gmail.com

The assumption that the heterogeneity of aquifers can be described with multilog-Gaussian distributions has been widely used (Law, 1944). However, the multilog-Gaussian assumption is inappropriate in alluvial aquifers (Zinn and Harvey, 2003). Alluvial aquifers, such as fluvial sediments containing paleochannels, present structures composed of interconnected bodies (Tidwell and Wilson, 1999). Alluvial aquifers can be described with binary distributions (Zinn and Harvey, 2003). Many authors have argued that the connectivity of alluvial aquifers is more important than the values of permeability K (Zappa et al., 2006). The connectivity of alluvial aquifers induces a channeling leading to significant increase in average flow rates and even more significant reduction of contaminant first arrival times (Molinari et al., 2019). Few works have performed three-dimensional detailed numerical simulations of groundwater flow and solute transport in binary distributions. In 2017, Jankovic et al. choose to study the effective permeability, the plume mean velocity, the BTC and the mass flux in multiLog-Gaussian, connected and disconnected K -fields introduced by Zinn and Harvey in 2003 (Jankovic et al., 2017). The bulk of the BTC was predicted quite accurately by the solution of the advection dispersion equation based on the first order approximation. In this work, the asymptotic value of the longitudinal dispersivity λ is numerically estimated in three-dimensional multiLog-Gaussian, connected, intermediate and disconnected, K -fields from Monte Carlo parallel numerical simulations in advection –diffusion cases with a Peclet number $Pe = \langle u \rangle l_c / d_m = 100$ where $\langle u \rangle$ is the mean flow velocity, l_c is the correlation length of K -fields and d_m is the diffusion coefficient. The following figure shows that the evolution of λ with respect to the deviation $p-p_c$ presents a mountainous form in all the tested cases. p and p_c are the volume fraction of low conductivity zones and the percolation threshold, respectively. The maximum value of λ is obtained just after the percolation threshold p_c . A detailed analysis will be performed by comparing the numerical results with the first order approximation and the percolation theory (Sahimi et al., 1986 ; Rubin, 1995).

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS21 / 282

Ganglia mobilization by purely elastic instability

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The flow of viscoelastic polymer solutions and their use as displacing agents in porous media are important for industrial applications, such as enhanced oil recovery and soil remediation. Complexity of flow and high elasticity of conventionally used viscoelastic polymer solutions can lead to purely elastic instability in porous media. In this work, we study the impact of elastic instability on displacing oil ganglia at low Reynolds numbers using a microfluidic approach. Our unique design consists of a single-capillary entrapment connected to two symmetric serpentine channels. This design excludes the effect of viscous forces and allows a direct focus on displacement driven solely by elastic forces. After the onset of purely elastic instability, an unstable base flow is observed in the serpentine channels. We argue that the pressure fluctuations caused by this unstable flow create an instantaneous non-equilibrium state between the two ends of the oil ganglia. This provides the driving pressure to overcome the capillary threshold pressure and eventually displace the entrapped oil. In our geometry, we observe that the displacement coincides with the emergence of a fully developed elastic turbulent state.

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MS15 / 284

Upscaling of Realistic Discrete Fracture Simulations Using Machine Learning

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Fine-scale discrete fracture simulations provide a natural means to model fluid flows in fractured reservoirs. However, an application of discrete fracture modeling on the field scale is challenging due to uncertainties in fractures' properties, difficulties in creating conforming meshes, and the computational complexity of fluid flow simulations. Upscaling of flows in fracture networks has been traditionally used to cope with these challenges. One common approach is to use the dual porosity/dual permeability (DPDP) model (Hill and Thomas, 1985), where all fracture properties are encoded in effective coarse-scale fracture porosity, permeability, and a mass transfer term accounting for the crossflows between the fractures and the matrix.

Recent results (Andrianov and Nick, 2021; Andrianov, 2021) show that it is possible to map the pixelated fine-scale fracture geometry to the DPDP model closures via a convolutional neural network (CNN), and that the DPDP single-phase flow simulations with both reference and learned model closures agree reasonably well with each other. The goal of the present contribution is to extend these results to the case of two phases.

To this end, we simulate the fine-scale single-phase flow in each fractured coarse-scale grid block with a customized Discrete Fracture-Matrix (DFM) module of the open-source numerical simulator DuMuX (Flemisch et al., 2011). These simulation results are used to calculate the reference upscaled fracture permeabilities and to obtain the shape factors, which characterize the fracture-matrix mass transfer.

We demonstrate that the predicted model closures can be obtained by using the pre-trained CNNs from and implement the two-phase DPDP model on top of the dual porosity module of the open-source numerical simulator MRST (Lie, 2019). The DPDP results agree well with the fine-scale two-phase DFM solutions for a realistic fractured outcrop geometry.

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References:

Andrianov N. and Nick, H. M. 2021. Machine learning of dual porosity model closures from discrete fracture simulations. *Advances in Water Resources*, 147:103810. doi.org/10.1016/j.advwatres.2020.103810.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS05 / 285

Optimization of injection strategies for field-scale leakage remediation using microbially induced calcite precipitation

Authors: Sverre Tveit^{None}; David Landa Marbán¹

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In large-scale geological storage of CO₂ one of the key factors for effective storage capacity is how much one can inject before reaching critical pressure build-ups. If potential leakage paths in the caprock experience pressure value beyond their critical threshold, sequestered CO₂ might leak out of the storage site. Several sealing technologies have been suggested to close leakage paths in case they develop, where microbially induced calcite precipitation (MICP) is a novel technology that has gained much attention in recent years. MICP consists of accelerating the production of calcite (i.e., the sealing agent) using suitable bacteria, and requires injection of several components: microbial solution of pre-cultivated bacteria; growth solution to establish biofilm at leakage location; and cementation solution to initiate the calcite precipitation. A major challenge in applying MICP in CO₂ storage sites is the possibility of leakage paths developing several tens-of-meters away from the injection well. Thus, placing the components needed in MICP at the correct location and completely sealing the leakage paths without negatively impacting the rest of the storage site, i.e., sealing the near-well area, is a difficult task. Adding to the challenge is sealing the leakage paths in the least amount of time to avoid long shutdown of CO₂ injection.

To maximize sealing of leakage paths while penalizing total MICP operational time, we have developed an optimization procedure with a new injection strategy where growth and cementation solutions are injected in separate well segments. With the proposed injection strategy, we minimize the production of biofilm, and subsequent calcite, in other places than in the leakage paths after an initial injection of microbial solution. The optimization procedure uses a newly developed field-scale MICP mathematical model [1] implemented in the Open Porous Media (OPM) simulator. The

model approximates the chemical and physical processes to capture the necessary field-scale behavior of MICP at relatively low computational cost compared to contemporary models. To solve the optimization problem, we use a stochastic approximation of the gradient known as the ensemble-based optimization (EnOpt) method. The EnOPT method allows for easy parallelization, requires only input-output interaction with the simulator, and has been shown to perform well in realistic optimization studies.

The optimization procedure was applied to 3D synthetic test cases involving various scenarios with explicitly modeled leakage paths. The control variables were the injection and no-flow periods associated with our proposed injection strategy. The numerical results showed that in all scenarios, the leakage paths were effectively sealed, measured by comparing CO₂ leakage before and after optimization. The distribution of calcite in each scenario was localized in and around the leakage paths, with no unnecessary clogging elsewhere in the reservoir. Furthermore, the total injection and no-flow time was low in the final optimization results.

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References:

[1] Landa-Marbán, D., Tveit, S., Kumar, K., Gasda, S.E.: Practical approaches to study microbially induced calcite precipitation at the field scale. *Int. J. Greenh. Gas Cont.* 106, 103256 (2021).

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS06-B / 286

Unstable invasion during imbibition in regular porous media

Authors: Zhongzheng Wang¹; Jean-Michel Pereira²; Emilie Sauret¹; Yixiang Gan³

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The unstable fluid-fluid displacement patterns in porous media with rough invasion fronts and trapping of the defending phase are often observed in drainage, i.e., when the solid is non-wetting to the invading phase. Reversely, during imbibition, compact and faceted growth is expected in regular porous media with geometrically homogeneous pore structure due to the favoured overlap event at the pore scale. Here, we report the irregular growth of invading fluid during an imbibition process in two-dimensional regular porous media. The ramified invasion patterns associated with thin fingers and trapping of the defending fluids are reminiscent of capillary fingering, which are often observed only in drainage conditions. Through examining the capillary pressure signals and type of pore-scale invasion mechanisms during multiphase flow, the differences between compact and

faceted displacement and unstable growth are revealed. We analyse the critical events at pore-scale that determines the pore-filling process, which leads to a phase diagram describing the dominance of event type across a wide range of porosity and wetting conditions. Through conducting systematic quasi-static radial injection simulations, excellent agreement is observed on the transition boundary from faceted and compact displacement patterns towards irregular and dendritic invasion morphologies. This is reflected by the overlap of the transition boundaries from analytical prediction, type of pore-scale invasion events, and macroscopic morphology quantified by the fractal dimension. This work provides new insights on the role of geometrical features of solid structures during fluid displacement processes with emphasis on the porosity and wettability of regular porous media. The findings would assist in guiding the design of microfluidic devices to deterministically control the multiphase flow, transport and reaction processes.

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Time Block A (09:00-12:00 CET)

Participation:

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MS10 / 287

Optimising Micro-CT Imaging Reconstruction Using Iterative Methods

Authors: Puyan Bakhshi¹; Chloé Maucuer²; Omid Shahrokhi¹; M. Mercedes Maroto-Valer¹

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X-ray micro-CT is a non-invasive 3D imaging technique that allows the visualisation of the inner structure by obtaining 2D X-ray images at different angles. In recent years, micro-CT scanning has been extensively used for in-situ imaging of transport phenomena in porous media at the pore scale. However, the mentioned studies using lab-based micro-CT devices are generally limited to static imaging, given that the scanning times required for acquiring high-quality images are usually in the order of hours. While acquiring high-resolution images using a synchrotron beamline is in the order of seconds to minutes, which easily facilitates the in-situ imaging of dynamic processes, the access to these high flux sources is still limited in contrast with lab-based devices. Therefore, to approach dynamic in-situ imaging of flow processes with benchtop micro-CT scanning, reducing the image acquisition time of these devices with minimal loss of image quality is crucial. A practical approach to meet that end is decreasing the number of projections. Nonetheless, the conventional methods (analytical algorithms) to reconstruct 2D radiograms into 3D models need a large number of projections to provide high-quality images. In contrast, iterative reconstruction (IR) algorithms have been introduced to overcome the limitations of the analytical methods. IR methods have shown their capability in generating high-quality reconstructed images from under-sampled data. Despite that, since these algorithms use multiple repetitions to update the image until the best solution is found,

their computational demand is much higher than that of analytical ones. Hence, finding the right balance between image quality and computation time and demands is of absolute necessity. Accordingly, the objective of this work is to optimise micro-CT image quality and acquisition time by determining the suitable method of reconstruction and the sufficient number of projections. Here, we investigated two widely used IR methods, namely the simultaneous iterative reconstruction technique (SIRT) and the conjugate gradient least squares (CGLS) approach, in comparison with the most common analytical reconstruction method for cone-beam CT, the Feldkamp, Davis, and Kress (FDK) algorithm. We used the open-source ASTRA Toolbox on a micro-CT dataset acquired of a Doddington sandstone sample containing air and doped brine. We first reconstructed four different projection numbers of this dataset by using FDK, SIRT, and CGLS and then analysed the quality of the resulting images by calculating the signal-to-noise ratio (SNR) and quantifying the image sharpness. As the assessment of the analytical and iterative reconstruction algorithms based merely on pixel-based image quality determination methods may lead to an unfair comparison, we have also evaluated the discussed methods based on physical measures. For that purpose, we compared the segmented images of a number of selected reconstructions against a pre-set reference image. Our results indicated the clear advantage of CGLS compared to the other two algorithms in the optimisation of the number of projections required for reconstruction. CGLS showed to be capable of significantly reducing the acquisition time, down to a quarter of the original time, while providing significant improvement to the SNR and image sharpness, as compared to FDK.

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Time Block A (09:00-12:00 CET)

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MS09 / 288

Copper leaching in low-grade ore: A reactive-transport modelling study revealing controls on local reactions on mineral surfaces

Authors: Ralf R. Haese¹; Eric O. Ansah¹; Black Jay R.¹; Apoorv Jyoti¹

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The global copper demand is rapidly increasing with the electrification of the energy sector, requiring new ore deposit discoveries and more efficient copper recovery. Copper leaching occurs in piles of low-grade ore aggregate also known as heaps, which typically contain 2-5% copper mostly associated with the mineral chalcopyrite (CuFeS₂). The reagent for the dissolution of chalcopyrite is sulfuric acid with variable and complex ionic composition. Predicting and optimising the rate of chalcopyrite dissolution in heaps is complex because of a number of conditions including the following:

- Two competing reactions lead to the dissolution of chalcopyrite (Kimball et al., 2010): proton-promoted dissolution and ferric iron-promoted dissolution, where the latter requires iron oxidation in solution to maintain high ferric iron concentrations.
- Chalcopyrite is mostly surrounded by microporous gangue minerals such as quartz and not directly exposed to the reagent.
- Chalcopyrite is mostly surrounded by microporous gangue minerals such as quartz and not directly exposed to the reagent.
- Secondary minerals, mainly jarosite ((K,Na)Fe₃(SO₄)₂(OH)₆), can form on the chalcopyrite surface leading to surface passivation.

In order to better understand the controls on copper dissolution at the surface of chalcopyrite, we developed a combined pore- and continuum-scale reactive-transport model for a single grain of chalcopyrite surrounded by gangue mineral (quartz). The model was developed in iCP, where COMSOL is coupled to PhreeqC (Jyoti and Haese, 2021). Micro-porosity was assigned to the gangue mineral layer, while the chalcopyrite surface layer was resolved at pore-scale allowing us to determine local reaction rates of chalcopyrite dissolution and potential jarosite precipitation and associated changes in the solid phase at the mineral surface. Ferrous iron oxidation by oxygen in the aqueous phase was enabled. All reactions were kinetically controlled. The inflow composition, flow velocity, porosity of the gangue mineral and the thickness of the gangue mineral layer were varied in simulations to constrain the main controls on reactions at the mineral surface. We wanted to understand which dissolution reaction mechanism dominates under given conditions, whether the dissolution reaction is rate- or transport-limited and what conditions lead to surface passivation. The dissolution was simulated using injection fluids with a pH 1 and 2 and with Fe³⁺(aq) concentrations between 0.1M and 0.01M. To understand the role of physical effects, the radius ratio of the chalcopyrite to quartz grains were varied between 1:2 to 1:4 and the flow velocity varied between 1.2e-6 and 1.2e-4 m s⁻¹.

Initial results indicate an increase in copper recovery with increasing ferric iron concentration and decreasing pH. The dominant chalcopyrite dissolution mechanism is the ferric iron promoted reaction, except for a case with a pH of 1 and a very low (0.01 M) Fe³⁺(aq) concentration where proton promoted dissolution dominates. The copper recovery increased by about 50% for a radius ratio of 1:4 relative to a 1:2 ratio. Finally, the highest copper recovery was attained with the slowest injection fluid velocity of 1.2e-6 m s⁻¹, with concentrations measuring two orders of magnitude higher than with the fastest fluid velocity of 1.2e-4 m s⁻¹.

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References:

Kimball, B.E., Rimstidt, J.D., Brantley, S.L., 2010. Chalcopyrite dissolution rate laws. *Appl. Geochemistry* 25, 972–983, doi.org/10.1016/j.apgeochem.2010.03.010

Jyoti A. and Haese R.R., 2021, Validation of a multi-component reactive-transport model at pore scale based on the coupling of COMSOL and PhreeqC. *Computers and Geosciences* 156, doi.org/10.1016/j.cageo.2021.104870.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS01 / 289

CO₂ degassing kinetics in porous media

Authors: Chris Boeije¹; Cas Verweij¹; Pacelli Zitha¹; Anne Pluymakers¹

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Geothermal fluids often contain significant amounts of minerals and gasses such as CO₂ and N₂. As these fluids are extracted, a change in pressure and temperature will occur in or near the production well. These changes disturb the equilibrium the water is in with its dissolved minerals and gases and can result in degassing, that is, the formation of free gas bubbles. These bubbles take up space inside the reservoir's pore space, which limits the ability for the water to flow, thus leading to reduced production of geothermal waters. This project is aimed at experimentally investigating the conditions at which the onset of the degassing process starts (i.e. the conditions where the first free gas bubble forms) inside porous media. Furthermore, the influence of the degassing process is on the apparent permeability of the porous medium (i.e. the extent to which the water's ability to flow is altered). Knowledge on these parameters will enable operators to adapt their procedures such that fluid production can be maintained in the long-term.

To this end, coreflood experiments were performed in which CO₂ along with water (tap water or brine with a higher salinity) were co-injected into either a Bentheimer or Berea sandstone core under a variety of conditions. The first sets of coreflood experiments were carried out under moderate conditions (tap water, p = 50 bar and T = 30 °C). Here, the onset of the degassing process can be predicted accurately using CO₂ solubility values obtained from Henry's law combined with the Van 't Hoff equation (Smith (2007)). At these conditions CO₂ degassing near the wellbore will cause the apparent permeability to decrease by a factor 2 to 5 in a high permeability, 2.3 Darcy, Bentheimer sandstone core. At the same conditions the apparent permeability will decrease by about a factor 10 in a low permeability, 140 millidarcy, Berea sandstone core. The change in apparent permeability is gradual in the Bentheimer sandstone while in the Berea sandstone the change is near-instant. For rocks with small pore sizes and low initial permeability, the reduction in apparent permeability is larger and the rate of permeability decrease is faster. The onset of the degassing process is not influenced by the pore size and initial permeability.

Experiments at temperatures between 30 and 90°C show that with increasing temperature the onset of degassing shows deviates more from Van 't Hoff theory. The pressure where degassing initiates increases with temperature, but is still significantly lower than that predicted by the Van 't Hoff equation. Using a high-salinity brine (1.5 M CaCl + 2 M NaCl) leads to further deviation from theory, with bubbles forming at significantly higher pressures compared to the tap water experiments. However, the observed reduction in apparent permeability is similar for both sets of experiments.

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References:

1. F. L. Smith, Environmental Management Where do Henry's constants come from? (2007).

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS09 / 290

A pore-scale level-set approach to Ostwald ripening of gas bubbles in porous media in the presence of residual oil and water

Authors: Deepak Singh¹; Helmer Andre Friis¹; Espen Jettestuen²; Johan Olav Helland³

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CO₂ storage and foam injection in hydrocarbon reservoirs involve three-phase processes in porous media where interactions between gas bubbles occur in the presence of both residual oil and water. Gas-bubble interactions by Ostwald ripening is a thermodynamic process where bubbles with higher chemical potential lose mass to those having a lower chemical potential. This mass transfer can lead to coarsening and induce mobility in isolated gas bubbles, reducing both the lifetime of residual trapping in CO₂ storage and the effectiveness of foam in EOR. Previous studies of two-phase systems have shown that Ostwald ripening can cause subsurface fluid redistribution at length scales ranging from pore to field [1], and bubble evolution depends on both local capillary pressure and pore geometry [2]. However, the impact of a third phase, like residual oil, on fluid redistribution caused by Ostwald ripening is still unexplored.

In this work, we present a methodology for simulating Ostwald ripening of gas bubbles in three-phase fluid systems at the pore scale that combines a level-set method for three-phase capillary-controlled displacement [3] and a “ghost-bubble” method for mass transfer driven by chemical potential differences. The approach extends our previously presented two-phase work to three-phase systems [4].

We have carried out simulations on 2D idealized porous media and 3D pore-space images of a water-wet sandstone, using the Soave-Redlich-Kwong (SRK) equation of state to calculate gas bubble fugacity at reservoir conditions. The 2D simulations evaluate impacts of the gas-bubble distribution evolution with respect to (i) the assumption of idealizing a gas/oil/brine system as a gas/oil or gas/brine system and (ii) variations of the initial spatial arrangement of gas and oil ganglia surrounded by brine. Finally, the 3D sandstone simulations show the impacts of Ostwald ripening on residual three-phase fluid configurations with isolated oil and gas ganglia obtained after a water-alternate-gas invasion cycle. We quantified the evolution of pressure, volume, and the number of residual bubbles, for different initial gas and oil saturations.

A significant result of our work is that the equilibrium distribution of residual gas bubbles after Ostwald ripening in porous media depends strongly on the initial three-phase fluid configuration and its properties (e.g., interfacial tension, wetting state, and interfacial area), in addition to local capillary pressure and pore geometry as previously seen in the ripening of two-phase systems. The presence of oil ganglia speeds up the local coarsening process and influences the equilibrium location of gas bubbles. The initial gas pressures of isolated bubbles in oil and water depend on oil-water capillary pressure, gas-liquid contact angle, and pore geometry. We find that a three-phase scenario can create higher initial pressure differences in gas bubbles, which leads to larger mass transfers and different residual bubble sizes in the two liquids. Large residual sizes can create new gas flow paths by merging bubbles. During fluid redistribution, we also identify cases where the bubble coarsening leads to capillary instabilities and three-phase double displacements (e.g., oil displaces a gas bubble that displaces water), which in turn can lead to lower residual gas trapping.

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References:

[1] Xu, K., Mehmani, Y., Shang, L., Xiong, Q. (2019). Gravity-Induced Bubble Ripening in Porous Media and Its Impact on Capillary Trapping Stability. *Geophysical Research Letters*, 46(23), 804-813. <https://doi.org/10.1029/2019GL085175>

[2] de Chalendar, J.A., Garing, C., Benson, S.M. (2017). Pore-scale modelling of ostwald ripening. *Journal of Fluid Mechanics*, 835, 363-392. <https://doi.org/10.1017/jfm.2017.720>

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS06-A / 291

Wettability effect on Pore-filling events during two-phase flow

Co-authors: LIFEI YAN ; Bernhard Weigand ¹; Amir Raouf ²; Johannes Müller ¹

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Wettability is a crucial factor for pore-filling events in multiphase flow. If the fluid interface passes an abrupt variation in the cross-section of the porous medium, a sudden redistribution takes place, commonly known as Haines Jump. Different wettabilities of the solid substrate affect the global displacement pattern, the fluid trapping and the hysteretic saturation. Furthermore the effect of wettability needs to be considered in numerical and analytical models to enable the accurate description of the pressure response during such a pore-filling event.

To better understand the effect of wettability, we conduct a series of microfluidic experiments of drainage and imbibition processes with three displacement velocities for two-phase flow. The PDMS micro-models are designed with a depth of 100 μm and with one square pore body of 800 μm in width and length which is connected to 4,000 μm long inlet and outlet channels with a height of 150 μm . The models are rendered with three surface wettabilities of 40°, 95° and 150° static contact angle (measured with the sessile drop method for a water droplet on PDMS in air). Three fluids are used, fluorescent-dyed water, Fluorinert-FC 43 and crude oil, to investigate the displacement of: water-air, water-fluorinert and water-crude oil. By reversing the flow direction after each pore-filling experiment, also the corresponding drainage or imbibition process was captured. Confocal laser scanning microscopy (CLSM) is applied to recognize the fluid interface and monitor its movement. With an inserted pressure transducer in the upstreaming plastic tube, the pressure change during the events was continuously measured. The collected pressure curves are compared with existing analytical solutions. Due to the limitations of these solutions and to enable the prediction of the interface movement for a variety of wettabilities, we are correspondingly developing a numerical model based on the volume of fluid method (VOF) which will be validated with the presented experimental data. We found for the two cases with contact angles of 95° and 150° similar residual saturation levels of the wetting phase for all imbibition and drainage processes. For the case with 40° contact angle, the wetting phase can almost fully saturate the pore after imbibition and can be fully displaced by the non-wetting phase after drainage. Besides, we noticed that wettability plays an important role in thin-film generation and the thickness of the film during displacement. In our case, the crude oil shows non-irregular interfaces in pore-filling behavior during imbibition and drainage, and easily forms a slug flow of water in the micro-channel for the relatively high capillary numbers ($3.1\text{E-}7$ and

1.5E-6). Furthermore, crude oil, which is the wetting phase to PDMS, has remarkable residuals on the top and bottom surfaces of the channel compared to the experiments with fluorinert which is also wetting PDMS, due to the chemical heterogeneity of the components with various adsorption to the PDMS.

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS03 / 292

An experimental study of nonlinear flow behavior in fractured porous media by 3D printing technology

Author: Yunlong WU^{None}

Co-authors: Jean-Philippe CARLIER ; Nicolas BUR ; Jean-Baptiste COLLIAT ; Yun JIA

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Fluid flow in fractures is an important issue in natural gas and oil engineering. The fabrication of some morphologically controllable fracture models is very useful to understand and identify the evolution of fluid flow in fractures. For example, Suzuki et al. [1] investigated fracture networks with smooth surfaces using 3D printing technology. Based on this, Li et al. [2] improved the models by replacing the smooth fracture surfaces with rough surfaces.

In the present work, by using 3D printing technology, single fractures with controlled morphology are generated, each of them constituted of two parallel planes, one smooth, one of controlled roughness. Varying the fracture openings (mean distance between planes ranging from 0.1 to 0.8mm) and roughness (quantified in terms of Hurst exponent [3], ranging from 0 for smooth planes to 0.8), a series of samples are printed with identical length and width of fractures (typical dimensions are: 4.6 cm long and 1.8 cm wide) using an Anycubic MonoX printer (figure 1)

Anycubic MonoX is a Stereolithographic Apparatus (SLA) printer, using a photopolymerisation process on a UV-sensitive resin [4]. This process has been chosen for its simplicity and two major reasons: a compromise between model scale and precision (printing layer thickness of 50 μm), and printing material properties (mechanical resistance and low X-ray absorption to perform X-ray microtomographic analyses of the samples).

A series of hydrodynamic test are then performed on these samples: under prescribed water pressure gradient conditions, the variations of fluid flow in the fractures are studied to assess the effects of fracture surface roughness and fracture opening on water flow patterns. Following an extensive experimental design, a total of 26 samples are tested.

As expected, for smooth surface fractures, the ratio flow rate/pressure gradient to the mean opening of the fracture satisfies the classical cubic law [5]. In contrast, for rough surface cases, an impact of fracture roughness is observed in the experimental investigation. These observations are coherent with numerous experimental and numerical studies [6]. Primary analyses show an influence of the

fractal dimension of the rough plane, quantified in terms of Hurst exponent: when Hurst exponent becomes larger, the effective opening of fracture becomes smaller.

Based on the obtained experimental results, the influence of local wall roughness is taken into account by correcting the mean opening of fracture in the cubic law, via a correcting coefficient (α). This coefficient (α) is defined as the ratio between the fracture opening (mean distance between the walls) and can be linearly related to Hurst coefficient. Finally, the effective opening can be calculated by inversion of the cubic law (figure 2).

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS06-A / 293

The Transition from Connected to Disconnected Pathway Flow Regime : Understanding the Combined Effects of Wettability and Flowrate

Author: Rumbidzai Nhunduru¹

Co-authors: Amir Jahanbakhsh¹; Krystian. L Wlodarczyk¹; M. Mercedes Maroto-Valer¹; Omid Shahrokhi¹; Susana Garcia¹

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The contribution of pore-scale properties is often neglected in large scale (macro-scale) models describing subsurface fluid processes (1). Pore-scale flow properties, such as wettability have a significant impact on macro-scale flow functions, such as relative permeability, capillary pressure, saturation distribution and displacement efficiency (2). Upscaling multiphase flow from Pore-to-Darcy

scale is one of the largest unresolved problems in the field of porous media research that has attracted the interest of many researchers for decades (3). One of the key challenges is addressing connected and disconnected fluid fractions (4)(5).

In this work, the combined effects of wettability and fluid flowrate on dynamic fluid connectivity and the saturation function are investigated. Direct numerical simulations involving immiscible displacement of decane by water were performed in a 2D digital model of a Berea sandstone rock. In all simulations performed, the Berea sandstone model was initially saturated with decane and then water was injected to displace it from the pore spaces. Invading fluid Darcy velocities investigated ranged from 0.03m/s ($Ca = 5.45 \times 10^{-4}$; Reynold's number (Re) = 0.36) to 30m/s ($Ca = 5.45 \times 10^{-1}$; $Re = 360$). Wetting conditions investigated were for contact angles 45° (water-wet), 90° (neutrally-wet) and 150° (oil-wet).

Connected pathway flow (CPF) and two disconnected flow regimes were observed. The first disconnected flow regime was classified as ganglion dynamics (GD), where the invading fluid propagated through the pore network in the form of large, disconnected ganglia. The second disconnected flow regime was a drop traffic flow (DTF), where the invading fluid propagated through the pore network as very small fluidic elements (droplets).

At the lowest capillary number ($Ca = 5.45 \times 10^{-4}$), the CPF regime dominated under the neutrally wet state whilst the GD flow regime dominated for the oil- and water-wet cases. A connectivity index (Λ) derived from the Euler characteristic (χ), a fluid topological descriptor, was used to track the temporal evolution of fluid connectivity as the simulations progressed. For all wetting conditions investigated, ganglia of the defending fluid became smaller and more disconnected with increasing flow rate. At the highest capillary number ($Ca = 5.45 \times 10^{-1}$), the DTF flow regime dominated for all wetting states. In cases where the GD regime dominated, low flow cohesion was observed between discrete ganglia whilst high flow cohesion was observed where the CPF regime was dominant. Although more discrete fluid elements were present in the DTF regime in comparison to the GD regime, higher flow cohesion was observed in DTF dominant cases. The transition from low cohesion to high cohesion flows was found to have a consequential effect on the kinetics of the displacement process and the shape of the saturation function. Displacement efficiency increased by up to 35% for highly cohesive flows in comparison to flows with low ganglion cohesion.

Acknowledgements

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

Poster / 294

Quantifying risks of salt contamination of freshwater aquifers during Aquifer Thermal Energy Storage

Authors: Geraldine Regnier¹; Pablo Salinas¹; Matthew D. Jackson¹

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Aquifer Thermal Energy Storage (ATES) has significant potential to decarbonise heating and cooling in regions with seasonal climate variations. These systems often target freshwater aquifers, which are also used to produce drinking water. Therefore, a major concern when developing ATES is to ensure that operation of the system will not create or redistribute pollutants in the targeted aquifer such that it compromises drinking water supply. A key potential pollutant is saline water, which often underlies the shallow freshwater zone. Groundwater abstraction can lead to up-coning of the saltwater interface, causing an increase in salt concentration in the aquifer. However, unlike simple abstraction, the saline water during ATES operation is recycled from the abstraction well into the injection well in each warm and cool cycle, creating potentially complex patterns of contamination. Here, we report a methodology to model fluid flow, heat and salt transport in ATES systems with Dynamic Mesh Optimisation (DMO). DMO allows the mesh to refine in areas of high temperature and concentration gradients, whilst remaining coarse elsewhere. We validate the method against an analytical solution for up-coning of a freshwater –saltwater interface under a single abstraction well in a homogenous aquifer. The method is then applied to ATES operation using a well doublet. Simulated saltwater concentrations are monitored at the well heads and downstream from the ATES operation. Sensitivities to key parameters of an ATES installation are studied including the depth of the interface, injection flowrates, background flow of the aquifer, and aquifer heterogeneity, to understand their impact on contamination risk. Initial results suggest that the zone of contamination is limited to the hydraulic radius, which migrates downstream if there is background groundwater flow. However, aquifer heterogeneity can significantly increase the hydraulic radius compared to the homogenous case and must be accounted for when assessing risk.

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MS07 / 295

Differentiation in biological porous media: a role for diffusio-phoresis and surface instabilities

Author: Jacques Huyghe¹

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Biology is often explained in terms of biochemical pathways. In order for these pathways to work out, substantial logistics are needed to bring molecules to find their counterparts. Diffusion is typically the magic word that comes to rescue the transport mechanisms needed. Diffusion, however, results in homogenizing the medium, while differentiation is repeatedly the observed fact. This lecture will explore the potential of diffusio-phoresis and surface instability to elicit intelligent transport of cells and molecules in biology. Experiments as well as simulations will be presented.

1. Florea D., Musa S., Huyghe J.M., Wyss H.M. Long-range repulsion of colloids driven by ion-exchange and diffusio-phoresis. *Proc Nat. Acad. Sci. USA*, 111(18): 6554-6559 (2014).
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Poster / 296

Pore-scale modelling of polymeric solutions in porous media

Author: Amna Al-Qenae^{None}

Co-authors: Rouhi Farajzadeh ¹; Vahid Niasar ²

¹ Delft University of Technology

² University of Manchester

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Enhance Oil Recovery (EOR), especially Chemical EOR (CEOR) methods are applied to extract by-passed or capillary-trapped oil from subsurface formations. These methods have the potential to reduce the carbon intensity of the produced oil and therefore will play important role during energy transition. Water-soluble polymers with non-Newtonian behavior are usually added to water to increase the viscosity of the displacing fluid and hence to obtain a more favorable mobility ratio between the displacing phase and the in-situ oil. Ideally, the concentration or mass of the injected chemicals should be minimized while the oil recovery should be maximized to obtain a favorable chemical utilization factor (kg-c/bbl), a proxy for economic evaluation of the process. Moreover, the success of polymer EOR projects depends largely on the propagation of the injected polymer to maintain the mobility control at the displacement front. This is in turn determined by the retention of the polymer governed by physical adsorption and mechanical entrapment.

In this modelling study, we focus on polymer trapping and adsorption in porous media using pore-network modelling. In the model non-Newtonian fluid properties as well as adsorption characteristics are used to simulate the flow and transport of polymeric solutions in porous media. The pore-scale modelling offers a better understanding of fluids rheology, viscosity, thermostability and flow diversion. We observe that the ratio between the size of the pore and the polymer molecule and the wetting state of the porous medium are essential parameters in propagation of the polymer. In a water wet system, the polymer molecules block the smallest pores in the medium. With injection of sufficient amount of polymer, an area of the medium becomes inaccessible to the polymer solution, which is beneficial because the small pore contain water rather than oil. On the other hand, by exclusion of a fraction of the injected polymer the concentration of polymer at the front decreases, which results in viscosity loss. The results of our simulation can be used in design of polymer injection processes to obtain a favorable polymer utilization factor.

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Participation:

Online

MS21 / 297

Some analytical results about countercurrent capillary imbibition.

Authors: benoit Noetinger^{None}; Benjamin Braconnier¹; Frederic Douarche¹; Michel Quintard²; Sina Momeni¹

¹ IFPEN

² *Institut de Mécanique des Fluides de Toulouse*

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Capillary imbibition is a major process that controls many transport phenomena in porous media for many applications. In the countercurrent case, the process may be represented as the solution of a strongly non-linear diffusion equation $\partial S(x, t)/\partial t = \nabla \cdot [D(S(x, t))\nabla S(x, t)]$ in which $S(x, t)$ denotes the wetting fluid saturation at position x at time t . The function $D(S)$ depends non linearly on S through an expression involving relative permeabilities and capillary pressure. $D(S)$ vanishes as a power law near the extreme saturations, leading to a singular boundary problem that was investigated by many authors. Considering a finite block, two time regimes can be observed: a short time regime involving the Boltzmann variable x/\sqrt{t} , and a long time asymptotic regime that remains to be elucidated. We found an ansatz was proposed that yields a complete analytical determination of the spatial part of the asymptotic long time behavior of $S(x, t)$. The corresponding flux at the boundary of the block exhibits a two regimes that may be represented as a non-linear exchange term involving the average saturation on the block, weighted by a shape factor. This feature is well-suited for setting-up a macroscopic dual porosity description.

Selected references.

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- Braconnier, Douarche, Momeni, Quintard and Noetinge, About non-linear diffusion in porous and fractured media: Early- and late-time regimes, submitted

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

A probabilistic approach dedicated to the prediction of the reactive mass transport in porous media

Author: Thomas SAYET¹

Co-authors: Lukas Jakabcin¹; Athanasios Batakis²

¹ *Laboratory of mechanics Gabriel Lamé*

² *Denis Poisson Institute*

Corresponding Authors: athanasios.batakis@univ-orleans.fr, lukas.jakabcin@univ-orleans.fr, thomas.sayet@univ-orleans.fr

It is known that the degradation refractory processes are mainly related to high temperatures and aggressive working environments. In industrial plants, refractories are in contact with complex chemical components such as slags, fumes, ashes, etc. An optimal design of the refractories rests on a multiphysics model which accounts for the significant physics that take place in the real process.

In this paper, we only focus on the complexity of the non reactive transport modelling. Classical numerical approaches accounting for the reactive transport phenomena are based on the resolution of partial differential equations that requires a high computational cost and are often subjected to spurious oscillations. In the case of coupled multiphysics problem, those oscillations lead to inaccurate stress fields and therefore unreliable lifespan of refractory materials.

This work aims to introduce a new probabilistic approach based on gradient percolation theory and called Self-organized Gradient Percolation. The method, the algorithm, the boundary conditions and the link with the physical problem are presented. The results obtained in 1D and 2D are free of spurious oscillations and the calculation time is drastically reduced compared to finite element simulations.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS15 / 299

Machine/Deep Learning Methods for Pore-Mineral Characterization and Surface Areas Analysis

Authors: Lauren Beckingham¹; Parisa Asadi²

¹ *Auburn University*

² Auburn university

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Pore-scale imaging and modeling have advanced crucially through the integration of machine learning (ML) with imaging techniques. These integrated image analysis workflows can accelerate the mineral characterization of a given geological sample. The obtained parameters such as porosity, mineral composition, mineral accessible surface area data, and segmented mineral map are utilized to parameterize reactive transport simulations. This study evaluates the potential of ML methods for parameterizing reactive transport simulations of a given sample over various image resolutions in 2D and 3D. Random Forest and U-Net deep learning methods were trained and evaluated for semantic segmentation of 3D X-ray computed tomography (CT), and a scanning electron microscopy-backscatter electron using energy dispersive x-ray spectroscopy images of thin sections captured at different resolutions. The results showed both methods had an acceptable performance with the U-Net model showing the best results due to the ability to consider spatial as well as pixel-wise information. Considering a specific method but varying resolutions, the results showed a minimum variation for mineral abundances of relatively bigger granular phases (e.g., quartz) calculated from predicted images compared to minority classes. However, considering simulated mineral accessibilities as a metric showed, the simulated accessibility of clay particles (smectite/illite) decreased due to misclassification of pores and clays resulted in higher effective surface areas for the majority classes.

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Time Block C (18:00-21:00 CET)

Participation:

Online

MS11 / 300

Probing Multiscale Dissolution Dynamics in Natural Rocks through Microfluidics and Compositional Analysis

Authors: Bowen Ling¹; Mo Sodwatana²; Arjun Kohli³; Cynthia M. Ross³; Adam Jew⁴; Anthony Kavscek²; Ilenia Battiato²

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Mineral dissolution significantly impacts many geological systems. Carbon released by diagenesis, carbon sequestration, and acid injection are several examples where geochemical reactions, fluid flow, and solute transport are strongly coupled. Yet, the dynamics of mineral dissolution and fluid-solid interaction remain poorly understood. The complexity in these systems involves interplay between various mechanisms that operate at time scales ranging from microseconds to years. Current experimental techniques only characterize dissolution processes using static images that are acquired with long measurement times and/or low spatial resolution. These limitations prevent direct observation of how dissolution reactions progress within an intact rock with spatially heterogeneous mineralogy and morphology. We utilize microfluidic cells embedded with thin rock samples to visualize dissolution with significant temporal resolution (100 ms) in a large observation window (3×3 mm). In this study, we injected acidic fluid into eight shale reservoir rock samples ranging from 8 to 86 wt % carbonate minerals. The pre- and post-reaction microstructures are characterized at the scale of pores (0.1 - 1 μm) and fractures (1 - 1000 μm). We observe that non-reactive particle exposure, fracture morphology, and loss of rock strength are strongly dependant on both the relative volume of reactive grains and their distribution. Time-resolved images of the rock cell unveil the spatiotemporal dynamics of dissolution in real-time and illustrate the changes in the fracture interface across the range of sample composition. The newly developed platform and experimental workflow provides real time characterization of geochemical reactions and has the potential to inform various subsurface engineering processes.

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MS22 / 301

Sherwood number correlation for reverse osmosis membrane systems in turbulent regime

Authors: Siqin Yu¹; Bowen Ling²; Ilenia Battiato¹

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² *Chinese Academy of Sciences*

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Evaluating and understanding mass transfer in reverse osmosis membrane (ROM) systems is critical for improving their filtration performance. Previous studies show that the Sherwood number (Sh), a dimensionless measure of mass transfer rate, is significantly impacted by Reynold number (Re) in laminar regime. Although Reynolds number in ROM systems could reach values around 10,000, to the best of our knowledge, the impact of turbulent flows on Sh - Re correlation in ROM system has never been investigated. In this work, we develop a numerical framework in the OpenFOAM platform which couples flow, mass transfer and foulant accumulation for both laminar and turbulent regimes. Reynold-Averaged Navier-Stokes equations (RANS) and mass transport equations are

employed and validated to simulate turbulent flow and mass transport in ROM systems at high Re numbers. For the first time, Sh-Re correlation in spacer-filled channels are numerically derived for ranges of Re numbers that span both laminar and turbulent regimes. The Sh-Re correlation, calculated numerically, are in agreement with theoretical calculations in both low and high-Re flows. Our results show that mass transport is significantly enhanced in turbulent flows due to unsteady vortex shedding and increase of effective diffusivity.

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MS15 / 302

Morphology Decoder: Untangling Heterogeneous Porous Media Texture and Quantifying Permeability and Capillary Pressure by Semantic Segmentation

Author: Omar Alfarisi¹

Co-authors: Aikifa Raza ; Mohamed Sassi ; Djamel Ouzzane ; Mohamed Abdelsalam ; Salem Alzaabi ; TieJun Zhang

¹ *Khalifa University of Science and Technology*

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Determining porous media physical properties, like permeability and capillary pressure, in heterogeneous porous media, like carbonate rock, is one of the most challenging tasks for scientists in the digital rock physics domain. One of these challenges is the untangling of the heterogeneous texture. Another challenge is the image's resolution, which controls the visible details of the texture. The third challenge is the size of the representative sample, where the resolution and size form an inverse relationship. At the same time, the fourth challenge is the pore network simulation, which holds lots of assumptions with error accumulation. Finally, the fifth challenge is the high computation power and related high power consumption and long calculation time. Therefore, we propose a solution for untangling the heterogeneous texture: the morphology decoder of image resolution-independent, sample size-independent, simulation free, and machine learning-driven [1-86].

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS09 / 303

Variation of the representative elementary volume (REV) in heterogeneous rocks with changing CT image resolution

Authors: Marcel Reinhardt^{None}; Saeid Sadeghnejad¹; Frieder Enzmann^{None}; Michael Kersten²

¹ *Department of Petroleum Engineering, Faculty of Chemical Engineering, Tarbiat Modares University, Tehran, Iran*

² *Johannes Gutenberg-University Mainz, Germany*

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The two paradigms of digital rock physics, chemistry, and biology are imaging and computation (Sadeghnejad et al. 2021). An unbiased characterization of rocks not only requires a sample with a sufficient volume (i.e., representative elementary volume, REV) to account for sample heterogeneity but also requires a high-resolution image with enough pore-scale details (Lin et al. 2019, Jackson et al. 2020). However, imaging at the highest resolution is expensive; therefore, there should be an optimum resolution wherein the accuracy of the pore-scale studies can be guaranteed.

REV can be computed both deterministically or statistically. Deterministic REV's can be computed by finding a field-of-view (FOV) in which the property of interest (e.g., porosity, permeability, tortuosity) no further fluctuates. However, a statistical REV is defined as the representative volume below which the statistics (e.g., mean, standard deviation, coefficient of variation) for a quantity of interest vary with the scale. Different properties may have different REV's. Moreover, from one porous medium to another or depending on the overall dimensions of the problem, the REV size will typically vary among different scale ranges (Hommel et al. 2018).

Berea sandstone samples of 10 –15 mm length and 4 mm diameter were drilled from one sample block. The samples were scanned in various resolutions by utilizing X-ray microtomography (μ XCT) and an X-ray synchrotron light source. The grey value images were segmented by applying a random forest classifier. Rock properties (including porosity, permeability, tortuosity, Minkowski measures) were computed on FOVs of varying size by applying the commercial GeoDict software package (Math2Market, Kaiserslautern, Germany) and coding in Python. In this study we aim to analyse whether REV's for properties with high computational costs (i.e., permeability) might be replaced with REV's of other properties (e.g., surface area, Minkowski measures), which have lower computational demands. Furthermore, an analysis of deterministic and statistical REV's revealed different REV sizes for the computed parameters and a dependence of REV size on the spatial resolution.

Acknowledgement

The second author (S.S.) gratefully acknowledges financial support from the Alexander von Humboldt Foundation for his visiting research at the Johannes Gutenberg University at Mainz, Germany.

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Hommel, J., E. Coltman and H. Class (2018). "Porosity–permeability relations for evolving pore space: a review with a focus on (bio-) geochemically altered porous media." *Transport in Porous Media* 124(2): 589-629.

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Sadeghnejad, S., F. Enzmann and M. Kersten (2021). "Digital rock physics, chemistry, and biology: challenges and prospects of pore-scale modelling approaches." *Applied Geochemistry*: 105028.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS01 / 304

Modeling and Simulation of Long-term Wettability Alteration on CO₂ Storage Efficiency and Containment

Authors: Sarah Gasda¹; David Landa Marbán¹; Abay Kassa¹; Kundan Kumar²; Tor Harald Sandve¹

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Geological CO₂ storage can be successfully implemented in deep saline aquifers that have sufficient storage efficiency and are overlain by a competent sealing caprock. Constitutive functions that govern macroscale capillary pressure and relative permeability are central in constraining both storage efficiency of the formation and sealing properties of the caprock. Capillary pressure and relative permeability functions for porous systems are in part determined by wettability, which is a pore-scale phenomenon that has direct influence on macroscale displacement processes. While wettability of saline aquifers and caprocks are assumed to remain water-wet when CO₂ is injected, there is recent intriguing evidence of contact angle change due to long-term exposure to CO₂. This phenomenon weakens the strength of capillary forces which subsequently alters capillary pressure and relative permeability functions dynamically over time.

Recently, new dynamic models have been developed for both capillary pressure and relative permeability functions that captures the impact of wettability alteration (WA) due to long-term CO₂ exposure. These dynamic macroscale saturation functions are driven by CO₂ exposure time that is calculated from the saturation history. In this paper, the dynamic functions are implemented into a two-phase two-component simulator to study the impact of long-term WA dynamics on field-scale CO₂ storage systems. We simulate horizontal migration patterns for CO₂ injection affected by WA dynamics for different flow regimes. Our results show that the impact of WA dynamics leads to a complex CO₂ migration behavior that is not captured by static saturation functions. Also, we find that storage efficiency can be described effectively by the capillary number. In addition, we simulate buoyancy-driven migration in the caprock caused by loss of containment due to dynamics WA. We develop scaling models for CO₂ migration into the caprock caused by dynamic wettability that show that long-term WA poses little risk to CO₂ containment over relevant timescales.

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MS17 / 307

Pin-fin shape and orientation effects on heat transfer and fluid flow in gas turbine blade

Authors: saida chatti^{None}; chekib ghabi^{None}; abdallah mhimid^{None}; mohamed Sassi^{None}

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Gas turbine blades are usually exposed to a hot gas environment. Thus, it is essential to apply effective cooling technique to extend the blade lifetime. Turbine blades employ wedge-shaped channels for trailing edge internal cooling. Many experimental and numerical studies have been conducted on the heat transfer and flow structures in a wedge-shaped channel. In this work, we focused on a prototype based on laminar flow and wall heat transfer characteristics inside a blade trailing-edge. The numerical simulation was given by the thermal Lattice Boltzmann Method. A validation code was achieved by our previous research. In this study, five baseline configurations were used. These configurations were obtained by varying the shape and orientation against the incoming airflow. They presented a similar layout with five-row pin-fins in the main coolant region and one-row fillet circular pin-fin in the exit region. As a result, we found that the pin-fin shape and its orientation have considerable effects on the wall heat transfer proprieties. Indeed, some factors, such as higher heat transfer coefficient and pressure loss, depend on the rotation of the pin-fin.

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Time Block A (09:00-12:00 CET)

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MS07 / 308

A multipoint stress-flux mixed finite element method for the Stokes-Biot fluid poroelastic structure interaction model

Authors: Sergio Caucao¹; Tongtong Li²; Ivan Yotov²

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We develop a fully mixed formulation of the Stokes-Biot model for fluid poroelastic structure interaction and its mixed finite element approximation. The Stokes formulation is based on weakly symmetric deviatoric stress, velocity, and vorticity. The elasticity formulation is based on weakly symmetric stress, displacement, and rotation. The porous media flow formulation is based on Darcy velocity and pressure. Well posedness of the variational formulation is established. The multipoint stress mixed finite element method is employed for the discretization of the Stokes and elasticity equations. The multipoint flux mixed finite element method is utilized for the Darcy flow. The methods are based on the lowest order BDM spaces for the stresses and the Darcy velocity. A vertex quadrature rule is employed for the bilinear forms involving these variables, which allows for their local elimination, as well as the local elimination of vorticity and rotation. This results in a symmetric and positive definite cell centered system involving only Stokes velocity, displacement, and pressure. We study the stability and accuracy of the method and present numerical experiments.

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Time Block C (18:00-21:00 CET)

Participation:

In person

MS15 / 309

10,000-cubed Digital Rock Analysis: Beyond Hardware Super Resolution Imaging and Efficient HPC Modelling

Authors: Ying Da Wang¹; Ryan Armstrong^{None}; Peyman Mostaghimi^{None}

¹ *UNSW*

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The trade-off between the field of view (FOV) and the resolution of micro-computed tomography (micro-CT) is a hardware bottleneck that limits the capturing of both heterogeneity and micro-structure detail for analysis and modelling. Rather than choosing between high resolution or wide FOV, efficient super resolution methods can achieve both, while efficient modelling methods permit full analysis of the resulting large image. Low resolution images of porous rock and 4x scale high resolution images train an efficient 3D super resolution convolutional neural network (SRCNN). An unseen test image of a full coreplug with an otherwise unsegmentable wide FOV and low resolution is then super resolved to 10,000-cubed, and its permeability, flow field, and 2-phase flow is calculated with a High Performance Computing (HPC) cluster using efficient hybrid implementations of Semi-Analytical Solvers (SAS), Morphological methods, and Lattice Boltzmann Methods (LBM). A similar result is also obtained with other types of porous structures, such as a Proton Exchange Fuel Cell. This extent of resolution-FOV is 2 orders of magnitude above hardware limitations, and brings digital rock analysis closer in scope to conventional core-plug analysis.

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Wang Y.D., Blunt M.J., Armstrong R.T., Mostaghimi P.
Deep learning in pore scale imaging and modeling
Earth-Science Reviews (2021), p. 103555, 10.1016/j.earscirev.2021.103555

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS08 / 310

Pattern formation in carbonate precipitation in confined geometry

Authors: Negar Shahsavari¹; Xiaojing Fu^{None}; Benzhong Zhao^{None}

¹ *Ph.D. Student*

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Carbon capture and storage (CCS) is a promising technology to significantly reduce the amount of carbon dioxide (CO₂) emissions in the atmosphere. In CCS, CO₂ is captured at concentrated point sources and injected deep underground for permanent storage. Geochemistry is an important consideration in CCS projects since the injected CO₂ will dissolve in the ambient brine and interact with the host rock, resulting in either rock dissolution or mineral precipitation. In contrast with the wealth of studies on CO₂-driven dissolution, mineral precipitation is less well understood. This is partly due to the conventional wisdom that mineralization occurs on a much longer timescale compared to dissolution. However, recent field studies have demonstrated significant, fast mineralization when CO₂ is injected in reactive rocks such as basalt (Matter et al., 2016). The mineralization

alters the permeability around the injection well, and it has significant implications for the injectivity of the storage operation.

Here, we investigate the interplay between CO₂ injection, carbonate precipitation, and permeability evolution via simple microfluidic experiments. Specifically, we perform constant-rate injection of sodium carbonate into a radial Hele-Shaw cell filled with calcium chloride. Sodium carbonate readily reacts with calcium chloride to form calcium carbonate precipitate. We perform the experiments over a wide range of Péclet numbers (i.e. relative importance between advection and diffusion). At a low Péclet number, we observe a stable precipitation band that expands radially outward. However, at higher Péclet numbers, we observe viscous fingering-like precipitation patterns at the precipitation band, even though the fluids are of the same viscosity. This hydrodynamic instability arises as a result of precipitation, which locally decreases the effective mobility of the defending fluid. The precipitates generated at the interface of the fingers travel much slower than the precipitation band, which allows them to capture other precipitates through collision and aggregation. Therefore, our results demonstrate that the interplay between hydrodynamics and reaction can have an important control on permeability evolution in CO₂ storage in reactive formations.

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Time Block C (18:00-21:00 CET)

Participation:

Online

Poster / 311

Investigation of coupled processes in fractures and the bordering matrix via a micro-continuum reactive transport model

Authors: Qian Zhang^{None}; Hang Deng^{None}; Yanhui Dong^{None}; Sergi Molins^{None}

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In multi-mineral fractured rocks, the altered porous layer on the fracture surface resulting from preferential dissolution of the fast-reacting minerals can have profound impacts on subsequent chemical-physical alteration of the fractures. This study adopts the micro-continuum approach to provide further understanding of reactive transport processes in the altered layer, and mass exchanges with the bordering matrix and fracture. The modeling framework couples the Darcy-Brinkman-Stokes (DBS) solver in COMSOL Multiphysics and the geochemical modeling capability of CrunchFlow. 3D steady state simulations with systematically varied chemical-physical parameters of the altered layer were performed to examine the impacts of individual factors and processes. Our simulation results confirm previous observations that dissolution of the fast-reacting mineral (i.e., calcite) is largely controlled by diffusion across the altered layer. We also show that dissolution of the slow-reacting mineral (i.e., dolomite), which controls altered layer development and fracture enlargement, increases with surface area and has a complex dependence on different local rate-limiting processes. In particular, advection can result in evident spatial variations in the local dissolution rates of dolomite, although it does not affect the bulk chemistry significantly. The difference in the spatial patterns between simulations with and without advection in the altered layer is more noticeable in the locations

with smaller apertures, with up to 20% difference in local reaction rates. Therefore, it is important to include a full depiction of advection, diffusion and reactions for accurately capturing local dynamics that control long-term fracture evolution.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS01 / 312

CO₂ dissolution patterns with precipitation reaction under different permeability

Author: Shuai Zheng¹

Co-authors: Ke Xu ¹; Dongxiao Zhang

¹ Peking University

Corresponding Authors: dxz@pku.edu.cn, kexu1989@pku.edu.cn, shuaiz@pku.edu.cn

After CO₂ is sequestered into deep saline aquifers, it dissolves into underlying brine, with extensive precipitation reactions emerging. Whether and how precipitation reactions impact CO₂ dissolution is still an open question that affects the evaluation of sequestration safety and efficiency.

We conduct visualized experiments in a visible chamber. Calcium hydroxide (Ca(OH)₂) solution saturated in bead-pack is positioned into CO₂ atmosphere under 1 Mpa, 25 °C. Ca(OH)₂ concentration is one order of magnitude lower than the saturated CO₂ concentration. Permeability (k) is tuned by using glass beads with different sizes. pH indicator is added into the liquid to visualize the reaction front. Front velocity (U) is recorded that represents the dissolution rate.

In all experiments, we observe clear reaction front where pH quickly transients from 5 to 10. We also observe circumflux between the reaction front and the liquid surface, which is induced by buoyancy-driven hydrodynamic instability. However, dissolution patterns in the high/low permeability media are remarkably different, as shown in Figure 1:

- In high-permeability regime, strong hydrodynamic instability is observed, and precipitated CaCO₃ particles flow with the circumflux that emerge in large region. With the increasing of permeability, the U increases sub-linearly with k , approaching to its maximum in the condition without porous structure.
- In low-permeability regime, surprisingly, no pore-blocking happened and even no solid CaCO₃ particles are observed during the dissolution process. The U linearly increases with the increasing

of permeability. This linear $U - k$ dependence is also observed for CO_2 dissolution in DI water without Ca^{2+} .

We rationalize this difference by highlighting the role of porous structure. If the pore size is below a critical size, CaCO_3 is trapped and quickly consumed in the pore where it precipitates, so the density at the reaction front is thus the minimum in the system. As a result, mass transfer is dominated by buoyancy-driven convection above the reaction front, and by molecular diffusion beneath the front. Decreasing permeability results in quick compromise of convection but mild change in diffusion. Therefore, in low permeability condition, convection above the front limits the dissolution rate, resulting in a proportional $U - k$ correlation. In contrast, when permeability is high, diffusion beneath the front becomes the limiting factor of dissolution, resulting in a sublinear the $U - k$ correlation. In addition, at extremely high permeability with large pore, precipitated CaCO_3 is no longer trapped in the pore and complicates the dissolution kinetics.

We further implement same experiments but using DI water instead of $\text{Ca}(\text{OH})_2$ solution, in which case dissolution is completely governed by buoyancy-driven convection. As expected, U in this precipitation-free system keeps linearly correlated to k , without sublinear segment in large k regime. It thus highlights the key role of CaCO_3 precipitation in high-permeability scenario.

This work suggests permeability as a key factor that fundamentally reshape CO_2 storage mode and efficiency, by (1) regulating the immigration of precipitated CaCO_3 , and (2) modifying the limiting factor of mass-transfer.

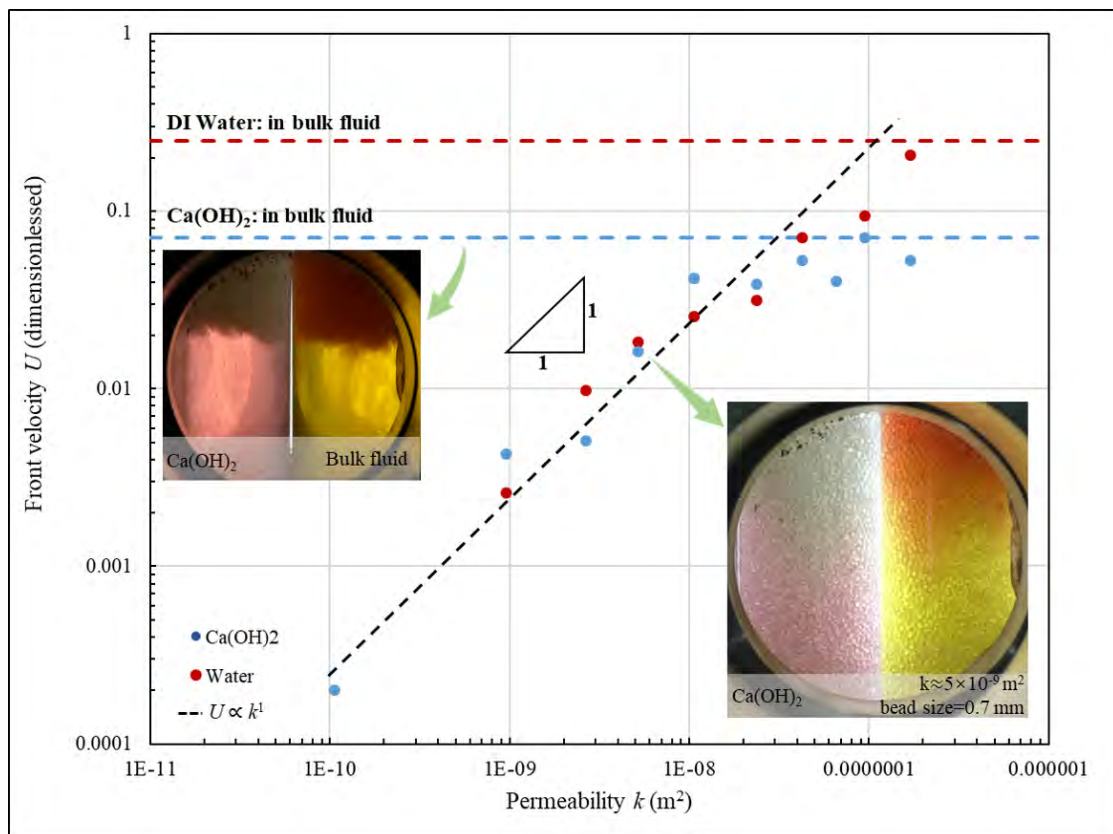


Figure 1: $U - k$ correlations for $\text{Ca}(\text{OH})_2$ /water and insets captured during dissolving.

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MS09 / 314

Pore-scale modeling of the dynamics of interface-coupled dissolution-precipitation

Authors: Hang Deng¹; Jenna Poonoosamy^{None}; Sergi Molins²

¹ *Peking University*

² *Lawrence Berkeley National Laboratory*

Corresponding Authors: smolins@lbl.gov, j.poonoosamy@fz-juelich.de, hangdeng310@gmail.com

In interface coupled dissolution-precipitation (ICDP) systems, pore structures change following the dissolution of the primary mineral and the precipitation of the secondary mineral. In order to predict the dynamics of the mineral-fluid interface, it is important to understand the interplay between macroscopic flow regimes and microscopic reaction mechanisms (e.g., nucleation and crystal growth pathways). In this study, we use a micro-continuum pore-scale reactive transport model to investigate ICDP processes with explicit consideration of surface passivation and the diffusion process through the precipitating layer. Our model results highlight that the drastically different coating behaviors at the macroscopic scale and their dependence on solution supersaturation observed in previous column experiments are primarily controlled by the interplay between mineral reaction rates, advective flow, and diffusion through the dynamically forming coating layer. Furthermore, in order to examine the controls on the textures of precipitates that will largely dictate the diffusion properties of the coating layer, we developed a probabilistic nucleation module building upon the classical nucleation theory. This new capability allowed us to consider saturation-dependent nucleation rate and the stochastic nature of the nucleation process, and the results highlight the complex dependence of precipitates' texture on solution chemistry and substrate properties. The modeling observations also underscore the necessity of further investigations to better characterize the properties of the coating layer and to improve modeling descriptions of the nucleation processes.

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Deng, H., Poonoosamy, J., Molins, S., 2022. A reactive transport modeling perspective on the dynamics of interface-coupled dissolution-precipitation. *Applied Geochemistry*, 105207, <https://doi.org/10.1016/j.apgeochem.2022.105207>.

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Participation:

Unsure

Poster / 315**Evaluation of fluid flow behavior and trapped non-wetting phase saturation with modified pore morphological approach in clastic reservoirs****Author:** Fatime Zekiri¹**Co-authors:** Gordon Burmester¹; Hrvoje Jurcic¹; Pit Arnold²; Holger Ott³¹ *OMV Exploration & Production*² *Montanuniversität Leoben*³ *Montanuniversität Leoben***Corresponding Authors:** fatime.zekiri@omv.com, burm2011-public@yahoo.com, pit.arnold@unileoben.ac.at, hrvoje.jurcic@omv.com, holger.ott@unileoben.ac.at

The quantification of fluid flow properties and residual non-wetting phases in petroleum reservoirs is essential to understand hydrocarbon recovery or CO₂ storage capacity of the subsurface reservoirs. Specific core experiments used to derive such properties, e.g., trapping curves and relative permeabilities can be time-consuming, difficult to conduct and sometimes not representative for the entire reservoir. Recent developments in Digital-Rock-Physics (DRP) are promising for effective prediction of fluid flow behavior based on 3D pore-scale images of rock samples. In this study, we will focus on the pore morphological approach (PMM) and its applications for OMVs clastic reservoirs.

The PMM is a quasi-static method that predicts the distribution of two fluids inside a porous medium and assumes that capillary forces are dominant. The method distributes the fluids using morphological operations to model drainage and imbibition processes. PMM shows very good results for primary drainage, but has shortcomings, when describing imbibition processes. Therefore, modifications were necessary to improve this simulation part, which is key in understanding hydrocarbon recovery. Sub-resolution wetting layers, which can swell while running a waterflood simulation and the possibility to assign different wetting conditions, by using multiple contact angles, were implemented in the application. Furthermore, a combined modeling of an imbibition and drainage sequence, allowed to extend the imbibition branch from spontaneous to forced imbibition.

The modified PMM was tested on clastic water-wet reservoirs, which have good to medium quality reservoir properties (e.g. porosities > 10 % and permeabilities from 100 –5000 D). The primary drainage and imbibition processes were simulated for several plugs covering two rock types per reservoir. The initial and the residual non-wetting phase saturations were used to derive trapping curves. The simulated results were then compared to industry-wide accepted correlations, such as the Land correlation, and to available core data. The comparison showed good agreement between simulated and measured data. Furthermore, two-phase fluid flow simulations for the imbibition process were conducted with the modified PMM approach for all rock types and compared to available core data. Again, the simulated relative permeabilities match well with available core data per rock type. If core data was not available, we compared it to analogue data from our internal rock-fluid database and subsequently with log upscaling.

Overall, the results from modified PMM showed that the simulations for the imbibition processes are in line with expected trends, e.g. the residual non-wetting phase saturation decreases with increasing contact angle and that the results are in good agreement with core and log data. After simulation of imbibition relative permeabilities, there are still some snap-offs mainly in intermediate rock types for the non-wetting phase branch observed, which results quickly in connectivity loss and therefore steep decrease of non-wetting phase relative permeabilities. However, these are topics to be addressed in follow-up studies in the upcoming year next to addressing mixed wet and heterogenous reservoirs.

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MS07 / 316

A One-domain approach for flow near porous media boundaries

Authors: Francisco J. Valdés-Parada¹; Didier Lasseux²

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Momentum transport near porous media boundaries has been the subject of intense work for more than half a century since the pioneering work of Beavers and Joseph in 1967 [1,2]. Currently, there are two modeling strategies to study this subject: 1) A one-domain approach (ODA), where the spatial variations of average properties are accounted for in the transition zone and 2) a two-domain approach (TDA), where these variations are collapsed in a boundary condition [3]. The TDA has received much more attention than the ODA due to the practical use of jump conditions, whereas a closed-form of the ODA has been typically made obscure and dependent of pore-scale solutions in the entire system. Nevertheless, the derivation of a jump condition for the TDA requires that the ODA be developed first. In this work, a practical formulation of the ODA is presented, that is valid for a porous medium sharing boundaries with a free fluid [4], another porous medium or a solid material. It has the simple structure of a Darcy-like model involving a position-dependent permeability tensor that is predicted from the solution of an ancillary closure problem. The performance of the model is exemplified in the vicinity of a fluid channel, near the boundary of two porous media (either in direct contact or separated by a fracture) and for flow between a porous medium and an impervious wall [5]. In all cases, the model predictions are validated with pore-scale simulations showing an excellent agreement. Furthermore, in the case of a fluid-porous medium boundary, the model is also validated with experimental data [4]. The simplicity and versatility of the new ODA model provided here make it an interesting alternative to existing approaches in the literature.

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Poster / 318

Parameter estimation for unsaturated flow with an efficient encoder-decoder convolutional neural network

Authors: Mohammad Reza Hajizadeh Javaran¹; Mohammad Mahdi Rajabi¹; Benjamin Belfort²; Marwan Fahs²

¹ *Civil and Environmental Engineering Faculty, Tarbiat Modares University, PO Box 14115-397, Tehran, Iran*

² *Université de Strasbourg, CNRS, ENGEES, ITES UMR 7063, F-67000 Strasbourg, France*

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Variably saturated flow in porous media is an important process of interest in many applications related to agriculture, geotechnics, sustainable water resources management. Its modeling has great issues in engineering and research & development, and the use of the “quite classical” model combining the Richards’ Equation (RE) and constitutive laws (e.g., van Mualem –van Genuchten or Brooks – Corey) remains a delicate challenge due to the necessity to deal with complex geometries, large space and long time simulations, variable boundary conditions, and often high non-linearities occurring in the simulations. Besides, hydraulic parameters related to the porous media have to be defined as input parameters of the computational model (Rajabi et al., 2020). This characterization - i.e., parameter estimation - can be achieved by inverse modeling approach, and in the context of unsaturated flow, many studies have tried to estimate these input parameters using different methods such as cloud computing and data-driven models. In this work, we aim to investigate the performance of the encoder-decoder convolutional neural network (ED-CNN) (Rajabi et al., 2022) as an optimizer tool to estimate the input parameters of flow employing the concept of image to image regression using input-output pairs through a supervised learning process. Input-output couples include maps of water content during an unsaturated flow experiment and parameters maps, respectively. Images of 3 relevant parameters, including $[k]_s$, which is saturated conductivity, α , the parameter related to the mean pore size, and n , the parameter reflecting the uniformity of the pore size distribution, are combined in a single parameters map. The training dataset is generated and then stored as PNG images using a numerical code based on RE which simulates the drainage phase of the laboratory experiment carried out by Belfort et al. (2019). The ED-CNN is then trained and evaluated using different evaluation metrics such as root mean squared error (RMSE) and relative errors. RMSE for $[k]_s$, α , and n is about 0.14, 0.12, and 0.12, respectively. Moreover, the relative error amount is

0.07, 0.03, and 0.02 for estimated parameters, respectively. Hence, to further assess the efficiency of the network as an optimizer, we compared real maps of parameters with ED-CNN predictions. We got a good agreement between them and low relative errors. The network's accuracy and speed revealed promising results as an inverse modeling tool for a transient simulation, indicating its potential for future subsurface and groundwater engineering applications and any other image-based kind of data.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS08 / 322

Gravity shapes permafrost melting after saline water invasion

Author: Yumin Wang¹

Co-authors: Yuheng Zhang²; Ke Xu³

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Invasion and retention of seawater into surface caves and fractures in permafrost land induces melting, as salt lowers water freezing point. Melting of permafrost region changes surface energy balance by modifying sunlight reflection rate and adsorbing latent heat, which may finally impact the global

climate mode. Therefore, it is of environmental significance to investigate ice melting in soil porous media with saline water invasion.

Visualized experiments are conducted in 3D-printed porous micromodel and bead-packs. A porous region saturated with ice is in contact with a vertical fracture/vug saturated with saline water. Dye is added into the saline water to characterize the melting front evolution as well as to visualize the concentration profile. Melting process is recorded by camera and microscope.

Surprisingly, we find that very little melting at the top –instead, a preferential melting region is observed at the bottom of the frozen porous media (shown in Fig.1). Strong upward convection along the inclined melting front is identified, implying the major role of gravitational force induced by the density contrast between just-melted pure water and original saline water.

Theoretical analysis demonstrates that this preferential melting emerges when the characteristic Peclet number $Pe > 1$, corresponding to pore size of $> 0.1\text{mm}$. When pore size is larger, gravity-driven convection dominates over diffusion that results in this preferential melting; when pore size is smaller, diffusion takes dominance and the melting front is relatively uniform. Analytical model of the preferential melting kinetics is derived that predicts experimental results well. As more than 70% particles in permafrost soil are larger than 0.1mm , this preferential melting should be highlighted in practice.

This preferential permafrost melting may lead to the formation of discrete permafrost islands floating on a melted mud layer. It alters (1) the heat transfer between the frozen surface and the environment, and (2) the mechanical performance of the permafrost surface. It thus should be seriously considered for accounting surface energy balance and evaluating civil construction at permafrost region.

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MS09 / 323

Pore network simulation of salt subflorescence growth in a porous medium

Author: oumayma fekih¹

Co-authors: Marc Prat²; nour sghaier¹

¹ LESTE

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Corresponding Authors: sghaier_nour@yahoo.com, fekihoumaima92@gmail.com, marc.prat@toulouse-inp.fr

Salt precipitation in porous media is of central interest in several applications, such as the salt crystallization induced damages in building materials, the underground storage of CO₂ or the evaporation process from soils and the soil salinization issue, to name only a few. When the salt precipitates inside a porous medium, the resulting salt structure is called subflorescence. The experiment reported in 1 shows that the subflorescence is itself a porous structure and that its growth is controlled by the distribution of the evaporation flux at its boundary.

The objective of the present work is to develop a pore network model (PNM) so as to analyze the subflorescence growth in more depth. The first step is to perform the simulation of the experiment reported in 1 where the subflorescence growth is observed in a 2D model porous medium made of a monolayer of glass beads sandwiched between two glass plates. The pore network model combines a drying algorithm [2] with the salt structure growth mechanisms identified in 1 and [3]. The main subflorescence formation and growth mechanisms will be described as well as the PNM developed. Simulations of the subflorescence development will be presented in conjunction with the experiment 1.

1 N.Sghaier, S.Geoffroy, M.Prat, H.Eloukabi, S. Ben Nasrallah, Evaporation driven growth of large crystallized salt structures in a porous medium, *Physical Review E* 90, 042402 (2014)

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2 M.Prat, Recent advances in pore-scale models for drying of porous media, *Chem. Eng. J.* 86: 153-164 (2002).

3 G.Licsandru, C. Noiriél, P.Duru, S. Geoffroy, A. Abou-Chakra, M.Prat, Dissolution-precipitation driven upward migration of a salt crust. *Physical Review E* 100, 032802 (2019).

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS09 / 324

Mobilization erases bubbles' hysteresis in porous media

Authors: Chuanxi Wang¹; Ke Xu¹

¹ Peking University

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In a d -dimensional porous medium, $d+1$ Minkowski functionals are required to fully characterize the status of two-phase immiscible fluids (1, 2). If fewer variables are available, which is practically common, the hysteresis effect emerges that disables unbiased estimation of fluid properties. Therefore, researchers are making major efforts to reduce the number of functionals under certain circumstances (3, 4). Here, we show that, once bubbles (or droplets, ganglia) are mobilized, their hysteresis in porous media can be largely erased, which may significantly simplify the characterization of the multi-fluid dynamic porous medium.

We inherit a conceptual model describing bubbles residing in a homogeneous porous medium (5). An external field is imposed, whose intensity is evaluated by a modified Bond number Bo_m , defined as the ratio of the external field potential drop to capillary pressure, P_c . We track the bubble evolution under increasing Bo_m .

A surprising “normalization” effect is revealed before a bubble is finally mobilized: regardless of its multiple possible initial pore-occupancies, capillary pressures, and surface area (5), the bubble gradually evolves towards a specific morphology when Bo_m keeps increasing. During the normalization, the bubble behaves as a wriggling worm that repeats two modes: (1) reversibly deforms to balance the external field without changing pore occupancy, and (2) irreversibly marches its head outwards or withdraws its tail inwards thus changing pore-occupancy by one. [Fig.1a] Finally, at the critical $Bo_{m,c}$, the bubble starts to flow, and it reaches a *final state* with a minimum total energy [Fig.1b&1c].

Furthermore, we find that P_c of bubbles in their *final states*, regardless of their sizes, fall into a very narrow interval around a constant, P_c^* , although their initial P_c vary in a much wider range. This *final* P_c^* depends only on the pore-throat structure, regardless of bubble size and initial morphology [Fig.1d]. Similar evolution towards a constant also happens for the specific surface area or molar free energy. Thus, we can now give an unbiased and precise estimation on dispersed phase properties, without the need to know pore-scale details like Euler characteristics, pore occupancy, etc., if the bubbles experienced mobilization. In other words, mobilization erases bubbles’ hysteresis.

Despite limitations in heterogeneity and wettability, we believe our simple analysis successfully captures the essence of how bubbles are mobilized under external fields and how mobilization erases hysteresis. This discovery is aligned with previous simulations and experiments that we re-visit (6, 7), and could be applied to significantly simplify the modeling of two-phase immiscible flow in porous media.

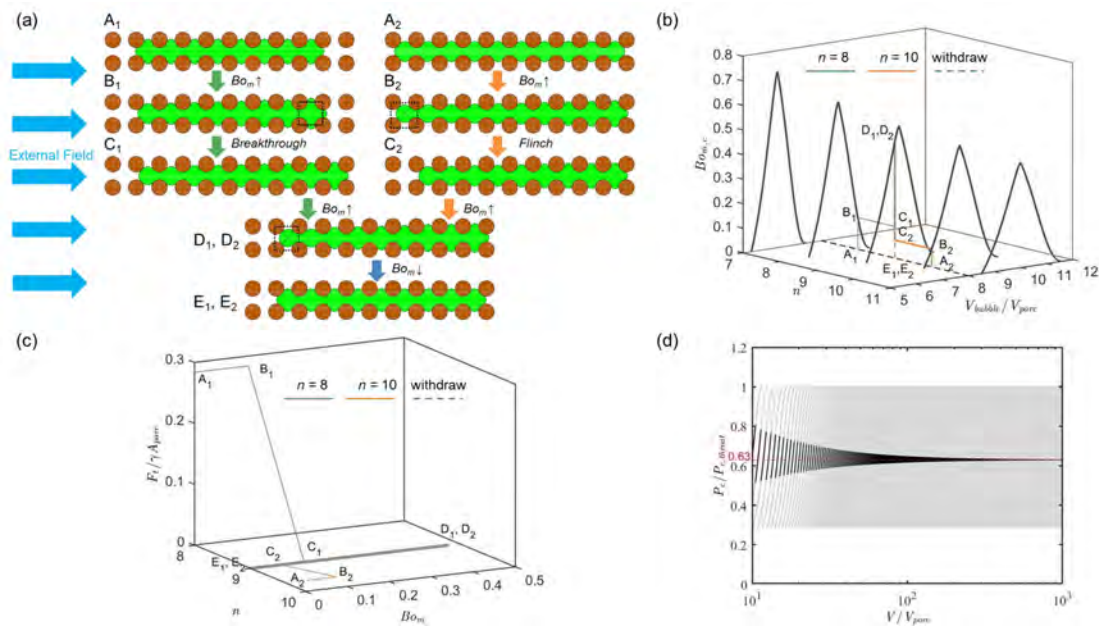


Figure 2: (a) A bubble wriggles like a worm under first increasing and then decreasing Bo_m . (b)(c) Evolution of the bubble morphology and total energy during mobilization and subsequent immobilization. (d) The $P_c - V$ relation for bubbles after mobilization and subsequently immobilization (black lines), while the red line represents the almost constant P_c for large bubbles. Gray lines represent metastable bubbles in the absence of the external field. The pore throat aspect ratio is set to be 6 in all figures.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

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Poster / 325

Pore level vs. continuum level model for solar thermochemical fuel production**Authors:** Da Xu¹; Meng Lin¹¹ *Southern University of Science and Technology***Corresponding Authors:** xud2020@mail.sustech.edu.cn, linm@sustech.edu.cn

For the solar-driven thermochemical fuel production redox cycle, the porous media design significantly determines the solar-to-fuel efficiency and per mass loading conversion efficiency of each redox cycle by governing the heat and mass transfer properties. Thermodynamically, porous media is expected to have a large surface area for fast reaction rate and a large mass loading for high fuel production amount. It has been concluded from the literature that the reduction step is surface area limited in micro/nano powder thermogravimetric study, while the particle size is also reported to become the other limitation as its size gets large enough to hinder the bulk oxygen vacancy diffuse. To optimize the porous media design, a comprehensive modeling framework for Triply periodic minimum surface (TPMS) structures, which are well-known for their mathematic equation-driven modeling and flexibility in design, has been developed to identify the volume-averaging geometrical properties, mass and heat transfer properties in our previous study. To analyze how the redox reaction is influenced by porous media's structure design, a new continuum level model is developed. It introduces rough surfaces in addition to the millimeter-scale TPMS structure. The surface roughness is simply treated as a correction factor of the surface area, which amplifies the reaction rate. However, this amplification will not influence the reaction equilibrium. The probable impact of porous media structure on bulk diffusivity cannot be observed either. Therefore, we are proposing a pore-level model to capture the mass and heat transfer behavior of extract three-dimensional porous media, coupled to thermochemical reaction with the consideration of bulk diffusion, surface exchange, and gas-phase diffusion. The micrometer-level spheric holes are randomly excavated over the TPMS structure to create the secondary pores (surface roughness). In this model, the surface exchange governing region and bulk diffusion governing region are identified at various combinations of surface area and particle size distribution. Additionally, the particle size is optimized to avoid bulk diffusion limitation.

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MS06-B / 326

Marangoni Effect Maintains Fast Evaporation in Near-Fracture Porous Media

Author: Yandong Zhang¹

Co-authors: Ke Xu¹; Fei Yu

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When dry CO₂ is sequestered into saline aquifer, CO₂ preferentially goes through high-permeability pathways, leaving the water in unswept low-permeability porous media evaporating into the CO₂ phase. Similar scenarios that volatile liquids evaporate into high-permeability pathways can also be observed in gas condensate reservoir recovery, shale gas recovery, and fuel cell water management, etc. Evaporation changes fluid saturation as well as local temperature and pressure that determines the flow and transport performance of abovementioned natural and engineering processes. Specifically, when extensive evaporation occurs, significant temperature and concentration gradients may occur that complicates the flow dynamics.

In this study, we conduct visualized micromodel experiments to investigate the evaporation of volatile liquids in porous media after dry gas flowing through an adjacent fracture. The porous medium is saturated first with pentane (for fast evaporation tests) or isoheptane (for mild evaporation tests), and air is then continuously injected to flow through the fracture. Evaporation rate is controlled by the choice of liquid and the injection rate. Peclet number (Pe) in the fracture ranges from ~0.1 to 107.

Surprisingly, the evaporation pattern under extensive evaporation and mild evaporation are qualitatively different, even under same (and negligible) shearing from gas flow in the fracture. When the evaporation is mild (1.2×10^{-4} kg/m²/s), the air invades into the porous media layer-by-layer, in a classic “capillary fingering” pattern, and forms a dry fracture/matrix interface. The evaporation rate gradually slows down by scaling $dS/dt \sim t^{-1/2}$, as a natural consequence of enlarging mass transfer distance from the drying front to the fracture. However, when the evaporation is ten thousand times faster (0.7 kg/m²/s), the evaporation front and the displacement front separates: the gas invades deep into the porous medium through preferential paths, while the main drying front keeps unmoved and stable at fracture/matrix interface (see Figure 1), even when the displacement rate is still in the “capillary fingering” regime. As long as the evaporation front is pinned, the evaporation rate keeps constant without slowing down.

Isothermal theory cannot rationalize this dramatic contrast behaviors of mild and extensive evaporation in near-fracture zone. We therefore use infrared camera to record the experiment, and discover a strong cooling belt around the interface at high evaporation rate. The existence of significant temperature gradient in this condition implies the involvement of Marangoni effect: strong evaporation cools down the fracture-matrix interface, resulting in higher interfacial tension (IFT) near the fracture than in deeper region of the porous matrix. This IFT gradient along the liquid-gas interface drives liquid in deeper matrix towards the fracture that supplies the evaporation front. As a result, the evaporation front is pinned at the fracture/matrix interface that maintains a constant evaporation rate.

This discovery that Marangoni effect reshapes evaporation pattern in near-fracture zone highlights the significance to take non-isothermal effect into consideration, when extensive phase changes emerge in CO₂ sequestration, hydrocarbon recovery and fuel cell design.

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Poster / 327

Microplastics Effects on Evaporation Dynamics and Cracking Morphology in Drying Porous Media

Authors: Sahar Jannesarahmadi¹; Nima Shokri¹

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Global production of plastics has increased exponentially over the past few decades. Annual production of plastics increased nearly 200-fold in 2015 compared to the production of nearly 2 million tones per year in 1950 (1). Estimates suggest that of the estimated 6.3 billion tones of plastics produced up to 2015, almost 80 percent has not been disposed of properly (2). Soil represents a large reservoir for plastics disposal. The improperly disposed plastics could serve as a major and long-term source of contamination. Degrading into microplastics (MP), they can affect soil properties and structure. The accumulated MP could enter food chains posing serious risks to food security and environmental health.

Within this context, the present study aims at analyzing effects of MP on water evaporation from porous media and cracking morphology induced by drying. A series of evaporation experiments were conducted under laboratory conditions. Quartz sand (particle size: 0.4-0.8 mm) and bentonite clay were used for evaporation experiments. Powders of Polyethylene (PE) with particle size ranges of 34-50 μm and Polyvinylchloride (PVC) were used as MP. Dry sand particles were mixed with PE and PVC at the concentration of 0.75% and 1.5% (by mass). The mixture of sand and MP was saturated by water and packed into cylindrical glass containers (200mm in height and 80 mm in diameter). An additional sand column was prepared without MP serving as the reference. Sand columns were mounted on digital balances to record evaporation dynamics in a climate chamber at constant temperature of 30°C and relative humidity of 30%. Each experiment lasted nearly 16 days and repeated four times. For the cracking analysis, the drying sample composed of 1:2 ratios of sand and bentonite clay (by mass). Sand-bentonite mixtures were mixed with PE and PVC at the concentration of 0.75%, 1.5%, 4.5%, 6%, 8% and 10% (by mass). Reference samples were also prepared without MP. Mixtures of sand-bentonite-MP were mixed with water at two different ratios of 1:4 and 1:5 (solid to water ratio by mass). Resulting pastes were poured into Petri dishes (15 mm in height and 145 mm in diameter) placed in the climate chamber at constant temperature of 30°C and relative humidity of 40%. Each experiment was replicated three times (resulting in 78 drying samples). After nearly one week of drying, the crack morphology was recorded using a digital camera. To analyze cracks patterns and characteristics, a code was developed in MATLAB. Our preliminary results confirm evaporation dynamics and cracking morphology in desiccating clays are influenced not only by MP concentration but also by MP physical and chemical characteristics. Our results will show how the cumulative mass loss as well as the length, density and area of cracks formed as a result of drying are influenced by type and concentration of MP and will shed new lights on effects of MP on soil water evaporation.

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1. Crawford, C.B., Quinn, B. (2017). Microplastic Pollutants, Elsevier, <https://doi.org/10.1016/C2015-0-04315-5>.
2. FAO (2021). Assessment of agricultural plastics and their sustainability –A call for action. Rome. <https://doi.org/10.4060/cb7856en>

Time Block Preference:

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MS03 / 328

Miscible displacement in near-fracture porous media with non-Fickian Diffusion

Author: Fei Yu^{None}

Co-authors: Yandong Zhang¹; Ke Xu¹

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Miscible displacement in fractured media is ubiquitous in many scenarios such as CO₂ sequestration, shale gas recovery, and reactive transport in groundwater, etc. In dilute solution cases, coupling Fick's law and Darcy's law works well in predicting the displacement behavior, which has been incorporated into commercial simulation software such as CMG, UTCHEM and Eclipse. However, non-dilute miscible displacement, which is the more common scenario for subsurface CO₂ sequestration and shale gas recovery, has been rarely investigated. Whether the Fick-Darcy coupling still works remains untested.

In this study, we experimentally investigate miscible displacement in a 3D-printed micromodel that mimics a near-fracture porous medium. The micromodel is first saturated with liquid paraffin (200 cp), and tetradecane (2 cp) is injected into the fracture. Liquid paraffin in the near-fracture porous media is thus displaced by and mixed with tetradecane. Peclet number (Pe) in our experiments ranges from $O(1)$ to $O(10^5)$, and the sweep efficiency (S) is recorded to characterize displacement kinetics.

The displacement kinetics in low Pe experiments are well predicted by reservoir simulator adopting Fick-Darcy coupling. However, the prediction is less and less accurate with increasing Pe . When $Pe \sim O(10^5)$, the Fick-Darcy coupling completely fails to characterize the displacement, with an anti-intuitive wedge-like displacement pattern (Fig. 1(a)) observed. We identify strong convection deep in the matrix and far from the fracture when displacement front sweeps over, which cannot be rationalized by the Fick-Darcy coupling. The evolution of S in experiments follows a novel scaling of $S \sim t^{1/2}$, while the Fick-Darcy coupling predicts a much slower, sub-diffusive kinetics, as shown in Fig. 1(c) &(d).

By conducting careful comparative experiments, microscopic visualization and numerical simulations, we demonstrate that this deviation is a consequence of non-Fickian diffusion at the displacement front, where the concentration gradient is so extensive that strong convection is induced. By adopting the concept of “effective interfacial tension”, we successfully rationalize the displacement kinetics.

We thus highlight the significance to take non-Fickian effect into consideration for future modeling of CO₂ sequestration and shale oil recovery, where non-dilute miscible displacement emerges.

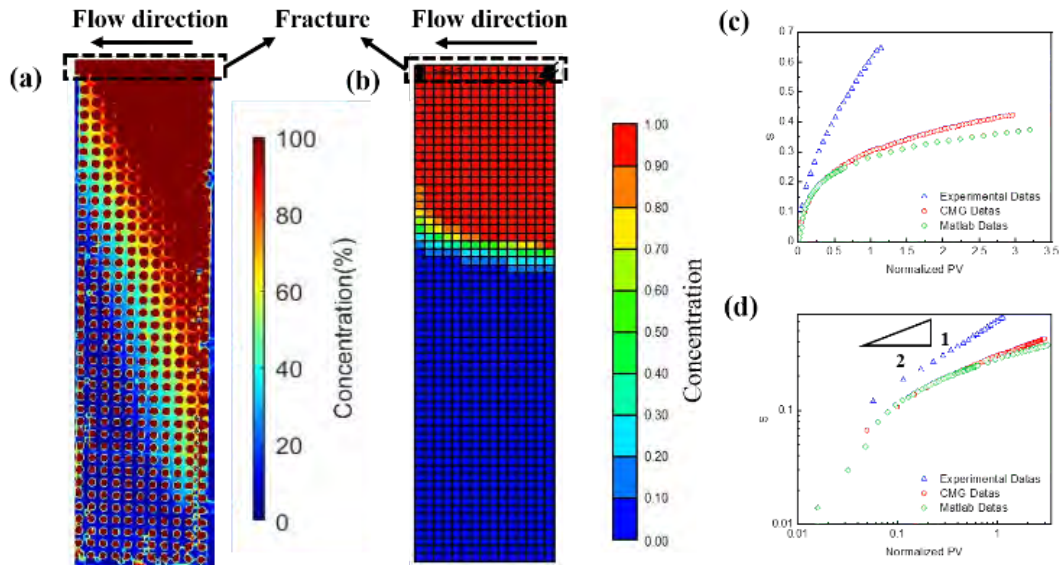


Figure 3: Figure 1. Concentration profile at 42mins after tetradecane injection along the fracture from (a) experiments and from (b) CMG simulation adopting Fick-Darcy coupling. The Pe in fracture is 1.04×10^5 . The flow patterns in experiment and simulation are qualitatively different. The evolution of tetradecane displacement efficiency in the domain is plotted in (c) linear scale and (d) log-log scale, where the diffusive scaling in experiment cannot be reproduced in simulation adopting Fick-Darcy coupling.

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MS01 / 329

Understanding CO₂ transport and carbonate formation in portland cement-based materials using X-ray micro-CT

Author: Laura Dalton¹

Co-authors: Dustin Crandall²; Karl Jarvis³; Mohammad Pour-Ghaz⁴

¹ North Carolina State University

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Two experimental studies focused on understanding the reactive transport properties of CO₂ in cement-based materials are discussed. In the first study, we investigate the kinetics of water sorption into air-entrained mortar specimens when purged with different gas phases CO₂, CH₄, and N₂. The rate of water sorption in the presence of different gases was measured using an engineered flow system built inside an X-ray micro-computed tomography (CT) scanner located at the U.S. Department of Energy's National Energy Technology Laboratory. The CO₂-purged specimen absorbed water 200 times faster than N₂- and CH₄-purged specimens revealing that the role of gas solubility and reactive sorption is expedited in the presence of CO₂ in portland cement-based materials. In a follow-up study, the influence of both the CO₂ state (gas, liquid or supercritical) and different degrees of saturation (0, 50, or 100%) on the transport properties and carbonate formation in portland cement-based materials was studied using the same X-ray micro-CT setup. It was found that the fluid transport, as well as the extent and formation of carbonates in different pore sizes change with the degree of saturation. These findings have implications for predicting mass transport in cement-based materials, ensuring the long-term safety of carbon storage structures, and sequestering CO₂ in the form of carbonates.

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Poster / 330

Microfluidic experiments on constrained oil remobilization induced by water transport in the oil phase

Author: LIFEI YAN^{None}

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¹ *Utrecht University*

Corresponding Authors: s.m.hassanizadeh@uu.nl, a.raoof@uu.nl, l.yan@uu.nl

Given the complex physical and chemical processes, several controlling mechanisms have been proposed to explain the oil remobilization due to low-salinity effects. Osmosis and water-in-oil emulsification are among these mechanisms. However, our knowledge of these processes is limited and their associated time scales are not well understood. To verify their roles, we conducted a series of microfluidic experiments by sequentially injecting high-salinity water, pure or surfactant-added synthetic oil, low-salinity water into the hydrophobized glass-based microchips. Several selected specific areas were continuously observed over at least 30 hours, with sandwiched systems of trapped high-salinity water along the solid grains, low-salinity water in bulk, and oil. The systems mimicked the contact status of these three fluids in the natural reservoir. In the experiments using pure oil, we found that the expending high-salinity water gradually squeezed the sandwiched oil phases out of the pores. The area of high-salinity water increased by 41.21% with an average rate of 141.88 $\mu\text{m}^2/\text{hr}$ after 70 hours of monitoring. In the experiments with adding surfactant (SPAN 80) in oil, we observed that the expansion rate of high-salinity water was 1.85 times higher than it without adding a surfactant, meaning that the emulsification contributed to accelerating water transport in the oil phase. Therefore, we proposed a hypothesis of emulsification and water diffusion in the oil phase. On the other hand, visualizations of water-in-oil emulsions were investigated from nano-scale to pore-scale. A corresponding series of experiments were carried out using Zetasizer to capture the size trend in water-in-oil emulsion around the oil/salinity-water interface under different salinity conditions. In the case of 2,000 ppm salinity, we found that the water-SPAN80-dodecane emulsions kept a primary size of around 50 nm for the first 4 hours, then generated a second primary size of 2 nm during 4-20 hrs. Finally, the small emulsions progressively dominated the size distribution around the interface, and relative big emulsions, e.g., 4,800 nm, occurred with the coalescence until the emulsification process reached equilibrium. This tendency matched well with the observation on the emulsion transformation in the microfluidic experiments and helped explain the process of high-salinity water expansion.

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MS01 / 331

The Role of Gas Composition on Injectivity in Surfactant-Alternating-Gas Foam Processes

Authors: JIAKUN GONG¹; William Rossen²

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Surfactant-Alternating-Gas (SAG) (also known as FAWAG) is the most common method of injection for foam EOR. Injectivity is a key factor of a foam EOR process for both process economics and diversion. We have examined liquid injectivity after a period of gas injection. During gas injection following foam, a bank of collapsed, or greatly weakened, foam propagates slowly from the inlet. During subsequent liquid injection, liquid quickly saturates the collapsed-foam region and then fingers through the weakened-foam bank ahead of the collapsed-foam bank in a way similar to liquid injection directly after foam. Mobility then rises substantially, as liquid dissolves gas trapped within the fingers. Over time, the fingers also grow slowly outwards as they dissolve surrounding trapped gas. Thus gas solubility is crucial to liquid mobility and liquid injectivity.

In this study, we conduct coreflood experiments in a Berea sandstone core sample with permeability 160 mD at 90°C with 40 bar back-pressure. Various types of gas, nitrogen, CO₂ and krypton, are adopted to investigate the effect of the gas solubility in water on the fluid behavior and injectivity in a SAG foam process. We examine gas injection following foam and liquid injection following a similar amount of gas injection. In one experiment, we partially pre-saturate injected liquid with CO₂.

We observe the same sequence of banks with the various types of gas. The liquid-finger sizes are similar, indicated by similar liquid break-through time during liquid injection following foam. The times for foam dry-out and collapse during gas injection following foam injection are also comparable among the gases. However, the process of dissolution of trapped gas into liquid fingers is strongly affected by the gas solubility, as expected. The lower the gas solubility in water, the slower the gas dissolution process, and the slower the rise in injectivity. The gas-dissolution process takes about 7 times longer with injection of liquid partially pre-saturated with CO₂ than with unsaturated liquid injection. The plateau value of pressure gradient during liquid injection is also affected by the gas type, in agreement with data on steady-state foam strength. One practical implication is that CO₂ SAG foam injectivity is substantially better than for foam made with other gases.

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Poster / 332

Study on quantitative identification method for lithology of pyroclastic rock

Author: Gang Hu¹

Co-authors: Zhiqiang Mao¹; Peiqiang Zhao²

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Pyroclastic rock is a transitional rock between magmatic lava and sedimentary rock. The content and particle size of pyroclastic are difficult to determine, thus, the identification of lithology is difficult. The traditional lithology identification methods including various kinds of cross-plot, cluster analysis and other methods, lack of geological concept and physical dependence. What's more, various mathematical methods are difficult to be quickly applied to the practical production. In this paper, based on the magmatic debris content of core sheet analysis and combining with RoqSCAN element content experiment, conventional and element logging data, the quantitative calculation model of magmatic debris content was constructed to solve the problem of quantitative evaluation of pyroclastic content. Based on the experimental data of core particle size, and the analysis of lithologic M-N crossplot (definition in well logging discipline) of different particle sizes, a quantitative calculation model of median grain diameter is established. Quantitative identification of lithology was realized by quantitative evaluation of pyroclastic content and particle size. This method is applied to reservoir lithology identification in Wuerxun Sag, Hailar Basin, China. Through the statistics of lithology identification results of 40 wells, the accuracy of lithology identification is 86%.

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Poster / 333

The First Experimental Design and Application of Large Horizontal Well Spacing Superheated Steam Flooding for Thin Heavy Oil Reservoir in Bohai Bay

Author: Guangming Pan^{None}

Co-authors: Lei Zhang ; Hao Li ; Lijie Yang ; Yike Luo

Corresponding Author: pgm_upc@126.com

The thinner the reservoir thickness is, the greater the heat loss after steam overpass, so there were few successful examples of steam flooding in heavy oil reservoirs less than 6 meters all over the world. However, similar thin-layer heavy oil reserves account for a large proportion in Bohai oilfield, so it is urgent to carry out steam flooding after huff and puff to further improve oil recovery. The target reservoir with formation oil viscosity 413~741mPa·s was developed by horizontal wells with large well spacing (250 m ~ 450 m) in the early huff and puff stage. The successful application of thick layer, directional well, small well spacing (70 ~ 100m) steam flooding development experience cannot be directly applied to the target oilfield. Therefore, based on the laboratory physical experiments and numerical simulation method with 13 years of huff and puff development history match, the steam flooding scheme was studied to optimize and obtain the key heat injection parameters,

and field practice has been successful carried out for half a year.

Research results show that: (1) formation pressure and formation oil viscosity are the main factors controlling the development effect of steam flooding with large well spacing of thin-layer heavy oil reservoir. The technical limit of formation pressure is $\leq 5\text{MPa}$, which guarantees big volume of steam to expansion displacement. The technical limit of formation oil viscosity is the ratio of viscosity to permeability $\geq 10\text{mD/mPa}\cdot\text{s}$ at reservoir temperature, which make sure the crude oil has natural flow ability in the reservoir temperature. (2) The enthalpy loss rate of steam flooding with large horizontal well spacing in thin-layer heavy oil is 48%, which is much higher than 11% of conventional steam flooding with small well spacing in thick layer. Therefore, it is recommended to inject steam with dryness above 80% at the well bottom (conventional 50%). In order to ensure the dryness of the bottom hole steam, it is recommended that the hot medium of the boiler outlet is 20°C superheated dry steam, rather than the conventional saturated wet steam. (3) In order to fully heat the reservoir and consider the economy, the heat injection intensity was optimized to be $1.4\sim 2.0\text{ m}^3/(\text{d}\cdot\text{Ha}\cdot\text{m})$. (4) The production/injection ratio was optimized to be $1.2\sim 1.6$ to ensure the continuous decline of formation pressure.

The above research results guided the development of the first offshore steam flooding field test with large well spacing. In half a year, 29000 tons of steam has been injected, 59 tons of oil has been increased per day, and the stage oil steam ratio is 0.85. The research results show that steam flooding can also be applied in thin heavy oil reservoirs with large well spacing.

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Poster / 334

A Novel Analysis Method for Water Breakthrough Mechanism in an Offshore Heavy Oil Reservoir with Bottom Water

Author: Guangming Pan^{None}

Co-authors: Kai Kang ; Jianting Huang ; Jifeng Qu ; PENG SHI

Corresponding Author: pgm_upc@126.com

A nitrogen-assisted steam stimulation test (NSST) was firstly carried out to evaluate potential for improving recovery of CN Reservoir, a typical heavy oil reservoir with high formation oil viscosity ($447\sim 577\text{mPa}\cdot\text{s}$) and strong bottom water drives. Unexpectedly premature water breakthrough and rapid water rising, however, occurred in a surrounding general production (SGP) well at early stage of first steam huff process. Reservoir characteristic with strong bottom water drives makes it difficult to diagnose this kind of phenomenon.

Through comprehensive analysis on the curves of water-oil ratio and water-oil ratio derivative, current change in current cards from electric submersible pump and formation water assay data, it was confirmed that the additional water produced of SGP well came from injected steam of NSST well, not bottom water coning. Improved Hall curve slope (IHCS) was derived, which can real-time reflect

injection resistance change during injection process of NSST well. IHCS curve was divided into three sections with different values, indicating the resistance effect decreased stepwise. Each segment had distinct characteristics, and it was suggested that slippage effect of heated nitrogen caused the rapid gas breakthrough at the stage of initial injection, and the formation of gas channeling induced the following water breakthrough. The analysis on the water breakthrough mechanism was consistent with real-time monitoring results.

This paper details how to analyze breakthrough mechanism using IHCS curve method, which can also be used to evaluate the injection effect efficiently in other steam stimulation tests because of its real-time diagnostic feature.

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MS10 / 336

Pore-scale imaging with measurement of relative permeability and capillary pressure in an altered-wettability limestone with bimodal porosity

Authors: Guanglei Zhang¹; Ali Qaseminejad Raeini²; Martin Blunt¹; Branko Bijeljic³

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Pore-scale X-ray imaging combined with a steady-state flow experiment is used to study the displacement processes during waterflooding in an altered-wettability carbonate, Ketton limestone, with distinct bimodal porosity. We simultaneously characterize macroscopic and local multi-phase flow parameters, including relative permeability, capillary pressure, wettability, and pore-by-pore fluid distribution. A more accurate method is applied for porosity and fluid saturation determination using differential imaging without image segmentation. Typical oil-wet behaviour in resolvable macro pores is measured from contact angle, fluid occupancy and curvature on micro-CT images. The capillary pressure is negative and decreases with brine saturation as brine is the non-wetting phase and forced into small pores and throats progressively. Micro-CT images show that brine initially flows through water-wet micro-porosity, and then fills the centre of large oil-wet pore bodies. The oil relative permeability drops quickly as oil is drained to low saturation and flows through connected oil layers. The brine flows through micro-porosity and its relative permeability remains very low until brine invades small throats and forms a connected flow path in macro-pores. Once brine breaks through macro-pores, its relative permeability increases significantly because macro-pores

are 3 orders of magnitude larger than micro-porosity. Due to Ketton wettability and distinct bimodal porosity, its relative permeability behaviour is markedly different when compared to other carbonates and sandstones. Overall, this work demonstrates that not only wettability but also pore size distribution have significant impacts on the displacement processes.

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MS08 / 338

Impact of flow rate on chemical gradients and mixing dynamics in porous media

Authors: Oshri Borgman¹; Régis Turuban²; Baudouin Géraud¹; Tanguy Le Borgne³; Yves Méheust⁴

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² *SISSA, Trieste, Italy*

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Solute mixing mediated by flow in porous media plays a significant role in controlling reaction rates in subsurface environments. Due to incomplete mixing, solute concentrations are inhomogeneous at the pore scale in many practical cases. Incomplete mixing will limit local and upscaled reaction rates, rendering their prediction by classical Darcy scale reactive transport models inaccurate. The lamellar mixing theory was recently introduced to give a more accurate description of mixing dynamics. The theory uses a Lagrangian kinematic description of solute filaments as material lamellae, which undergo stretching and deformation in the surrounding flow field. This theory has successfully explained the experimentally-observed impact of Péclet number variation on single solute lamellae mixing in a two-dimensional simple shear flow field 1. However, the applicability of these results to porous media, where pore-scale flow heterogeneity results in a complex fluid shear and stretching dynamics, remains an open question. To address it, we perform solute transport experiments in transparent, quasi-two-dimensional, soil analog models. These experiments investigate pore-scale solute dispersion and mixing under different flow rates, thus varying the Péclet number. We use Fluorescein as a conservative tracer and record its fluorescence intensity in monochrome images at fixed time intervals. We convert the fluorescence intensity to solute concentration fields and subsequently compute concentration gradients, which are indicators for solute mixing rates. Our images provide evidence for incomplete mixing at the pore-scale and show strong gradients transverse to the mean flow direction. The time evolution of the average value of the concentration gradients

exhibits the theoretically-expected behavior: the gradients' magnitude initially increases due to advective compression and later decrease due to diffusion and lamellae coalescence. The time to reach the maximum gradient value, or the mixing time, decreases with Péclet. We show that the scaling of the mixing time with Péclet is identical to the theoretical prediction based on simple shear flow, indicating that the theory accurately captures the pore-scale mixing dynamics in the porous medium. However, the scaling of the maximum gradient magnitude as a function of the Péclet number shows a weaker dependency than that theory predicts. We explain this discrepancy by considering the role of lamellae coalescence, which decreases gradient values. We observe that lamellae coalescence depends on the distance traveled by the solute front in the porous medium, i.e., the number of grains the solute front has encountered. Thus, coalescence begins earlier for higher Péclet values, reducing their maximum gradient values. So, in conclusion, we adapt the lamellar mixing theory formulation from the simple shear flow behavior to a more general configuration characteristic of two-dimensional porous media.

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1. Souzy, M., Zaier, I., Lhuissier, H., Le Borgne, T. & Metzger, B. Mixing lamellae in a shear flow. *J. Fluid Mech.* 838, R3 (2018).

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS06-B / 339

Pore-scale Assessment of Spontaneous Imbibition from Layer to Layer

Author: Jamal Alaamri¹

Co-authors: Viswasanthi Chandra¹; Hussein Hoteit²

¹ *King Abdullah University of Science & Technology*

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Spontaneous imbibition is a fundamental flow mechanism that plays a significant role in oil extraction from subsurface reservoirs. Understanding the imbibition behavior, which is driven by capillarity relative to the interfacial forces between the immiscible fluids within the porous media, is essential for designing and optimizing IOR/EOR recovery schemes. Conventional lab experiments with Amott cell, which is commonly used to quantify the oil recovery behavior from a core plug, do not replicate the actual field conditions, where imbibition occurs within the porous media, i.e., from layer to layer. The poor representation of field case conditions may underestimate the full potential

of the imbibition mechanism. In this study, we propose a new method to complement the conventional method by providing insights on the spontaneous imbibition behavior from layer to layer, mimicking cross-flow between reservoir layers. The concept is based on placing two different layers of glass beads, with different mesh sizes, in contact with each other in a closed-cell and observing the change in saturation and the cross-flow pattern at the pore-scale level, driven by capillarity and wettability difference. The fluid change will be only in the water-oil distribution, where water initially placed in one glass beads layer is expected to imbibe the other layer and vice-versa for the oil, i.e., counter-current flow. Computed Tomography Scan (CT scan) equipment was employed for this purpose. High-resolution time-lapse images were captured and reconstructed to represent the whole volume of the two layers. The imbibition front movement and the redistribution of the saturation were qualitatively analyzed and discussed. We were able to offer an understanding of the effects of heterogeneity and pore size distribution on the imbibition and cross-flow between the layers at the pore-scale level. X-ray attenuation, which is affected by the sample's density and atomic number, was used to quantify the change in saturation with time and construct the production curves. Results were used to enhance the obtained conventional spontaneous imbibition by Amott cell and provide a new concept about the imbibition mechanism across the contact of the two rocks. We also identified areas of preferred production sites as evidence of the wettability heterogeneity within the rock. The novelty of this work, which is the first of its kind, is that it provides a deep understanding of the pattern of the spontaneous imbibition that happened in the subsurface. The new method should complement the current Amott cell method to enhance the construction of the production curves. The use of micro-CT and time-lapse in-situ imaging facilitates visualizing and quantifying rock-to-rock imbibition within heterogeneous porous media, which cannot be achieved with the conventional methods.

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Poster / 340

Extended Allen-Chan phase-field equation for ternary fluid flows and phase-change process in binary fluid flows

Authors: Reza Haghanihasanabadi¹; Carl Fredrik Berg²; eirik flekkøy³

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Corresponding Authors: carl.f.berg@ntnu.no, reza.haghanihasanabadi@ntnu.no, flekkoy@fys.uio.no

Multiphase fluid flows are ubiquitous in many natural phenomena and industrial applications such as oil production, purifying water systems, heat exchangers, etc. Analytical analyses of multiphase

flow are limited to simplified cases due to the complex nature of real phenomena. Experiments can reveal main aspects of complex systems, but not concurrently provide detailed information about the individual effects of each involved property or parameter. As computer resources have developed in terms of speed and handling of large data, numerical simulation has received more and more attention and different models have been developed in the field of multiphase fluid flows. Such numerical modeling yields an alternative approach to obtain the physics of multiphase flow on structures of realistic complexity. The most commonly numerical models for interface capturing or tracking may be divided into two categories: sharp-interface models and diffuse interface models such as phase-field models. Phase-field models are mainly used to capture the interfaces between fluids, where the fluid velocity is determined by the Navier-Stokes equations. In general, there are two phase-field theories: Cahn-Hilliard (CH) and Allen-Cahn (AC) [1]. The former includes a fourth-order derivative in its diffusion term, which implies a more complex discretization and a higher dispersion error, while the latter contains only up to a second-order derivative, which makes it more efficient and less dispersive. In spite of the privileges that the AC equation has over the CH, it has received less attention, probably since it was originally proposed for complex interfacial pattern formation process. AC has recently modified to a phase-field model [2], and then reshaped into a conservative form (CAC) [3]. The CAC equation can be solved using conventional CFD models or using lattice Boltzmann method (LBM). Geier et al. [4] were the first to develop a LBM to solve the CAC. Due to the robustness of CAC compared to CH equation, it is of value to extend this equation to simulate ternary fluid flows and also phase-change process in binary fluid flows. In two different works, we extended CAC to handle ternary systems and binary systems with phase-change phenomena, and provided LB models to solve the developed equations. In the first paper [5], for the first time, we extended the CAC from its binary form to ternary systems, and developed a LB model to solve the equation. It was shown that CH-based models are not mass conservative, while the mass conservation does not violate in the proposed ternary CAC. Also, the current ternary CAC enables the elimination of unphysical apparition of one fluid at the interface of the other two fluids, a numerical artifact that exists in the CH-based models. In another paper [6], the CAC is extended to include mass transfer between liquid/vapor phases for modeling phase-change phenomena. Before that, all of the existing phase-field models for modeling the phase-change mechanism were based on the CH equation. Where available, different benchmark tests were conducted, and the results were in good agreement with analytical, experimental, and numerical data.

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Country:

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References:

- [1] S. M. Allen and J. W. Cahn, "Mechanisms of phase transformations within the miscibility gap of Fe-rich Fe-Al alloys," *Acta Metallurgica*, vol. 24, no. 5, pp. 425-437, 1976/05/01/ 1976.
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS15 / 341

Physics-enhanced Convolutional Neural Networks for Predicting Effective Dispersion in Porous Media

Authors: Ross Weber¹; Ilenia Battiato¹

¹ *Stanford University*

Corresponding Authors: ibattiat@stanford.edu, rweber3@stanford.edu

The effective dispersion coefficient is a key parameter for characterizing the transport capability of porous media. This coefficient depends not only on the pore-scale geometry but also the macroscale flow conditions and is traditionally expensive to compute as it requires the solution to a partial differential equation (PDE). In this work, a physics-enhanced Convolutional Neural Network (CNN) is developed to estimate effective dispersion given an image of the microstructural geometry and a Peclet number describing the flow condition. The CNN is trained with 100,000 computer-generated images of porous media, on which a PDE closure problem is solved to calculate the effective dispersion coefficient for various Peclet numbers. The CNN is enhanced by including Minkowski functionals and tensors as inputs, which are powerful morphological descriptors for porous media. Results demonstrate that enhancing the CNN with physics-based Minkowski functionals not only speeds up training time but also increases accuracy. This CNN dramatically reduces the computational cost of characterizing porous media while improving on the accuracy of frequently-used relationships and can have benefits in multiple fields including energy and energy storage.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Unsure

MS03 / 343

Consistent Treatment of Shear Failure of Embedded Discrete Fracture Networks Using XFVM

Authors: Giulia Conti^{None}; Rajdeep Deb^{None}; Stephan Matthai¹; Patrick Jenny^{None}

¹ *The University of Melbourne*

Corresponding Authors: jenny@ifd.mavt.ethz.ch, gconti@student.ethz.ch, stephan.matthai@unimelb.edu.au, rajdeep.deb@nmr.phys.chem.ethz.ch

Modeling the mechanical behavior of a fractured reservoir is important for various engineering applications such as enhanced geothermal systems, fracking and CO₂ capture. To understand the coupled mechanical and flow processes of fractured porous reservoirs, it is crucial that computational frameworks are able to capture the displacements of large number of active fractures with various topologies. To this end, we use the extended finite volume method (XFVM) to model poroelastic fractured rock. The fractures are embedded manifolds of lower dimension and are represented by special discontinuous basis functions. These functions have the important property that the displacement gradient is continuous over the fracture segments, which simplifies the computation of traction and compressive forces. Embedded discrete fracture models are cost efficient, since the mesh does not have to get adapted to the fractures and no remeshing is needed in case of fracture propagation; therefore, coarse meshes can be used. However, embedding fracture networks in non-conforming meshes is challenging, since any kind of fracture topology and number of fracture segments can be present within a grid cell. Here, we use a merging technique to locally simplify intersecting and branching fracture segments in grid cells and introduce the rule of weakest link to retain the mechanical property of the dominant segment. Shear displacement and tensile opening of a fracture network with locally merged intersections and under in situ conditions are analyzed. The hydraulic and void aperture changes due to shear displacement and tensile opening are included in the model. The aperture through shear slip is not only calculated a posteriori but is added in the equations such that its influence directly affects the stress-strain relation and displacement calculations. The results indicate that by using the local simplification of merging fracture segments the mechanical behavior of fractured reservoirs is retained. The merging technique is a flexible and simple method, which allows to employ embedded discrete fracture models for scenarios involving shear failure.

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Time Block B (14:00-17:00 CET)

Participation:

In person

MS08 / 344

Autocatalytic reaction-diffusion-advection fronts in radial geometry

Authors: Alessandro Comolli¹; Fabian Brau¹; Anne De Wit¹

¹ *Université libre de Bruxelles (ULB)*

Corresponding Authors: adewit@ulb.ac.be, alessandro.comolli7@gmail.com, fabian.brau@ulb.be

Reaction diffusion (RD) fronts are ubiquitously found in a wide variety of systems in chemistry, biology, physics and ecology, and understanding their properties is especially important for hydrogeological problems involving chemical reactions. The dynamics of RD fronts in geological media is

generally complex, due to the interplay of several physical and chemical processes. Autocatalytic fronts represent an important subset of RD fronts, for which that the coupling of diffusion and chemical processes gives rise to self-organization phenomena and pattern forming instabilities [1]. It has been shown that, when the reactant and the catalyst are put into contact and the interface is a straight line, the front behaves as a solitary wave. This means that, as the front travels at a constant speed towards the nonreacted species, its shape remains unchanged [2]. When uniform advection occurs, the properties of the system do not change, provided that a proper comoving reference frame is used for its description.

In this work we show that the geometrical properties of the injection source have a significant impact on the reaction front dynamics. Indeed, when the catalyst is injected radially into the reactant at a constant flow rate, the pre-asymptotic dynamics of the front is strongly affected by the presence of a nonuniform velocity field. Moreover, although at long times the front still behaves as a solitary wave, the efficiency of the reaction is strongly increased in virtue of the increasing volume occupied by the radial front. Changing the position of the species also impacts the front dynamics significantly. We show that injecting a finite amount of reactant into the catalyst gives rise to collapsing fronts, which we characterize in terms of their position, and width, as well as the production rate. In contrast, when the reactant is injected into the catalyst at a constant flow rate, a stationary regime is reached where, unlike the case of solitary waves, the autocatalytic front does not move.

References

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- [2] P. Gray, K. Showalter, and S. K. Scott, *J. Chim. Phys.* 84, 1329 (1987)

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Time Block A (09:00-12:00 CET)

Participation:

In person

Poster / 345

Comparison of Pore-network Simulation and Infiltration Experiment Performed on Coarse Sand

Authors: Tomas Princ¹; Michal Snehota²

¹ *Czech Technical University in Prague*

² *Czech Technical University in Prague, Civil Engineering*

Corresponding Authors: michal.snehota@fsv.cvut.cz, tomas.princ@fsv.cvut.cz

The research focused on the simulation of the previous experiment described by Princ et al. (2020). The relationship between entrapped air content (ω) and the corresponding satiated hydraulic con-

ductivity (K) was investigated for two coarse sands, in the experiment. Additionally the amount and distribution of air bubbles were quantified by X-ray computed tomography.

The pore-network model based on OpenPNM platform (Gostick et al. 2016) was used to attempt simulation of a distribution of the entrapped air bubbles after infiltration. Satiated hydraulic conductivity was determined to obtain the $K(\omega)$ relationship. The results from pore-network model were compared with the results from experiments. The using of special pore network, corresponds to distribution obtained by CT imaging, leads to obtaining satisfying results from simulations.

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References:

Gostick et al. (2016). Computing in Science & Engineering. 18(4), p60-74.
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 346

MODELLING OF FREEZING AND THAWING EXPERIMENTS OF SATURATED SAND COLUMN

Authors: Martina Sobotkova^{None}; Alexandr Zak^{None}; Michal Snehota^{None}; Michal Benes^{None}

Corresponding Authors: michal.benes@fjfi.cvut.cz, msobotkova@seznam.cz, michal.snehota@fsv.cvut.cz, zakal@centrum.cz

Freezing and thawing experiments were carried out in the laboratory on fully saturated sand sample (15 cm in diameter and 20 cm in height). The column sand, packed into the PVC container, was well insulated by foam materials at the bottom and on sides, whereas the top of the sample was covered by a stainless steel plate to allow the heat flux between the sand and the ambient environment in the climatic chamber. The freezing-thawing cycle started by equilibrating the sample temperature at +10°C then the temperature inside the climatic chamber was changed -10°C. The freezing-thawing cycle was repeated 4 times. The inner temperature of sand sample was monitored in three depths by thin temperature sensors horizontally inserted into the sample at three depths.

The experiment aims to provide information on freezing dynamics and thermal changes during the freezing and thawing cycles. Temperatures inside the sample achieved 9.6°C before freezing and were stabilized around 0°C after 12 hours. The same behavior was monitored within thawing cycle. The data were compared with simulations obtained by a numerical model. The model is based on the heat balance within the sample assembly and a modified heat equation for the porous medium temperature allowing for the phase transition below the freezing point depression. The comparisons of the thermal behavior show good agreements both in quantitative and qualitative sense.

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Participation:

In person

MS06-A / 347

Transition from viscous fingers to compact displacement during unstable drainage in porous media

Authors: Marcel Moura¹; Fredrik Kvalheim Eriksen²; Mihailo Jankov¹; Antoine Turquet³; Knut Jorgen Maloy⁴

¹ *PoreLab - University of Oslo*

² *Porous Media Laboratory*

³ *NORSAR*

⁴ *PoreLab, Department of Physics, University of Oslo, Norway*

Corresponding Authors: marcelmoura@yahoo.com.br, antoine@norsar.no, mihailo.jankov@fys.uio.no, f.k.eriksen@fys.uio.no, maloy@fys.uio.no

We have performed a series of drainage experiments in a radial porous Hele-Shaw cell where we systematically varied the viscosity of the defending (wetting) fluid, and the overpressure of the invading (non-wetting) fluid to map out the resulting invasion structures as a function of viscosity ratio and injection pressure (see Figure 1). We described a cross-over from the viscous fingering instability to a compact invasion regime during viscously unstable drainage of porous media, and we investigated the underlying mechanisms of this compact fluid displacement. We have shown that above a threshold of injection pressure and for low enough viscosity of the defending fluid, a more stable and compact invasion structure emerges within the viscous fingering patterns, i.e. a roughly circular displacement with viscous fingers on the outside. We found that the ratio between the length of the outer fingers and the size of the compact invasion scales with the viscosity ratio of the fluid phases and approaches an approximately constant value during growth, resulting in structures with proportionate growth and larger compact invasions for lower viscosity of the defending fluid. As opposed to the viscous fingering instability, we observed rich ganglion dynamics within the compact invasion structures and showed that the pressure gradient is not screened by the outer fingers. We introduced a new concept called the flipping matrix to study the ganglion dynamics. Two global measures derived over this matrix allowed us to give a quantitative description of the intensity of the ganglion dynamics activity.

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References:

1 F. K. Eriksen, M. Moura, M. Jankov, A. L. Turquet and K. J. Måløy, "Transition from viscous fingers to compact displacement during unstable drainage in porous media," *Phys. Rev. Fluids* 7, 013901 (2022).

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS21 / 348

Two-phase non-Newtonian flow in porous medium

Author: Federico Lanza¹

Co-authors: Alex Hansen²; Laurent Talon³; Tom Vincent-Dospital⁴; Alberto Rosso⁵

¹ NTNU, Université Paris Saclay

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⁴ University of Oslo

⁵ Université Paris-Saclay

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We study the evolution of an immiscible two-phase flow system in a porous material for which one of the two phases is a non-Newtonian fluid. In particular, we are interested in analyzing the displacement of a non-Newtonian fluid in a porous medium by invasion of a Newtonian fluid, and examining the spatial and temporal evolution of the interface separating the two phases. Simulations were carried out in the framework of the pore network model, adopting numerical techniques already employed for the study of a fully Newtonian two-phase flow system and adequately adapted taking into account the two-phase non-Newtonian rheology in a single channel. Experiments were also performed, in which air was injected in a 3d-printed isotropic porous model previously saturated by a non-Newtonian liquid. As for the fully Newtonian case, the phenomena of viscous and capillary fingering is observed, but now, due to the dependance of the viscosity of the non-Newtonian phase from the flow rate, the competition between capillary and viscous regime, as a function of the capillary number and viscosity ratio, is more complex, bringing to a rich variety of displacement patterns.

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Participation:

In person

MS04 / 349

Stress and Relax: Hydrogel swelling in a confined granular medium and relaxing after extraction

Authors: Jean-Francois Louf¹; Nancy Lu^{None}; Margaret O'Connell^{None}; H. Jeremy Cho²; Sujit Datta³

¹ *Auburn University*

² *University of Nevada Las Vegas*

³ *Princeton University, USA*

Corresponding Authors: jeremy.cho@unlv.edu, mgo2@princeton.edu, nblu@princeton.edu, ssdatta@princeton.edu, jlouf@auburn.edu

Hydrogels hold promise in agriculture as reservoirs of water in dry soil, potentially alleviating the burden of irrigation. However, confinement in soil can markedly reduce the ability of hydrogels to absorb water and swell, limiting their widespread adoption. Unfortunately, the underlying reason remains unknown. Here, we report the first direct visualization of hydrogel swelling within a model three-dimensional (3D) granular medium with tunable confining stresses and grain sizes. Our experiments enable us to measure, in situ, two key quantities that were previously inaccessible: the extent of hydrogel swelling and medium restructuring. Unlike an imposed osmotic or hydrostatic pressure, confinement in a granular medium subjects the surface of a hydrogel to a spatially nonuniform stress. We therefore extend the classic Flory-Rehner theory of hydrogel swelling by coupling it to Hertzian contact mechanics that explicitly treats the stresses exerted by the medium at the hydrogel-grain contacts. Using this approach, we show that the extent of hydrogel swelling is determined by the balance between the osmotic swelling force exerted by the hydrogel and the confining force transmitted by the surrounding grains. Furthermore, we demonstrate that a balance of the same forces, also including intergrain friction, determines the onset of restructuring of the surrounding medium. Our work therefore reveals the physical principles that describe how hydrogel swelling in and restructuring of a granular medium both depend on the properties of the hydrogel, the properties of the medium, and confining stress. We show that our theoretical framework not only describes our measurements but also helps to rationalize previous measurements of hydrogel water absorption in soil. Moreover, upon extraction of the originally spherical hydrogel spheres, we noticed multiple indentations, resulting in the gels having raspberry shapes. Such indentations relax at a characteristic time - the poroelastic time - that we were able to measure and confront to typical indentation measurements. Together, our results provide (1) quantitative principles to predict how hydrogels behave in confinement, and (2) a new cost-effective method to measure the poroelastic diffusion coefficient of hydrogels, potentially improving the use of hydrogels in agriculture as well as informing other applications such as oil recovery, construction, mechanobiology, and filtration.

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Under pressure: Hydrogel swelling in a granular medium
J-F Louf, N. B. Lu, M. G. O'Connell, H. J. Cho, S. S. Datta, *Science Advances*, 7, eabd2711 (2021)
DOI: 10.1126/sciadv.abd2711

Poroelastic shape relaxation of hydrogel particles
Jean-François Louf, and Sujit S. Datta,
Soft matter 17.14 (2021): 3840-3847
DOI: 10.1039/D0SM02243H

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS18 / 350

Estimation of aquifer permeability using aquifer testing with fiber-optic Distributed Strain Sensing

Author: Yi Zhang¹

¹ *Geological Carbon dioxide Storage Technology Research Association, Kyoto, Japan; Research Institute of Innovative Technology for the Earth (RITE), Kyoto, Japan*

Corresponding Author: zhangyi@rite.or.jp

Permeability & compressibility structures in aquifers are critical for predicting fluid flow behavior as well as utilizing and managing subsurface fluid resources. In conventional pressure-based well testing methods, formation investigation by the packer testing is difficult to operate and only the properties of thick sections can be acquired. In this study, based on the results of a field aquifer test, we show that fiber-optic Distributed Strain Sensing (DSS) can provide high-resolution aquifer formation characterization at fine scales. The strain changes indicate the spatial distribution of fluid pressure migration. Via the poroelastic modeling, we demonstrate that the strain changes, like the pressure changes, contain the information of formation permeability & compressibility. We further apply an inversion algorithm to estimate the fine-scale vertical permeability & compressibility profiles from field DSS records. Our study gives a new reservoir characterization method using DSS in aquifer testing.

Acknowledgment:

This presentation is based on results obtained from a project (JPNP18006) commissioned by the New Energy and Industrial Technology Development Organization (NEDO) and the Ministry of Economy, Trade and Industry (METI) of Japan.

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References:

1 Zhang, Yi., Lei, X., Hashimoto, T., & Xue, Z. (2021). Toward retrieving distributed aquifer hydraulic parameters from distributed strain sensing. *Journal of Geophysical Research: Solid Earth*, 126(1), e2020JB020056.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS03 / 351

Physics-driven interface modeling of multiphase flow in different scale of subsurface fractures

Authors: wenhui song¹; Masa Prodanovic²; Jun Yao¹; Kai Zhang³

¹ *China University of Petroleum*

² *The University of Texas at Austin*

³ *China University of Petroleum (East China)*

Corresponding Authors: zhangkai@upc.edu.cn, masha@utexas.edu, rcogfr_upc@126.com, song_wen_hui@hotmail.com

Multiphase flow and transport phenomena within fractures are important because fractures often represent primary flow conduits in otherwise low-permeability rock. Flows within the fracture, between the fracture and the adjacent matrix, and through the pore space within the matrix typically happen on different length and time scales. Capturing these scales experimentally is difficult. It is, therefore, useful to have a computational tool that establishes the exact position and shape of fluid/fluid interfaces in realistic fracture geometries.

We here propose a progressive quasi-static level set-lattice Boltzmann coupling algorithm to study multiphase flow behavior in different scales of fracture (hydraulic fracture and natural fracture). The proposed model finds detailed, pore-level fluid configurations satisfying the Young-Laplace equation at a series of prescribed capillary pressures. The fluid volumes, contact areas, and interface curvatures are readily extracted from the configurations. The method automatically handles topological changes of the fluid volumes as capillary pressure varies. It also accommodates arbitrarily complicated shapes of confining solid surfaces. The influence of fracture cementation and stress dependence on relative permeability and capillary pressure in different scales of fractures are discussed in detail. The simulated results establish a new, mechanistic basis for evaluating transfer functions in dual-porosity flow models.

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References:

1Song, W., Yin, Y., Landry, C. J., Prodanovic, M., Qu, Z., & Yao, J. (2021). A local-effective-viscosity multirelaxation-time lattice Boltzmann pore-network coupling model for gas transport in complex nanoporous media. *SPE Journal*, 26(01), 461-481.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 352

The Effect of Interfacial Elasticity of a Nanofluid/Surfactant system for EOR through a Visual Micromodel Study

Author: Hector Bonilla^{None}

Co-author: S. H. Hejazi¹

¹ *University of Calgary*

Corresponding Authors: shhejazi@ucalgary.ca, hector.bonilla@ucalgary.ca

Nanoparticles have proven to overcome several challenges above traditional chemicals used for EOR. Silicates compounds are the most abundant on earth, making silicon-based nanoparticles highly compatible with most of the reservoirs, environmentally friendly, and a cost-effective nanofluid option for EOR. Silicon-based nanofluids coupled with other chemicals such as surfactants and polymers can effectively recover extra amounts of oil compared to the chemicals with no nanoparticles. Silicon dioxide nanoparticles, on their own and combined, have shown a significant improvement in the characteristics required to improve the oil displacement such as ultra-low IFT levels, change in wettability, increase viscosity, and reduce the chemical adsorption into the surface. Despite the considerable benefits and the extensive proven in lab results for this technology, there are no in-field trials to prove their performance. Some of the recovery mechanisms remain unclear and still unexplored. The interfacial rheological properties of silicon oxide nanoparticles have been mostly neglected. Herein as a first stage I aim to provide fundamental insight into the interfacial and bulk viscoelastic response of water/oil interface in the presence of silicon oxide nanoparticles utilizing dilatational rheology. Then salt will be added to the nanofluid to simulate reservoir water conditions, the nanoparticles will be coupled with a surfactant to improve the stability and maximize their oil recovery performance. Finally, I will conduct a series of visual micromodel resembling the network of pores and throats in a target sandstone rock. An advanced imaging system is built to record the flow events in micromodels. The developed technique can be readily utilized for the rapid screening for other mechanism occurring systems or suspended particles used for heavy oil recovery. The results single out the ability of silicon dioxide nanoparticles to alter the interfacial viscoelasticity and to quantify its effects displacing oil.

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Time Block C (18:00-21:00 CET)

Participation:

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MS15 / 353

Multiscale modelling of permeability and effective dispersion coefficient in porous media: a deep learning approach**Author:** Agnese Marcato¹**Co-authors:** Gianluca Boccardo ²; Daniele Marchisio ¹; Matteo Icardi ³; Javier E. Santos ⁴; Masa Prodanovic ⁵¹ *Politecnico di Torino*² *Politecnico di Torino, Italy*³ *University of Nottingham*⁴ *University of Texas at Austin*⁵ *The University of Texas at Austin***Corresponding Authors:** agnese.marcato@polito.it, masha@utexas.edu, javierestradasantos@gmail.com, matteo.icardi@nottingham.ac.uk, daniele.marchisio@polito.it, boccardo.gianluca@gmail.com

The modelling of transport in porous media is of great interest in many fields of application in chemical and environmental engineering, such as packed bed chemical reactors, underground transport of contaminants or carbon capture and storage. Flow and transport in porous media are a multiscale phenomenon, in fact, both microscale and macroscale affect the transport properties of interest. We here focus on estimating the permeability and the effective dispersion coefficient of porous media.

In this work the flow and mass transport equations are solved numerically on both microscopic and macroscopic scales and are used to train and validate deep learning techniques. At the microscopic level the geometry of the porous medium is obtained by an in silico reconstruction or by the use of computer tomography, resulting in a domain for the solution of the relevant transport equations, most often the Navier-Stokes and advection-diffusion equations [1]. At the macroscale the porous media are not topologically detailed, and are instead described as permeability fields, which can be experimentally or mathematically reproduced. The Darcy equation can be solved at this scale, and homogenisation techniques can be exploited for the evaluation of the effective permeability and the effective dispersion coefficient in the porous media [2].

The computational cost of direct simulations together with the wide range of porous media structures impacting the permeability fields make the study of flow and transport in porous media a prime candidate for machine learning applications. The data-driven models trained can predict instantaneously new input data that could be useful in multiscale modelling or optimization problems. Neural networks can be trained on CFD data for the sake of obtaining data-driven models of highly non-linear problems, in particular, convolutional neural networks (CNN) can take as input image-like geometrical information and are employed for the prediction of integral descriptors and fields. In this work CNN were used to predict the velocity in the main direction of flow, the effective permeability and the effective dispersion coefficient of porous media. Discontinuous permeability fields were produced in silico by using a spectral method [3], varying local permeabilities and correlation lengths. The mean velocity is calculated by the solution of the Darcy equation, the effective permeability and the effective dispersion coefficient were calculated by a homogenisation of the Darcy and the advection-diffusion equation by solving the cell problem with spectral decomposition. The input of the CNN are the permeability fields, and the prediction are quite accurate with average errors lower than 6%.

Convolutional neural networks can be employed for the prediction of integral values or entire fields, such as the detailed local flow field [4] or the concentration field of a chemical species. In the case of transport applications, it is necessary to provide the network with more information, i.e. both the geometrical description of the porous media and the diffusivity of the chemical species or the boundary conditions. The tuning of these kinds of multiple purpose architectures could lead this methodology to be effectively employed in a wide range of applications.

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- 1 Marcato, A., Boccardo, G., Marchisio, D., 2021. A computational workflow to study particle transport and filtration in porous media: Coupling CFD and deep learning. *Chem. Eng. J.* 417, 128936. <https://doi.org/10.1016/j.cej.2021.128936>
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

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MS15 / 354

Semantic segmentation of rock images and ensemble approach for deep learning methods

Authors: Robert John Ringer¹; Hongkyu Yoon¹

¹ Sandia National Laboratories

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The segmentation of images obtained from different imaging techniques, such as X-ray computed microtomography (μ CT) and scanning electron microscopy (SEM), is a critical step towards quantitatively describing various features of geomaterials. In this work we evaluate the capability of convolution neural networks (CNNs) to segment both μ CT and focused ion beam-SEM (FIB-SEM) images. The performance of five different 2D CNN architectures (U-Net, Attention U-Net, VGG16, ResNet, and MultiResUnet) as well as a 3D CNN architecture (U-Net) is assessed on four independent datasets including sandstone, carbonate chalks, and shale. Each of these datasets is composed of three-dimensional image stacks and corresponding ground truth segmentation labels obtained using various traditional image processing techniques. Our results indicate that deep learning architectures can successfully be applied to the task of semantic segmentation for μ CT and FIB-SEM images with frequency weighted accuracy between 94% and 99% and can perform better than manual segmentation to recover the natural morphology of original images. We also find that ensemble solutions with multiple trained models obtained from single training process consistently improve prediction accuracy in comparison to single-model (i.e., the best model in the single training) approaches across multiple datasets. In addition, our results indicate that transfer learning can allow for models to converge more quickly during training and that generic image features (learned from a large dataset such as ImageNet) can be applied to improve model performance in some cases. A comparison in performance among different CNN architectures highlights the connection from classification outcomes to underlying features of each architecture and its hyperparameters. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS23 / 355

Global sensitivity analysis on a groundwater flow model in a regional-scale with uncertain parameters: a case study in the Middle Magdalena Valley- Colombia.

Author: Boris Lora Ariza¹

Co-authors: Luis Silva Vargas¹; Eduardo Castro Alcalá²; Leonardo Donado Garzón¹

¹ *Universidad Nacional de Colombia*

² *Universidad nacional de Colombia*

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The characterization of aquifer systems on a regional scale is one of the main challenges in the study of groundwater today. This is addressed, usually, from the implementation of hydrogeological models. However, these have implicit uncertainties associated with the lack of hydrogeological information [1,2]. In this study, a numerical hydrogeological model was implemented at a regional scale in the Middle Magdalena Valley - Colombia, a region with high potential for the exploitation of gas/oil in unconventional reservoirs, where it is required to have a high degree of certainty in the hydrodynamic behavior of the system.

For this, a global sensitivity analysis (GSA) was performed to determine the impact of each parameter considered in the conceptual model on the calibration, performed with hydraulic heads. The relative influence of the uncertainties of each parameter, including boundary conditions, on the behavior of the hydraulic head in steady state will be determined from a GSA approach based on the evaluation of the Sobol index, concluding that the recharge is the parameter with higher incidence followed by the regional flow, that enters the model, through the Quaternary deposits in the northeast border.

Acknowledgments

The researcher thanks the MEGIA Research Project, Contingent Recovery Contract FP44842-157-2018 funded by Minciencias and the National Hydrocarbons Agency.

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MS03 / 356

Coupled poro-elasto-plasticity of geomaterials: Simulation and validation

Authors: Maria Warren^{None}; James Bean¹; R Charles Choens¹; Mario Martinez¹; Alec Kucala¹; Hongkyu Yoon¹

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Coupled flow and deformation processes have a significant influence on subsurface activities such as carbon sequestration, geothermal recovery, and nuclear waste disposal. Success of these activities requires accurate numerical modeling of flow and deformation in geomaterials. In this work, the Sandia Sierra Multiphysics toolkit with the fixed stress scheme is used to evaluate poro-elasto-plasticity through the thermal/fluid mechanics module ARIA and solid mechanics module. Here, a Kayenta generalized plasticity model is employed where the Kayenta model uses a shear yield function to generate a differentiable yield surface including a “cap” at higher mean stresses. The accuracy of the solution under stresses that induce elasticity, elasto-plasticity, and full plasticity are numerically evaluated against two analytical solutions and validated against experimental data. For the numerical verification with analytical solutions, indentation over the flat surface with a sphere indenter and plane stress field with an injection through a central hole are considered. For experimental validation, the wellbore breakout testing with Mancos shale will be evaluated with detailed mapping of mineral phases and material properties. This problem is used to assess the effects of geomaterial parameters in the Kayenta model and convergence criteria on the fixed stress scheme. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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Poster / 357**Three-dimensional fractal model of hydraulically fractured horizontal wells in anisotropic naturally fractured reservoirs****Authors:** Rosa María Mariscal Romero¹; Rodolfo Gabriel Camacho Velázquez¹¹ *Universidad Nacional Autónoma de México***Corresponding Authors:** rosa.m.mariscal@gmail.com, camachovrodolfo@gmail.com

A 3D numerical model is presented to analyze the behavior of gas flow in hydraulically fractured horizontal wells in anisotropic heterogeneous naturally fractured reservoirs with triple porosity (organic and inorganic matrix, and natural fracture network). This model generalizes the models proposed previously in the technical literature so far in relation to the combined effects of fractality, present in the stimulated reservoir volume (SRV), triple-porosity, slip and viscous flow, Knudsen diffusion, and kerogen adsorption/desorption from the organic pore walls, geomechanics, anisotropy, and anomalous diffusion.

The proposed model considers the presence of a SRV due to the improvement of the original petrophysical properties of the natural fractures network caused by hydraulic fracturing process generating an anisotropic and heterogeneous distribution of properties around each one of the hydraulic fractures. As a result of the fractal distribution of properties, a consistent matrix shape factor distribution is obtained in this SRV. The model also includes the presence of anomalous diffusion both in the natural fracture network and in the organic and inorganic matrix matrices through the Caputo's fractional derivative, geomechanically effects of production on the petrophysical properties, correction in the apparent permeability with slip and viscous flow, Knudsen diffusion and the adsorption-desorption process of kerogen from the walls of organic pores, and high-speed flow in the hydraulic fractures.

In this work, the functionality/benefit of implementing the proposed model with triple porosity, anisotropic fractal geometry, anomalous diffusion and different transport mechanisms is analyzed in detail.

The accuracy of the proposed model is verified using approximate analytical solutions, previously presented in the literature, and asymptotic cases by means of a commercial simulator. The different flow periods are identified in the numerical solutions determined.

The results indicate that the shape of the pressure and rate decline curves are causally related to the anisotropic fractal exponents and the order of the fractional derivatives, which represent the density and connectivity of the natural fractures within the SRV and the degree of anomalous diffusion, respectively.

At long times the decrease in gas pressure produces an improvement in apparent permeability due to the sliding effect of the organic and inorganic matrices. In these times the desorption of gas from the organic walls also contributes to production.

The gas depletion process triggers the compaction of hydraulic and natural fractures, reducing the permeability and porosity of these media. This work shows the effect of the effective stress dependence of these properties.

This model allows the generation of well performance scenarios that are closer to reality and make decisions with less uncertainty.

The proposed model is presents for the first time production predictions which take into account the anisotropic permeability behavior of the SRV through the use of the fractal geometry, with associated distributions of porosity and matrix shape factor, and combines these petrophysical properties with the effects of triple-porosity, different scale-dependent transport mechanisms, geomechanics, and anisotropic anomalous diffusion.

The practicality of using these features together for reservoir simulation is evaluated against the benefits of more realistic production scenarios.

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Poster / 358

Hydrodynamic instabilities of immiscible fluids in a Hele-Shaw cell

Authors: Chekib Ghabi^{None}; Hamid Abderrahmane^{None}; Mohamed Sassi^{None}

Corresponding Authors: hamid.abderrahmane@ku.ac.ae, mohamed.sassi@ku.ac.ae, ghabichekib@yahoo.fr

Viscous fingering is a topic of interest for long period, it renewable with the beginning of computational fluid dynamics. Here we focus on the classical constellation of non-miscible displacement, as it has been investigated in Hele-Shaw cells. A first fluid front is entering with another second fluid that has different properties. The pure flow is destabilized by the Saffman-Taylor instability. Using COMSOL Multiphysics we investigate the solution of a 2D generic set-up in an Eulerian system. We explore the fingering solutions in terms of various numerical parameters. This led to an extensive comparison of the numerical results, for meshes of various type and refinement. For various solvers we examine the execution time, and the performance of the model.

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MS15 / 359

Reduced order modeling with Barlow Twins self-supervised learning: Navigating the space between linear and nonlinear solution manifolds

Authors: Teeratom Kadeethum¹; Francesco Ballarin²; Daniel O'Malley³; Youngsoo Choi⁴; Nikolaos Bouklas⁵; Hongkyu Yoon¹

¹ Sandia National Laboratories

² Catholic University of the Sacred Heart

³ Los Alamos National Laboratory

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We propose a unified data-driven reduced order model (ROM) that bridges the performance gap between linear and nonlinear manifold approaches. Deep learning ROM (DL-ROM) using autoencoders has been shown to capture non-linear solution manifolds but fails to perform adequately when linear subspace approaches such as proper orthogonal decomposition (POD) would be optimal [1]. Specifically, the proposed framework relies on the combination of an autoencoder and Barlow Twins self-supervised learning as first introduced in Zbontar et al. (2021) [2]. The framework is data-driven and can operate on unstructured meshes, which provides flexibility in its application for various cases including standard finite element solvers, observation data, or a combination of these sources. Through multiple benchmark problems regarding natural convection in porous media, we show that our framework provides a speed-up of 7×10^6 times compared to a finite element solver and achieves a relative error of 4% in the worst case scenario. Moreover, this framework mitigates the limitation of the previous DLROM framework by providing comparable results to POD-based approaches for problems where the solution lies within a linear subspace, as well as DL-ROM autoencoder-based approaches where the solution lies on a nonlinear manifold. Hence, it would bridge the gap between linear and nonlinear reduced manifolds. We have illustrated that our framework achieves these results due to a proficient construction of the latent space. Hence, it is easier to map these latent spaces using regression models. SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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- 1 Kadeethum, T., Ballarin, F., O'Malley, D., Choi, Y., Bouklas N., Yoon, H. Non-intrusive reduced order modeling of natural convection in porous media using convolutional autoencoders: comparison with linear subspace techniques. *Adv. Water Resour.* 104098 (2022).
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Participation:

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MS15 / 360

U-FNO - an enhanced Fourier neural operator-based deep-learning model for multiphase flow

Authors: Gege Wen¹; Zongyi Li²; Kamyar Azizzadenesheli³; Anima Anandkumar²; Sally Benson¹

¹ *Stanford University*

² *California Institute of Technology*

³ *Purdue University*

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Numerical simulation of multiphase flow in porous media is essential for many geoscience applications. However, these numerical simulations are often very time-consuming and computationally intensive since they require fine spatial and temporal discretization to accurately capture the flow processes. Data-driven machine learning methods can provide faster alternatives to traditional simulators through the inference of neural network models trained with numerical simulation data mappings. Convolutional neural network (CNN)-based models have been successful in providing fast and accurate predictions for high-dimensional and complex multiphase flow problems. However, CNN-based models are often prone to overfitting, therefore requiring large numerical simulation data sets that can be unmanageable as the problem dimension grows. To resolve this problem, we present U-FNO, a novel neural network architecture for solving multiphase flow problems with superior speed, accuracy, and data efficiency.

U-FNO is designed based on the newly proposed Fourier neural operator (FNO) that learns an infinite-dimensional integral kernel in the Fourier space. The FNO has shown excellent performance on single-phase flow problems with great generalization ability and is significantly more data-efficient than CNN-based methods. We extend the FNO-based architecture to a CO₂-water multiphase problem in the context of CO₂ geological storage and propose the U-FNO architecture to enhance the prediction accuracy in multiphase flow systems. We apply the U-FNO architecture to predict dynamic pressure buildup and gas saturation in 2D-radial reservoirs with wide ranges of permeability and porosity heterogeneity, anisotropy, reservoir conditions, injection configurations, flow rates, and multiphase flow properties.

Through a systematic comparison among a state-of-the-art CNN benchmark and three types of FNO variations, we show that the U-FNO architecture has the advantages of both the traditional CNN and original FNO, providing significantly more accurate and efficient performance than previous architectures. Using the U-FNO architecture, the mean absolute error for gas saturation is reduced by 50% while the mean relative error for pressure buildup is reduced by 24% compared to the state-of-the-art CNN benchmark.

The U-FNO predicted gas saturation and pressure buildup is 6×10^4 times faster compared to traditional numerical simulators while maintaining similar accuracy, as long as the ranges for the test case input are within the training data range. The significant improvement in computational efficiency can support many engineering tasks that require repetitive forward numerical simulations. For example, the trained U-FNO model can serve as an alternative to full physics numerical simulators in probabilistic assessment, inversion, and site selection, tasks that were prohibitively expensive with desirable grid resolution using numerical simulation.

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MS01 / 361

Porous ceria foams coated with Ca-doped lanthanum manganite perovskites for solar thermochemical CO₂/H₂O splitting**Authors:** Amir Masoud Parvanian¹; Ehsan Baniasadi²¹ *Postdoctoral Researcher at University of Isfahan*² *Associate Professor***Corresponding Authors:** e.baniasadi@eng.ui.ac.ir, m.parvanian@gmail.com

The solar thermochemical fuel synthesis method utilizes concentrated solar radiation to drive a series of reduction/oxidation (RedOx) reactions for splitting the abundant CO₂/H₂O into CO/H₂ known as syngas. In the following, the syngas will be catalytically converted into solar fuels through a commercially proven process such as Fischer–Tropsch. However, the commercialization of the process needs further improvement of the splitting efficiency. The exceptional properties of porous materials could trigger the commercialization of solar fuels by providing an enhanced surface area for such surface-controlled reaction kinetics. In this study, porous ceria foams are used as the RedOx materials. To increase the ceria oxygen exchange capacity, the porous foams were coated by Ca-doped lanthanum manganite perovskite active materials. The coated samples were tested in a thermochemical CO₂/H₂O conversion process and compared to uncoated powder forms of the materials. The results revealed a significant enhancement of the reduction reaction for perovskite coated foams compared to uncoated powders. The enhanced reduction extent had a beneficial effect on the oxygen release rate and thus nonstoichiometry leading to a higher total amount of fuel produced by CO₂ and H₂O splitting. The results of this study will be practically used in the commercialization of solar fuels.

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MS18 / 362

Pore-scale hydrodynamic and biogeochemical controls on manganese biomineralization in granular media

Authors: Eleanor Fadely¹; Gaitan Gehin¹; Lena Ray¹; Veronica Morales¹; Jasquelin Peña¹

¹ University of California, Davis

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Manganese (Mn) biomineralization is a ubiquitous biogeochemical process with promising applications for *in situ* bioremediation of contaminated soils and sediments. This process involves the enzymatic oxidation of aqueous Mn(II) to form reactive solid-phase Mn(III)/Mn(IV) oxides that aggregate around Mn-oxidizing bacteria. This transformation can immobilize Mn from flowing groundwater, and the resulting oxide particles can sequester co-occurring toxicant metals prevalent at sites impaired by mine drainage and industrial processes. While Mn biomineralization has been investigated in well-mixed batch systems, no studies have considered the effect of incomplete fluid mixing in heterogeneous porous media on this biogeochemical process.

To enhance the ability of Mn biominerals to react with environmental contaminants, it is crucial to understand the extent to which biomineral formation can be externally controlled by tuning flow conditions. Both size and distribution of Mn oxide aggregates must be optimized to maximize the reaction between the biominerals and contaminants in flowing groundwater. Specifically, biominerals should be distributed uniformly but not be so abundant that the pore network becomes clogged. Our research investigates the pore-scale **transport and mixing mechanisms** that control **biomineral formation extent** (location, percent coverage of pore network) and **morphology** (aggregate size, shape). We use “soil-on-a-chip” **microfluidic reactors** to simulate the geometry of a sandy soil pore network and visualize biogeochemical activity at the microbe-mineral scale with brightfield and epifluorescence microscopy.

In this study, we performed experiments to i) quantify the **spatial distribution and aggregation of the microbial inoculum** (*Pseudomonas putida* GB-1, a Mn-oxidizing bacterium), and ii) characterize the **extent and morphology of the biominerals** formed after the introduction of aqueous Mn(II) into the microfluidic reactor for conditions of variable flow rate (slow, medium, high), flow continuity (intermittent or continuous), and feeding regime (nutrient-rich or minimal salts medium). Preliminary results for experiments using a continuous fluid injection at medium flow rate (0.1 mL/hr) show that the bacteria in the inoculum distribute evenly throughout the pore network and coalesce over time into large microbial aggregates in pore throats and at grain contacts. Mn oxidation occurs at microbial aggregate boundaries in contact with the pore fluid. We are currently developing image processing methods to quantify the size distribution and percent coverage of microbial aggregates across the microfluidic pore network as well as the prevalence of Mn oxides relative to grain surfaces.

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MS06-A / 364

Preferential Flow of Emulsion through Homogeneous Porous Media

Authors: Ke Xu¹; Qingrong He¹; Wei Yang¹

¹ Peking University

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We experimentally identify major preferential paths for emulsion and foam flow, even at steady-state in homogeneous porous media. Therefore, even identical parallel channels cannot be assumed equivalent when emulsion or foam flows through them. This discovery challenges previous approaches that upscale single pore/channel-scale rheology to Darcy-scale simply by linear summation and integration adopting the “bundle-of-tubes” approach.

We construct a general form of emulsion/foam rheology model at single channel scale that is compatible with most reported models. We investigate ΔP - Ca correlation when fixing the dispersed fluid flow rate and droplet/bubble size. Surprisingly, the ΔP - Ca curve under these constraints is non-monotonic, consisting of an ascending segment at low Ca (regime I), a descending segment at higher Ca (regime II), and another ascending segment when Ca goes to infinity (regime III), regardless of exact channel geometry and fluid properties. The origin of preferential flow in homogeneous porous media is rigorously rationalized by linear stability analysis from this non-monotonicity.

Microfluidic experiments validate the abovementioned theory. The non-monotonic ΔP - Ca correlation is experimentally reproduced. Specifically, three different flow patterns are observed in the three curve segments: (1) in regime I, droplets fulfil almost every single pore but only very few droplets are mobilized, by droplet-droplet squeezing (Fig.a); (2) in regime II, not all pores are occupied by droplet, and only few droplets are mobilized, by droplet-droplet replacement (Fig.b); (3) in regime III, droplets distribute sparsely and all droplets independently mobilize along with the continuous phase (Fig.c). Capillarity-viscosity interplay explains the change of droplet flow behavior in different regimes.

Due to the emergence of preferential flow, a stable fluid distribution pattern has to be solved before constructing a rheology model. In addition, regular upscaling methods for non-Newtonian fluid flow in porous media is physically incorrect for emulsion and foam, due to varying phase ratio in different flow paths. This work thus brings light to constructing a physics-based rheology model for emulsion and foam in porous media.

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Poster / 366

Physics Informed Neural Networks for Fluid Flow in Porous Media

Author: Waleed Diab¹**Co-author:** Mohammed Saad Al Kobaisi ¹¹ *Khalifa University***Corresponding Authors:** 100049411@ku.ac.ae, mohammed.alkobaisi@ku.ac.ae

Physics Informed Neural-Networks (PINNs) is an emerging field that is gaining credence among the scientific computing community. By embedding domain knowledge into machine learning models, PINNs allow for long-term, accurate, consistent, and generalizable spatiotemporal predictions that are rooted in physics while leaving room for data assimilation. In addition, the PINNs approach is mesh-free, avoids truncation errors, and can solve inverse problems as easily as it can solve forward problems. In this work, we present a PINNs approach for the simulation of fluid displacement in porous media. Specifically, we solve the non-linear hyperbolic Buckley-Leverett (B-L) problem with a nonconvex flux function, and we extend the PINNs solution to a 2D heterogeneous problem. The contributions of our work are threefold. First, we present a PINNs approach to solving the hyperbolic B-L problem by regularizing the neural network residual with more physics. Second, we show that it is possible to obtain extremely accurate solutions using the Adam optimizer with a residual-based adaptive refinement (RAR) algorithm that achieves an ultra-low loss. Our solution method can accurately capture the shock-front. Third, we extend the PINNs application to stratified and heterogeneous porous media in a 2D setting.

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MS09 / 367

On a workflow for efficient computation of the permeability of tight sandstones

Author: Vladislav Pimanov¹**Co-authors:** Ekaterina Muravleva ¹; Denis Orlov ¹; Dmitry Koroteev ¹; Oleg Iliev ²; Vladislav Lukoshkin ¹; Pavel Toktaliev ²¹ *Skolkovo Institute of Science and Technology*

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We present a workflow for fast pore-scale simulation of single-phase flow in tight reservoirs typically characterized by low, multiscale porosity. Multiscale porosity implies that the computational domain contains porous voxels (unresolved porosity) in addition to pure fluid voxels. In this case, the Stokes-Brinkman equations govern the flow, with the Darcy term needed to account for the flow in the porous voxels. As the central part of our workflow, robust and efficient solvers for Stokes and Stokes-Brinkman equations are presented. The solvers are customized for low-porosity binary and multiclass images, respectively. Another essential component of the workflow is a preprocessing module for classifying images with respect to the connectivity of the multiscale pore space. Particularly, an approximation of the Stokes-Brinkman problem, namely, the Darcy problem, is investigated for the images that do not have pure fluid percolation paths. Thorough computational experiments demonstrate efficiency and robustness of the workflow for simulations on images from tight reservoirs.

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Participation:

In person

MS17 / 369

Modeling of Powder Bed Dynamics in Thermochemical Heat Storage

Authors: Torben Prill¹; Marie Gollsch¹; Henrike Schmies¹; Marc Linder¹; Thomas Jahnke¹

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Storing energy in the form of heat has been under long-standing investigation for prospective applications, such as the capturing of excess heat from industrial processes as well as storing energy in concentrated solar power plants. Investigated mechanisms for the heat storage include the adsorption in porous media, materials undergoing phase changes and thermochemical reactions. Among these, thermochemical heat storage provides a large energy capacity and next to perfect reversibility. More specifically, storage in the CaO/Ca(OH)₂-System is investigated because of the low price and environmental friendliness of the reactants.

In the project THEMSE, DLR is developing models and simulations as well as experimental characterization methods for thermochemical heat storage in the CaO/Ca(OH)₂-System. In this talk, we shall give an overview over the project with a focus on the modeling activities.

Special attention is given to the investigation of how the cycling of the material influences the heat and mass transport in the powder bed inside the reactor. This happens through mechanical and physical alteration of the powder bed, mainly through three mechanisms. First, the gas flow through the reactor exerts a force on the powder particles, compacting the powder bed. The resulting densification of the bed increases its flow resistance, while improving the heat transport. Second, the agglomeration of powder particles, where bonds between the particles form, turning the bed into a solid. The exact mechanism of the agglomeration is yet unknown, but it can be characterized by mechanical measurements. Third, the expansion of the powder particles through water uptake during the hydration stage, and the corresponding contraction during dehydration.

To model the compaction and solidification of the powder bed during cycling, we present a mechanical model based on Drucker-Prager-Cap plasticity, which has been used previously for powder compaction, see e.g. [1]. The parameterization of the model, i.e., the plastic yield surface, is done via flow tester experiments. The changes in the powder bed during cycling are modeled by hardening mechanisms, i.e., a changing yield surface, corresponding to powder compaction and agglomeration, respectively.

Then, the plastic model is coupled to a reactor scale model, simulating the heat and mass transport, as well as the thermochemical reaction using a model, similar to [2]. This enables the study of the powder bed dynamics under different boundary conditions during cycling, such as pressure drop, water vapor fraction and reactor geometry.

Finally, an outlook will be given on the multi-scale modeling of the reactor. The geometrical micro-scale characterization of the material is done using micro computed tomography (μ CT). From the μ CT-Images, effective transport parameters, such as diffusivity and permeability are computed for different stages of agglomeration. These are then used in the reactor-scale model to produce predictions, which can be verified on the reactor-scale.

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References:

[1] Wu, C.-Y & Ruddy, O.M. & Bentham, A.C. & Hancock, B.C. & Best, Serena & Elliott, James. (2005). Modelling the mechanical behaviour of pharmaceutical powders during compaction. *Powder Technology*. 152. 107-117. 10.1016/j.powtec.2005.01.010.

[2] Nagel, Thomas & Shao, Haibing & Singh, Ashok & Watanabe, Norihiro & Roßkopf, Christian & Linder, Marc & Wörner, A & Kolditz, Olaf. (2013). Non-equilibrium thermochemical heat storage in porous media: Part 1 –Conceptual model. *Energy*. -. 10.1016/j.energy.2013.06.025.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS21 / 371

The anomalous moisture transport in cementitious materials: causes and models

Author: Zhidong Zhang¹

Co-author: Ueli Angst¹

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The moisture condition in concretes is closely related to their durability. Liquid water is the intermedia for the penetration of aggressive agents (e.g., chloride). The empty pores provide paths for the diffusion of gases (e.g., CO₂). These processes can lead to concrete deterioration or steel corrosion. Therefore, appropriate methods to determine moisture state in concrete are essential for predicating structures durability. Conventional moisture transport models are based on the Darcy's or Fick's law. However, they do not work for anomalous moisture transport, often reported for cementitious materials.

Anomalous moisture transport is caused by various reasons and we have developed different models to explain these causes. The present work summarizes the available models in the literature for anomalous moisture transport. The first type of models considers that the microstructure of cementitious materials is altered by water transport. To consider this change, a straightforward way is to use the time-dependent transport coefficient (e.g., water permeability [1–3]). The second type of models was developed by simplifying the complex pore structure as a two-porosity system, so that a dual-porosity/permeability can be applied [4]. Both types of models have been calibrated by experimental data. The other causes and potential ways to develop new moisture transport models will be also discussed in this work.

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References:

1 C. Hall, Capillary imbibition in cement-based materials with time-dependent permeability, *Cem. Concr. Res.* 124 (2019) 105835.

[2] Z. Zhang and U. Angst, Modeling anomalous moisture transport in cement-based materials with kinetic permeability, *Int. J. Mol. Sci.* 21 (2020) 837.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS09 / 372

Pore-scale study on convective drying of porous media by the lattice Boltzmann method

Authors: Linlin Fei¹; Feifei Qin¹; Jianlin Zhao¹; Dominique Derome²; Jan Carmeliet¹

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In this work, a multi-component multiphase lattice Boltzmann method (LBM) is proposed and applied to convective drying of a dual-porosity porous medium at pore-scale. The pore-scale information can be directly resolved by the proposed numerical model. The drying dynamics are analyzed in detail in terms of pore-scale drying patterns, saturation profiles versus height, vapor concentration boundary layers, evaporation rate and periods as well as the behind mechanisms. From the numerical simulations, it is found the convective drying process of a dual-porosity porous medium follows the pattern that the evaporation front invades the large pores first and then penetrates the smaller pores. The evaporation rate undergoes a transition from a constant rate period (CRP, the first phase) to the falling rate period (FRP, the second phase). It is found that in the CRP, the evaporation rate increases with the inflow Reynolds number (Re), while in the FRP the evaporation curves almost collapse at different Re . The underlying mechanism is elucidated by introducing an effective Péclet number (Pe). It is shown that convection is dominant in the CRP, and diffusion in FRP, as evidenced by $Pe > 1$ and $Pe < 1$, respectively. Within the considered parameter range, we find a log-law correlation of the average evaporation rate in the CRP regime with the inflow Reynolds number. The present work provides new insights into the drying physics of porous media and its direct modeling at the pore scale.

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MS06-A / 373

Advanced Digital-SCAL measurements of gas trapping in sandstone

Authors: Ying Gao¹; Tibi Sorop¹; Hilbert van der Linde¹; Ab Coorn¹; Niels Brussee¹; Steffen Berg¹

¹ *Shell Global Solutions International B.V.*

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As a key parameter, trapped gas saturation (S_{gr}) plays an important role in subsurface processes involving gasses such as carbon capture and storage, H₂ storage efficiency and also the production of natural gas. However, the gas compressibility, partitioning/solubility and diffusion effects can be important impact factors for the spatial evolution of fluid and gas phases and directly contribute

to the overall mobility. Thus, Sgr is difficult and challenging to measure in the laboratory or field. We have indications that the conventional method of measurement- low-rate unsteady-state core flooding - is often impacted by gas dissolution effects, resulting in large uncertainties of the measured Sgr. Moreover, it is not understood why this effect occurs even for brines pre-equilibrated with gas. The hypothesis is that it is related to the effective thermodynamic behavior inside the porous medium which due to the geometric confinement could be different than the phase behavior of bulk fluids.

Therefore, in this study, we used high resolution X-ray CT imaging techniques to be able to investigate such effects at the pore scale. We conducted in-situ experiments in Bentheimer sandstone using X-ray computed micro tomography which allowed direct visualization of the snap-off of gas phase and the shrinkage of the gas ganglia inside of the pore. Gas saturated brine was injected at very low rate (0.495 $\mu\text{L}/\text{min}$) using high pressure syringe pumps (Quizix), while applying with a back pressure of 5 bar to ensure that the pressure drop over sample is low enough to prevent experimental artefacts. The gas and water distributions in the pore space were scanned using a Zeiss Versa 520 micro-CT scanner with the voxel size of 4 μm at regular time intervals after injection of every PV. After injecting a total of 6 PV, 7 more images were taken every 24 hours to check the gas distribution in the rock sample after stopping the injection.

One of the key findings is that for pre-equilibrated brine, the remaining gas saturation was continually decreasing with more brine injected and even after the brine injection was stopped, resulting in very low Sgr values (possibly even zero) At the pore scale level, we were able to clearly observe the snap-off effect followed by a further shrinkage of the gas in each pore. This points to the hypothesis that indeed the gas dissolution plays a role during the experiment. The effect is likely linked to ripening dynamics which involves a coupling between phase equilibrium and dissolution/partitioning of components on the one hand and capillarity in the geometric confinement of the pore space on the other hand.

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MS03 / 374

Adaptive Conservative Time Integration with Higher Order Schemes for Transport in Fractured Porous Media

Author: Michael Liem¹

Co-authors: Patrick Jenny ; Stephan Matthai²

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² *The University of Melbourne*

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When transport (or any other hyperbolic partial differential equation) is solved with explicit time integration in a finite volume method (FVM), the Courant-Friedrichs-Levy (CFL) number needs to be below a critical value in order to ensure stability and accuracy. The CFL criterion provides an upper bound of the time step for every grid cell. In conventional methods, where the same time step is used for all grid cells, the lowest value of this upper bound is chosen as the global time step. When advection speed and/or grid spacing vary considerably throughout the domain, this can lead to unnecessary computational cost because many cells could be integrated with a much larger time step.

Various local time stepping methods have been developed which overcome this drawback by using customized step sizes for each cell. The adaptive conservative time integration (ACTI) scheme is a local time stepping method recently developed by Jenny (2020). The basis for this scheme is that all local time steps Δt_I are fractions of the global time step by powers of two, i.e., $\Delta t_I = \Delta t_{\text{Global}}/2^{L_I}$, where the integer variable $L_I \geq 0$ denotes the time refinement level of a particular grid cell. The grid cells are synchronized after each global time step and strict conservation at the global time resolution is guaranteed.

For tracer transport in two-dimensional discrete fracture and matrix models we demonstrate that ACTI reduces the computational cost by orders of magnitude compared to global time stepping. We obtain excellent results with a first-order upwind scheme which is still widely used in many applications. However, we notice that a combination of ACTI with a standard higher-order MUSCL scheme can lead to spurious oscillations in the solution even though this flux scheme is stable in combination with global time stepping. In this work, we study the influence of different slope limiters on the solution stability, and we propose a modified MUSCL scheme relying on advection of an inclined reconstruction (MUSCL-AIR). Empirically, we show that a more dissipative slope limiter can reduce the spurious oscillations that arise with the standard MUSCL scheme, albeit at the cost of slightly more diffusive concentration fronts. Combining ACTI with MUSCL-AIR results in accurate and stable solutions independent on the choice of slope limiter. This combination is therefore ideally suited for tracer transport in fractured porous media, but it is also very attractive for other applications where advection speed and/or grid spacing vary throughout the domain and a higher-order transport scheme is desired.

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JENNY, P. 2020. Time adaptive conservative finite volume method. *Journal of Computational Physics*, 403, 109067. doi: 10.1016/j.jcp.2019.109067

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

Poster / 375

Dynamic pore-network modeling of compositional flow and nanoconfined phase behavior in shale rocks

Authors: Sidian Chen¹; Jiamin Jiang²; Bo Guo¹

¹ *University of Arizona*

² *Chevron Energy Technology Co.*

Corresponding Authors: boguo@arizona.edu, jiamin.jiang@chevron.com, sidianchen@email.arizona.edu

The phase behavior of fluids becomes abnormal in shale formations due to the presence of extensive nanoscale pore spaces. Prior research has demonstrated that this so-called nanoconfined phase behavior—driven by the presence of significant capillary pressure and interaction between hydrocarbons and the pore wall (i.e., competitive adsorption)—is a function of the pore size and geometry. However, it remains unknown how the pore-size and -geometry dependent nanoconfined phase behavior manifests in complex multiscale nanopore structures representative of shale rocks. The interplay between the nanoconfined phase behavior and compositional gas-condensate flow adds further complexity. Here, we develop a novel dynamic pore-network model that couples nanoconfined phase behavior and compositional gas-condensate flow. The new modeling framework is comprised of 1) a phase-equilibrium model that accounts for the pore-size and -geometry dependent nanoconfinement effects and 2) a fully implicit dynamic pore-network modeling framework that couples the individual-pore nanoconfined phase-equilibrium formulation with the two-phase compositional flow. This new framework for the first time allows us to investigate the interactions between nanoconfined phase behaviors and compositional flow dynamics in complex multiscale pore structures representative of shale rocks, which we will illustrate by a series of numerical experiments on complex nanopore networks with pores varying in size and geometry.

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MS23 / 376

Structure and stochastic dynamics of hydrodynamic flow and transport in three-dimensional random fracture networks

Authors: Jeffrey Hyman¹; Marco Dentz²

¹ *Los Alamos National Laboratory*

² *IDAEA-CSIC*

Corresponding Authors: marco.dentz@csic.es, jhyman@lanl.gov

We study the upscaling and large scale modeling of anomalous transport in three-dimensional random fracture networks. Our approach is based on the continuous time random walk (CTRW) approach, which was pioneered in this context by Brian Berkowitz in his 1997 paper in *Phys. Rev.*

Letters on Anomalous Transport in Random Fracture Networks. Based on detailed flow and particle tracking simulations, we analyze the statistical properties of Lagrangian speeds along individual particle trajectories. Particle transitions are characterized by the conditional probability distribution of subsequent particle speeds separated by different lag distances. We observe that the correlation structure can be described by a Gaussian copula. This finding implies that the particle motion can be described stochastically by a CTRW combined with a Langevin equation for the evolution of particle speeds that is determined by the speed point distribution and correlation length. Mass transfer between the fracture and matrix domains is included in this framework by a compound Poisson process that accounts for particle trapping and retention. The results of the stochastic model are compared to the data from the detailed numerical simulations for solute breakthrough curves and the mean and variance of particle displacements. The model captures all features of anomalous dispersion, and can predict particle transport for different initial conditions.

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Online

MS09 / 377

How the Probabilistic Nature of the Nucleation Process Affects and Controls the Distribution of Mineral Precipitates in Porous Media

Authors: Mohammad Masoudi¹; Mohammad Nooraiepour¹; Helge Hellevang¹

¹ *University of Oslo*

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Nucleation and growth of secondary mineral phases is of great importance in a variety of processes in different fields. Mineral precipitation alters the morphology and hydrodynamics of the porous media by blocking the pore and throats and changing the tortuosity and permeability of flow paths. Even reaction rates are affected by the reshaping of available reactive surfaces. Any mineral precipitation process begins with the nucleation, which is a probabilistic phenomenon. It is often overlooked in studying the reactive transport phenomena. Nucleation controls the location and timing of crystal formation in a porous structure. The spatial distribution of stable secondary nuclei is crucial to precisely predict the hydrodynamics of the porous medium after mineral precipitation. Thus, a deeper understanding of the mineral nucleation and growth process is essential and it is necessary to develop a new probabilistic nucleation approach that could produce more reliable results. Accordingly, we have developed a new probabilistic nucleation model and incorporated it into a pore-scale Lattice Boltzmann reactive transport model to investigate the effect of various factors such as saturation ratio, flow rate, temperature, interfacial free energy, nucleation rate, and growth rates on the

distribution of precipitated secondary minerals. In our model, the probabilistic induction time statistically spreads around the measured or reported induction time, either obtained from experiments or approximated by the exponential nucleation rate equation suggested by the classical nucleation theory (CNT). We provide a detailed explanation on how to implement the developed probabilistic nucleation approach into pore-scale reactive transport models. We also gave a thorough description of each parameter of the probabilistic nucleation model and how to measure or calculate them for different fluid and rock systems. Additionally, we used a new approach to measure the disorder of the spatial mineral distributions. The developed models provide new insights into the spatiotemporal evolution of porous media during mineral precipitation. Furthermore, the outcomes provide the basis for implementing mineral nucleation and growth for reactive transport modeling across time-scales and length-scales.

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References:

Fazeli, H. et al. (2020) 'Pore-Scale Modeling of Nucleation and Growth in Porous Media', ACS Earth and Space Chemistry. American Chemical Society, 4(2), pp. 249–260. doi: 10.1021/acsearthspacechem.9b00290.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS16 / 378

Application of Screen Channel Liquid Acquisition Devices for Phase Separation in Microgravity

Author: Prithvi Shukla¹

Co-author: Michael Dreyer¹

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Phase separation is critical for the supply of gas-free liquid propellant from the tank outlet to the engine of a spacecraft. In a microgravity environment, surface tension and contact angle become

the governing mechanism for phase separation and dictate the position of the liquid-gas interface. Liquids with zero-degree contact angle tend to adhere to the tank wall, and gas stays in the center. Therefore, to maintain a constant supply of liquid to the outlet of the tank, a liquid acquisition device (LAD) is essential. Screen channel liquid acquisition devices (SC-LAD) are a type of LAD that work on the principles of capillary action. Liquid enters into the channel through a porous screen but the entry of gas is blocked as long as the pressure difference across the screen is below its bubble point.

In this project, the experiment is designed to test the phase separation in a microgravity environment with the help of a screen channel liquid acquisition device SC-LAD. For this purpose, a supply tank has been designed with a SC-LAD inside it. The screen used in the SC-LAD is DTW 200x1400. The liquid is removed from the supply tank with the help of a gear pump and a combination of valves in the liquid pipeline. A total of 22 drop tower tests are performed with 9.1 seconds of microgravity each. The analysis of the sensor data and the images obtained by the high-speed cameras shows a successful separation of phases through the SC-LAD in subcritical conditions and ingestion of bubbles at the critical condition. A combination of various complex phenomena and their effects on one another could be also observed visually during the experiments. The phenomena observed are reorientation of the free surface under microgravity, capillary rise of liquids between parallel plates, flow through screen pressure loss due to applied removal flow rate, and bubble point breakthrough of the screen.

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MS01 / 379

Analytical analysis of wettability in hydrogen-rock-brine systems

Authors: Farzaneh Nazari¹; Rouhi Farajzadeh²; Vahid Niasar³

¹ *The University of Manchester*

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³ *University of Manchester*

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The energy transition efforts have given rise to the demand for energy storage. Due to its desirable characteristics, hydrogen is a favorable medium for storing the excess low-carbon electricity. Subsurface porous formations provide the solution for large storage capacities required to facilitate the energy transition. A successful storage project requires accurate modeling of the hydrogen movement and extent of its trapping, which is partially determined by the wetting properties of the

hydrogen/water/rock system. The three-phase contact angle is an indirect means of quantifying wettability. Wettability and the resulting three-phase contact angles can be calculated using the surface force analysis. The interplay between the surface forces active in the contact region (namely, van der Waals (vdW), electrostatic, and structural/hydration forces) determine the film stability and the wetting behavior of the multi-phase systems.

In this study, we conduct a surface force analysis to investigate the wetting behavior of hydrogen in the presence of water and rock relevant for the underground storage systems. In light of surface forces, different parameters such as dielectric properties of the phases (water, hydrogen, rock), medium properties (water salinity and pH), and interface (water-rock and water-hydrogen) potentials/charge densities affect the magnitude of the vdW, electrostatic, and structural forces. The hydrogen contact angles for smooth surface can be calculated once the surface forces are quantified. Equilibrium and meniscus contact angles can be determined by means of the calculated total active force, the equilibrated film thickness, and capillary properties. An extensive sensitivity analysis on the model parameters controlling the wetting state of the considered system has been performed and critical parameters have been identified.

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Time Block B (14:00-17:00 CET)

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MS02 / 380

Imbibition dynamics in cellular, xylem-like nanoporous media

Authors: Olivier Vincent¹; Théo Tassin²; Erik Huber²; Abraham Stroock²

¹ *CNRS & Cornell University*

² *Cornell University*

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We built multiscale porous media resembling the architecture of water-conducting tissues in plants (xylem), using micro/nano-fabrication techniques with silicon and glass. These structures couple a nanoporous layer to arrays of microchannels of varying aspect ratio. We studied experimentally spontaneous water imbibition in these artificial systems, in a situation where imbibition is triggered by capillary condensation from water vapor in the atmosphere surrounding the samples. We show that the presence of the microchannels can dramatically affect the dynamics of imbibition in the nanostructure, resulting in faster dynamics globally, and in intermittent dynamics locally. We further show that these effects can be tuned not only by the choice of the geometry of the microstructure, but also by changing the filling state of the cavities (air vs. vacuum), which suggests strategies for dynamic control of the speed of imbibition.

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Poster / 381

On the CO₂/caprock interaction based on quantitative image analysis from in-situ x-ray tomography

Authors: Eleni Stavropoulou¹; Lyesse Laloui¹

¹ EPFL, Laboratory of Soil Mechanics, Lausanne, 1015, Switzerland

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Previous studies have highlighted the great potential of shales as geological barriers thanks to their favourable properties (very low permeability, high capillary entry pressure, swelling properties). However, the response of shales is governed by Thermo-Hydro-Chemo-Mechanical (THMC) couplings of high complexity, often making their study challenging. The difficulty arises mainly from the fact that the undergoing phenomena take place in a much longer time period compared to the time-scale of experimental campaigns and thus, most measurable responses have been observed only at the application of extreme, often non-representative, boundary conditions. Taking into consideration limitations related to boundary conditions, sample size and mineralogy the proposed work aims to investigate the CO₂/caprock interaction at the microscale level using for the first time live x-ray tomography.

X-ray tomography is a non destructive imaging tool that can provide precious insight into the 3D kinematics of heterogeneous materials and reveal localised response which otherwise is not depicted in the overall recorded measurements of typical hydromechanical testing methods. In order to improve both spatial (pixel size) and temporal (transport-related) resolution, very small cylindrical shale samples (d=h=5mm) are tested in a high resistance x-ray compatible cell. First, a better understanding of the contribution of the different mechanisms is demonstrated with simple isotropic CO₂ exposure on the sample, where the chemo-mechanical and thermo-mechanical impact of supercritical CO₂ on the material's microstructure is evaluated. A second series of tests follows where CO₂ injection under isotropic confinement is performed.

3D image analysis revealed that even at that small scale, pre-existing micro-fissures in shales cannot necessarily be avoided. Pre-existing cracks are more prone than intact matrix to opening/closing (increased localised strain activity) upon THM loading which here is imposed both by thermal loading and water evaporation in the anhydrous CO₂, they thus have a crucial role for the integrity of the entire storage system. Application of confinement closes pre-existing fissures (at least at a given resolution) but their contribution to the overall flow is yet to be quantified. CO₂ breakthrough has been identified from the volumetric response of the sample which locally expands in locations around pre-existing fissures. The current work shows that even at resolutions lower than the average pore size of the material, 3D image analysis can reveal important insight on the localised behaviour which in the context of CO₂ storage can be related to potential leakage paths.

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Boulin, P. F., Bretonnier, P., Vassil, V., Samouillet, A., Fleury, M., & Lombard, J. M. (2013). Sealing efficiency of caprocks: Experimental investigation of entry pressure measurement methods. *Marine and Petroleum Geology*, 48, 20-30.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS13 / 384

Operando Determination of Pore-filling Mechanism and Saturation of PEFC Catalyst Layer using Small-Angle X-ray Scattering

Author: Kinanti Hantiyana Aliyah¹

Co-authors: Christian Appel¹; Christian Prehal²; Manuel Guizar-Sicarios¹; Lorenz Gubler¹; Jens Eller¹

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Shortcomings in the water management of polymer electrolyte fuel cells (PEFC) need to be overcome for successful market penetration. Proper membrane humidification relies on ionomer hydration, which in turn affects the performance. In contrast, excess water retention in the pores results in blockage of the gas diffusion to the active sites of the electrochemical reaction, thus reducing performance and efficiency.

Various measurement techniques suitable with the length scale of PEFC components have been explored to address the PEFC water management challenge. For the gas diffusion layer (GDL), technological advances have permitted operando water saturation quantification and its mechanism with X-ray tomography with few microns resolution (1-4). Furthermore, sub-voxel information contained in the X-ray tomography data has demonstrated accurate water quantification in the nanoporous microporous layer (MPL) (5). However, in the nanoscale regime of the catalyst layer, the quantification

of water and the pore-wetting mechanism remains nontrivial. Studies involving imaging techniques dedicated to understand the water management in the catalyst layer have been carried out albeit with limited spatial resolution (6).

Small angle X-ray scattering (SAXS) is proposed as suitable candidate for a diagnostic tool to investigate the catalyst layer saturation under operating conditions. SAXS is well suited for diagnosing the presence of liquid water during operando experiments because of its sensitivity to electron density contrast, nanoscale observation window, high temporal resolution and adequate spatial resolution to distinguish the components in PEFCs. SAXS intensity profiles measured at the cSAXS beamline of the Swiss Light Source at the Paul Scherrer Institut with a recently developed SAXS-compatible operando PEFC (Figure 1 middle and right) are interpreted using representative morphology models and assuming different water filling mechanisms (Figure 1 middle and left). The presentation will summarize the structure morphology fitting approaches and provide insights on the actual pore filling mechanism.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS08 / 385

Modelling Transverse Anomalous Solute Transport in Highly Heterogeneous Porous Media

Authors: Aronne Dell'Oca¹; Marco Dentz²

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We study the intermittent transverse dynamics of solute transport through highly heterogeneous porous media. Considering a Lagrangian framework focused on the equidistant analysis of the particles motion, we identify two fundamental mechanisms that determine large-scale particle motion, namely, the relaxation towards a (non-zero) average transverse particle position and the short-scale correlated behavior of the transverse particles motion. Based on these mechanisms, we derive a theory that jointly predicts anomalous transverse and longitudinal dispersion in terms of Eulerian velocity distribution, key statistics of the system heterogeneity, and two additional parameters related to the particles relaxation process with a clear physical meaning.

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Time Block B (14:00-17:00 CET)

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Online

MS03 / 386

A Particle-Tracking Scheme with Adaptive Diffusion for Multiphase Flows in Fractured Porous Media

Author: Ranit Monga¹

Co-authors: Daniel Meyer²; Patrick Jenny

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Advection dominated transport processes in sub-surface formations are characterized by discontinuities in the fields of transported quantities, e.g., concentration in the context of solute transport, phase-saturation in multiphase flows. Realistic predictions are challenging for Eulerian schemes because they suffer from numerical dispersion. This, however, does not limit Lagrangian particle-tracking methods, which makes them particularly relevant for advection dominated processes [Michalak and Kitanidis, (2000)].

We are interested in transport in fractured porous media with a permeable matrix, and adopt an Embedded Discrete Fracture Model where fractures are treated as lower dimensional manifolds [Deb and Jenny, (2017)]. However, the fracture-matrix interface is not resolved. In Monga et al. (2020), we presented a conservative stochastic particle-tracking scheme for advective solute transport in single-phase flow. This scheme uses a two-state Markov chain with transition probabilities for inter-continuum particle transfer. The probabilities are pathline-specific and scale with the particle's modeled travel time through the grid cell.

The focus of the present work is to improve the efficiency of the mentioned stochastic particle scheme and extend it to model saturation evolution in two-phase immiscible flows. Saturation evolution is simulated by the motion of two particle ensembles, i.e., one for each phase [Tyagi et. al (2008)].

For flows with high Péclet numbers and without capillary pressure differences, saturation transport is hyperbolic in nature. With finite particle ensemble sizes, capturing saturation discontinuities becomes challenging due to inaccurate cell-saturation estimates and related instabilities at saturation fronts. We aim to tackle this by including an adaptive diffusivity to the system, which selectively acts in the vicinity of the saturation front and remains inactive away from the front. To this end, a Smagorinsky-type [Smagorinsky (1963); Lilly (1966)] diffusion coefficient is proposed, which scales with the magnitude of the saturation gradient. Our goal is to keep the expression quantifying the coefficient's magnitude generic, without the necessary adjustments for different flow scenarios.

The proposed particle scheme is potentially extendable to multi-species settings and enables the straightforward formulation of Lagrangian models for locally unresolved sub-grid processes such as phase dissolution or trapping.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Understanding the influence of pore-scale structural heterogeneity in CO₂ geo-sequestration

Author: Farshad Daraei Ghadikolaei¹

Co-authors: Anna Herring²; Mark Knackstedt³; Mohammad Saadatfar⁴

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1. Introduction

Of the viable strategies outlined by the Intergovernmental Panel on Climate Change (IPCC) for atmospheric emission reduction strategies and technologies, geological storage of CO₂ holds an enormous promise with the potentials to have significant impacts on emission and atmospheric CO₂ reduction. Predicting the behavior of CO₂-brine in the complex heterogeneous porous structure of reservoir rocks as well as the interaction between these fluids with minerals in rocks are important for designing and managing CO₂ storage sites in CCS technology. To increase the effectiveness of the underground CO₂ sequestration, the multiphase-flow and its relevant mechanisms that change the distribution and concentration of the underground CO₂ must be assessed. To date, CO₂ geo-sequestration as a complex multiphase fluid flow in heterogeneous rock systems has not yet been given enough attention due to various reasons including lack of high quality experimental data, coupled fluid-fluid-rock interaction that is made even more complex due to rock heterogeneity, difficulty of in-situ experimentation and acquisition of usable data etc.

2. Materials and Methods

The focus of this research is directed towards understanding the role of rock heterogeneity on the safety and capacity of CO₂ geo-sequestration at the pore and core scales. We will present a pore-scale tomographic and experimental study of CO₂ trapping mechanisms in homogeneous and heterogeneous sandstones. The in-situ experiments consist of multiple sets of drainage and imbibition experiments on three sandstone rocks with different types of heterogeneities. The working fluids in the experiments were super-critical CO₂ (scCO₂) and Potassium Iodide (KI) brine. High resolution X-ray micro Computed Tomography (XCT) scans were acquired to resolve pore scale features and fluid distribution in the system. The experimental setup 1 is composed of a high pressure/temperature triaxial flow cell for in-situ flow experiments.

3. Results and Conclusion

Rock heterogeneity at the pore scale can be mapped in 3D and we have correlated rock morphology with multi-phase fluid distribution. Our results show larger amounts of trapped scCO₂ in heterogeneous rock compare with the homogeneous ones at a high rate. Residual scCO₂ are mostly trapped in pores with larger radii with high aspect ratios. Moving toward pores with smaller radius and aspect ratio decreases the amount of scCO₂ in the pores. We have also conducted in-situ cyclic brine-CO₂ flooding experiments, and our results show that residual CO₂ accumulates in layers parallel to the low-perm lamination layers, and primarily below the layers present in the rock. Further, we observe that scCO₂ saturation profiles below the low-perm layers align after drainage. These results agree with the conceptual model that the cyclic fluid injection creates a preferential high-flow pathway below the low-perm layer [2]. We observe that at low flow rates; the capillary trapped CO₂ increases in volume as the number of injection cycle increases, however, at high flow rates, lower residual trapping of CO₂ is observed.

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1 P.E. Øren et al. <https://dx.doi.org/10.2139/ssrn.3366008>
[2] A. L. Herring, et al. <https://doi.org/10.1029/2021WR030891>

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

Poster / 388**Space-time upscaling of reactive transport in porous media****Authors:** Nicolae Suciu¹; Florin Adrian Radu²; Iuliu Sorin Pop³¹ *Tiberiu Popoviciu Institute of Numerical Analysis, Romanian Academy*² *University of Bergen, Norway*³ *Hasselt University***Corresponding Authors:** sorin.pop@uhasselt.be, sucIU@math.fau.de, florin.radu@uib.no

Reactive transport in saturated/unsaturated porous media is numerically upscaled to the space-time scale of a hypothetical measurement through coarse grained space-time (CGST) averages. The one-dimensional reactive transport is modeled at the fine-grained Darcy scale by the actual number of molecules involved in reactions which undergo advective and diffusive movements described by global random walk (GRW) simulations. The CGST averages verify identities similar to a local scale balance equation which allow us to derive expressions for the flow velocity and the intrinsic diffusion coefficient in terms of averaged microscopic quantities. The latter are further used to verify the CGST-GRW numerical approach. The upscaling approach is applied to biodegradation processes in saturated aquifers and variably saturated soils and the CGST averages are compared to classical volume averages. One finds that if the process is characterized by slow variations in time, as in homogeneous systems or in case of observations of reactive transport in heterogeneous aquifers made at large times or far away from the contaminant source, the differences between the two averages are negligible. Instead, the differences are significant if the averages are computed close to the source at early times, in case of aquifer simulations, and can be extremely large in simulations of biodegradation in soils. In the latter case, the volume average is totally inappropriate as model for experimental measurements, leading for instance to overestimations by 100% of the CGST average.

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Participation:

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MS15 / 389

Twisting the ensemble Kalman filter with random forest**Authors:** J. Jaime Gómez-Hernández¹; VANESSA A. GODOY²; Gian Napa³¹ *Universitat Politècnica de València*² *Universitat Politecnica de Valencia*³ *Research***Corresponding Authors:** godoyalmeida@gmail.com, jgomez@upv.es, giannagar@gmail.com

A reformulation of the ensemble Kalman filter is presented in which the updating step is changing from a linear combination of discrepancies between observed and predicted state variables onto a random forest regressor. The method is demonstrated in a synthetic aquifer and the advantage of the new formulation is discussed.

Research financed by grant PID2019-109131RB-I00 funded by MCIN/AEI/10.13039/501100011033 and the InTheMED project, which is part of the PRIMA Programme supported by the European Union's Horizon 2020 Research and Innovation Programme under Grant Agreement No 1923.

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In person

MS09 / 390

Pore scale modeling of the moisture transport in cementitious porous media**Author:** Luka Malenica¹**Co-authors:** Zhidong Zhang ¹; Ueli Angst ¹¹ *ETH Zurich*

Corresponding Authors: ueli.angst@ifb.baug.ethz.ch, zhangzhi@ethz.ch, lmalenica@ethz.ch

Understanding of moisture transport through cementitious porous media, such as concrete or mortar, is of great importance since it is directly related to degradation mechanisms and has great impact on durability of cement-based structures. Prediction of water transport throughout such a complex pore system is usually based on traditional models relying on a homogenization approach and requires different macroscopic properties such as porosity, permeability and tortuosity, among others¹. In recent years, the pore scale modeling of multiphase flow has received significant attention and started to be used as a predictive tool in many different porous media applications². These models account for complex microstructure heterogeneities and together with pore scale experiments (e.g. neutron and X-ray imaging) have potential to improve our understanding of multiphase flow processes and lead development of improved upscaled models by connecting microscale mechanisms with macroscopic properties required for large scale modeling. In the context of cementitious media, application of pore-scale modeling is still limited and yet an emerging tool. Thus, the goal of this work is to advance prediction of moisture transport in cement-based materials by using a pore scale modeling. Among different computational methodologies used for investigation of the multiphase flow at pore-scale, our focus is on direct pore scale modeling since this approach preserves the complexity of the pore-space geometry, while grid-based approach using finite volume discretization and interface capturing approach implemented in OpenFOAM code is used to get insight into relevant physical processes of multiphase flow at pore scale.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS06-B / 391

Intrinsic Mobility control by Foam-like Emulsion?

Author: Ahmad Kharrat¹

Co-authors: Bianca Brandstätter¹; Holger Ott¹

¹ *Montanuniversität Leoben*

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In an earlier study, we found that oil-water-surfactant systems can form foam-like emulsion phases under porous-media flow conditions (<https://doi.org/10.1016/j.jcis.2021.10.022>). Those phases are especially stable far outside optimum conditions as characterized by phase behavior experiments and displacement efficiency in microfluidics. The emulsion phase displaces the oil in film flow attached to the solid surfaces, in the lamella, as well as solubilized as micro emulsion in the aqueous phase in the compartments of the foam-like structure. The results and the close similarity to a foam texture explain some earlier observations on emulsion texture, and emulsion stability against coalescence, oil mobilization and potentially emulsion phase mobility. As in foam flooding, we expect this foam-like phase to show a strongly reduced mobility, which raises the question, whether out-of-optimum emulsion phases can be used for intrinsic mobility control of surfactant flooding. This would be in close analogy to foam flooding, which is considered and used for mobility control, potentially increasing the sweep efficiency of enhanced oil recovery (EOR) operations.

The present study investigated the emulsification and flow characteristics for different surfactant concentrations in microfluidics. The foam phase textures are imaged by optical and fluorescence microscopy and phase mobility is indicated in the differential pressure measurements. We discuss the displacement mechanisms and the relation to foaming/emulsifying in detail and find consistent results in different pore structures and for different injection rates. We conclusively show that the fluid-phase mobility is highest in the optimum, substantially decreasing for non-optimal surfactant concentrations. Therefore, the observed phase may provide an intrinsic mobility control provided that a favorable surfactant concentration gradient can be established across the flood front. This may be an attractive option to enhance oil recovery but requires further research.

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<https://doi.org/10.1016/j.jcis.2021.10.022>

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS23 / 392

Dynamic mesh optimisation for efficient density-driven flow simulations

Authors: Meissam L. Bahlali¹; Pablo Salinas^{None}; Carl Jacquemyn¹; Matthew D. Jackson¹

¹ *Imperial College London*

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Density-driven flows in porous media are frequently encountered in natural systems and arise from the gravitational instabilities introduced by fluid density gradients. They have significant economic and environmental impacts, and numerical modelling is often used to predict the behaviour of these

flows for risk assessment, reservoir characterisation or management. However, modelling density-driven flow in porous media is very challenging due to the nonlinear coupling between flow and transport equations, the large domains of interest and the wide range of time and space scales involved. Solving this type of problem numerically using a fixed mesh can be prohibitively expensive. Here, we apply a dynamic mesh optimisation (DMO) technique along with a control-volume-finite element method to simulate density-driven flows. DMO allows the mesh resolution and geometry to vary during a simulation to minimize an error metric for one or more solution fields of interest, refining where needed and coarsening elsewhere. We apply DMO to the Elder problem for several Rayleigh numbers. We demonstrate that DMO accurately reproduces the unique two-dimensional (2D) solutions for low Rayleigh number cases at significantly lower computational cost compared to an equivalent fixed mesh, with speedup of order x16. For unstable high Rayleigh number cases, multiple steady-state solutions exist, and we show that they are all captured by our approach with high accuracy and significantly reduced computational cost, with speedup of order x6. The lower computational cost of simulations using DMO allows extension of the high Rayleigh number case to a three-dimensional (3D) configuration and we demonstrate new steady-state solutions that have not been observed previously. Finally, applications of the present numerical framework to real-scale copper-rich fluid flow transport in sedimentary basins are considered.

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MS06-B / 393

Capillary Wave Tweezers

Author: Prashant Agrawal¹

Co-authors: Bethany Orme¹; Richard Fu¹; Matthew Unthank¹; Hamdi Torun¹

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Particle manipulation in a liquid has many applications at different length scales: from size-based particle sorting in industrial production processes to cellular manipulation for bio-sensing and analysis in microfluidic lab-on-a-chip devices. Many active methods employing various external fields, such as, optical, acoustic, magnetic and electrical have been used for tweezing particles, particle clusters and biological cells in a liquid volume [1,2,3,4]. However, these devices generally require complex and costly fabrication procedures and operations.

In this work, we use low frequency vibrations (~100 Hz) via capillary waves as efficient tweezers to control particle movement in a liquid volume. We demonstrate a mechanism to manually control the position of capillary wave nodes in an open liquid volume. We demonstrate that the capillary waves trap particles underneath their nodes and the particles follow these nodal positions as the capillary

waves are displaced in the liquid volume. We also characterise the effects of liquid volume, actuation amplitude and frequency on the particles' movement. This newly developed platform provides an adaptable solution to the collection and manipulation of microparticles in biomedical or chemical applications.

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3. C. Quanliang, H. Xiaotao, and L. Liang, "Two-dimensional manipulation of magnetic nanoparticles in microfluidic systems," *Appl. Phys. Express* 6, 025201 (2013).
4. P. Agrawal, P. S. Gandhi and A. Neild, "Microparticle Response to Two-Dimensional Streaming Flows in Rectangular Chambers Undergoing Low-Frequency Horizontal Vibrations," *Phys Rev Appl* 2, 064008 (2014).

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 394

High Precision Saline Intrusion Modelling in Heterogeneous Aquifers using Dynamic Mesh Optimisation

Authors: Pablo Salinas^{None}; Meissam Bahlali¹; Carl Jacquemyn¹; Christopher C. Pain¹; Adrian P. Butler¹; Matthew D. Jackson¹

¹ *Imperial College London*

Corresponding Authors: m.d.jackson@imperial.ac.uk, c.jacquemyn@imperial.ac.uk, a.butler@imperial.ac.uk, pablo.salinas@imperial.ac.uk, c.pain@imperial.ac.uk, m.bahlali@imperial.ac.uk

Saline intrusion (SI) in coastal aquifers is a global problem with the potential to contaminate groundwater used by over a billion people. The problem is becoming more widespread due to increased groundwater abstraction in response to urbanization combined with natural phenomena such as rising sea levels due to climate change or storm surges. Accurate modelling and prediction of SI in coastal aquifers is vital for aquifer management, development of regulatory frameworks and risk assessment. However, numerical modelling of SI is very challenging because the mixing zone at the saline front is often highly anisotropic, or order meters perpendicular to the front, but extending laterally over the order of km. Moreover, the aquifer may be highly heterogeneous, further complicating the movement and geometry of the front. Here, we present a parallel computational framework (using the memory distributed approach) with dynamic mesh optimization (DMO) for contaminant transport in density-dependent groundwater flow modelling. The use of DMO guarantees that precision is

placed where and when necessary to ensure accurate solutions and is especially effective when having to span many length scales without compromising the computational cost. The approach uses a double-control-volume-finite element method and is implemented in IC-FERST (the open-source Imperial College Finite Element Reservoir SimulaTor). We first validate the approach and study the precision and efficiency/speed up of DMO for SI modelling with the classic “Henry” problem. Next, we apply the framework to a realistic 3D case study simulating saline intrusion in a heterogeneous chalk aquifer. We study the efficiency and precision of DMO both in serial and in parallel, obtaining with the combination of the two a simulation speed-up of 120x.

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Participation:

In person

Poster / 395

Direct comparing the permeability derivation from Images: Empirical Modeling vs Physics-Based Simulation vs Deep Learning

Author: Lingyun Kong¹

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As the advantage of directly extracting microstructure information and simulating multiple petrophysical scenarios, estimating permeability from rock images became prevail for studying fluid flow in porous media, which is a fundamental problem in subsurface hydrocarbon recovery, CO₂ underground storage, and geothermal development. This study aims to directly compare three commonly-used approaches: empirical modeling, physics-based simulation, and deep learning on the same Berea sandstone 3D images data, and to lay out the advantages and disadvantages based on their performances. The empirical modeling method used in this study is Kozeny-carman equation which are based on pore-throat size and specific surface area. The physics-based simulation, referred to Lattice-Boltzmann method and Shan-Chen model, where Palabos, the open source LB simulator, is adopted in this study. Deep learning work implemented the MultiScale Network for hierarchical regression (MS-Net), a neural network trainer, on the rock images by using simulation results as the output. The study showed that empirical modeling is simple and easy to follow, but only provides rough estimate of the absolute permeability. LB-based simulation is more accurate and can calculate relative permeability by considering many types of scenarios such that a range of estimates are obtained. However, as the image data increases, simulation requires great time and computation costs. The deep learning results show potential in an efficient way by approaching the accuracy of simulation with increasing training efforts. This direct comparison shows the exact results of all three methods on the same image data and clearly gave the hints to the researchers depending on what they demand.

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Poster / 396

An optimization-based method for upscaling carbonate volumetric image data

Authors: Anup Kumar Shahi¹; Anil Kumar¹

Co-authors: Kumar Hemant Singh²; Ranjith Pathegama Gamage³

¹ *IITB-Monash Research Academy*

² *Indian Institute of Technology, Bombay*

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Extraction of information from volumetric core data is highly dependent on the quality of the acquired images and processing. Segmentation of the 3D image helps separate the pore networks from the rock matrix using the process of binarization. The processing done by the user turns out to be subjective and there exists a trade-off between resolution and field of view for the features of interest. The need for a principled way of processing these images is of utmost requirement in the rock physics modelling pipeline.

So, in this paper, we develop a simple optimization-based routine to improve the resolution of the 3D volumetric images using laboratory-based data such as mercury porosimetry. Optimization algorithms work by minimizing the error between the observed and modelled data. Solutions obtained by such algorithms are a function of initialization and the cost function. Regularization is often required when dealing with nonlinear data such as the arbitrary shapes of the pores. It is known that the porosimetry derived capillary pressure vs saturation curve is indicative of the pore size distribution in a rock core sample. This curve can be exploited to enhance the upscaling process using multi-point statistics (MPS). Conventionally, MPS mandates a careful selection of kernel parameters for capturing the spatial variation in volumetric data. The MPS method works by sequentially populating a 3D grid to emulate the observed 3D image. However, finding optimum kernel parameters is crucial to capturing the spatial characteristics. Also, when dealing with multiple images, finding a single set of kernel parameters might not be a trivial task. We show that the selection of these kernel parameters can be enhanced using the pressure vs saturation curve of the MICP data when formulated as an optimization problem and minimizing for this curve.

We test the proposed methodology on carbonate rock sample data show the results on multiple 3D samples and evaluate the upscaling performance using statistical metrics. For the workflow, a low-resolution 3D volume image sample is acquired using the X-ray microtomography instrument which was then subjected to MICP simulations and pore-scale statistical analysis. The result of the application of such a method naturally adheres to the pore size distribution of the samples while giving the user the confidence of real laboratory-based data.

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MS15 / 397

Stylolite detection and image classification from whole core images using convolutional neural networks

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² *Department of Petroleum Engineering, Faculty of Chemical Engineering, Tarbiat Modares University, Tehran, Iran*

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Abstract

Stylolites are natural rock-rock interlocked interfaces that may produce spectacular rough patterns in formation rocks [1]. They form by a localized dissolution process, and their interface contains minerals at concentrations different from that in surrounding host rocks. The presence of stylolites, with various amounts of clays, may affect fluid flow in hydrocarbon formations or underground geological storages (e.g., Hydrogen, CO₂). Stylolites could act as seals and stop the upward migration of fluid in formations [2]. Recent observations indicate that the stylolite permeability is anisotropic and that they may act both as seals and fluid pathways depending on the material that collects in them and the offset of sealing material at teeth [3]. Therefore, detecting stylolites in reservoir core samples can help us to have a better estimate of fluid flow through porous media.

In this study, a deep learning technique were used to detect and classify well depths showing stylolites from slabbed core images. The main approach of this study was using Convolutional Neural Networks (CNN) for analyzing core images. The CNN architecture was developed in Python using TensorFlow and Keras libraries and validated by the ground truth. The core data from of one the Iranian carbonate reservoirs with a length of 150 m were used. In the first step, the raw data of whole core images, photographed in white light, were pre-processed. 3,600 smaller square-shape

images with a size of 300x300 pixels were extracted. Five various classes were defined for core images: stylolite, induced cracks, vertical plug, horizontal plug, and intact rock. The data geometric augmentation method (e.g., flipping, cropping, rotating, contrast and brightness changing) was implemented to increase the size of the training database to 5,000 images per class (25,000 images for all classes). Two main networks (ResNeXt-50 and manually modified ResNeXt-50) were trained on the images of each class to measure the effect of network architecture and number of training image dataset on the classification performance. 80 % of each class data set were used for training and the rest 20 % used for testing. The pre-trained parameters of CNN models on more than million natural images from the ImageNet dataset were used as an input. Both architectures were then retrained on our core database for 500 epochs, where the models converged, and further training would result in minimal or no improvements. After improving and altering the model's hyperparameters, including the batch size and learning rate, the stylolite classification model could predict the five classes on unseen core tray images (20 % of the initial data set) with an accuracy of 94%. The results show that the deep learning approach used in this study can be easily implemented on core-scale images to classify macroscopic features from core image samples. Moreover, this approach can reduce the time for macroscopic core studies usually done by hand.

Acknowledgement

The 2nd author (S.S.) gratefully acknowledges financial support from the Alexander von Humboldt Foundation for his visiting research at the Johannes Gutenberg University at Mainz, Germany.

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References:

1. Rolland, A., et al., Modeling the growth of stylolites in sedimentary rocks. *Journal of Geophysical Research: Solid Earth*, 2012. 117(B6).
2. Toussaint, R., et al., Stylolites: A review. *Journal of Structural Geology*, 2018. 114: p. 163-195.
3. Koehn, D., et al., A new stylolite classification scheme to estimate compaction and local permeability variations. *Sedimentary Geology*, 2016. 346: p. 60-71.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

Poster / 400

Local wettability characterization of porous media under two-phase conditions using lattice-Boltzmann simulations

Authors: Hamidreza Erfani Gahrooei¹; Reza Haghani¹; Per Arne Slotte¹; James McClure²; Carl Fredrik Berg³

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Wettability is a controlling property for multi-phase processes, and therefore an important input to simulate multi-phase processes in porous media. Conventionally, wettability is assumed to be a constant property throughout the medium, despite the common knowledge that it is not uniform in natural porous media. Under two-phase conditions, every three-phase contact line conveys information about the local wettability. In this work we use μ -CT images of the distribution of two phases under no-flow boundary conditions to assess the wettability. We isolate the three-phase contact lines, and then conduct local lattice-Boltzmann (LB) simulations to replicate the relaxed fluid configurations in the pore-space. We take the affinity parameter of the LB color-gradient model as the tuning parameter, and optimize the fluid configuration compared to the observation from the μ -CT data to obtain local wetting descriptions. We later assimilate all the obtained information from different parts of the μ -CT image, and populate the final data into the whole sample. The obtained wettability map can be used to simulate displacement processes for the two given fluid phases in the imaged porous medium for digital rock physics analysis.

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Time Block B (14:00-17:00 CET)

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Poster / 401

Computational and experimental microfluidics for geosciences

Authors: Sophie Roman¹; Cyprien Soullaine²

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A fundamental understanding of multiphase flows in porous media is relevant to the process of CO₂ sequestration, remediation of contaminated aquifers, or Enhanced Oil Recovery. These processes are greatly influenced by a phenomenon known as snap-off. Snap-off is a complex pore-scale mechanism responsible for the break-up of the invading fluid at the entrance of a pore-throat, it leads to the storage of a droplet within the pore chamber. The snap-off and coalescence (merging of droplets) of a fluid phase during two-phase flow affect the quantities of residual trapping and thus affect the storage capacity of a reservoir.

In this work, we investigate trapping mechanisms of a fluid phase during two-phase flows. We use a combination of computational and experimental microfluidics to decipher physical processes using models of geological porous media. With this approach, we demonstrate that we can improve our prediction of residual trapping during two-phase flow. In particular, we observed and characterized cycles of snap-off and reconnection events that contradict the criteria that are generally used in numerical models for snap-offs.

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Poster / 403

Test of multi task XGBoost model and its application in Maokou-1 Member, east Sichuan Basin

Authors: Keran Li¹; Yingjie Ma²; Yang Lan³; Zhaokai Zhang⁴; Jianping Fan¹; Jinmin Song¹

¹ College of energy resources, Chengdu University of Technology

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The carbonate clastic shoal reservoirs in the Middle Permian Maokou Formation has been proved to be outstanding oil/ gas-generating strata. Clastical shoal reservoirs are mainly developed in Maokou-2 and Maokou-3 Members, where Maokou-1 Member is mostly wackstone and packstone. However, with the gas producing under the instructing of in-stu gas generating and enrichment theory, unconventional gas reservoirs are new targets in Maokou-1 Member. To predict porosity, permeability, TOC and lithogy in Maokou-1 Member, east Sichuan basin, this study designs a new multi taks XGBoost model and compares it with traditional random forest models and XGBoost models in single tasks. Multi task XGBoost model has four parts. The first part is inputting all well logging data and responding porosity/permeability/TOC/lithology (labels). Then all labels re encoded. After mixing-training in one shared XGBoost model, the model splits into four independent XGBoost models. Comparision shows single XGBoost models have higher accuracy than single random forest models (the best model is selected by grid search algorithm). Multi task XGBoost model reaches higher accuracy than single XGBoost models. To tesct multi task XGBoost model, this study collects data from YF-1 and Y66-1 (untrained) and put into multi task XGboost model. Result shoew the accuracies for lithology/porosity/permeability/TOC are 91.3%, 90.4%, 94% and 92% repectively, while for single XGBoost models, the accuracies are 72%, 81%, 77.3% and 80.8%. With multi task XGBoost, central and

southeastern parts of east Sichuan Basin are the most potential zones unconventional gas reservoirs develops based on Based on Fuzzy Evaluation Method.

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MS15 / 404

Machine learning to accelerate nonlinear solvers applied to multiphase porous media flow

Authors: Vinicius Santos Silva¹; Pablo Salinas²; Matthew Jackson²; Christopher Pain²

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² *Imperial College London*

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We present a machine learning strategy for accelerating the nonlinear solver convergence for multiphase porous media flow problems. The presented approach dynamically controls an acceleration method based on numerical relaxation. The methodology is implemented and demonstrated in a Picard iterative solver; however, it can also be used with other types of nonlinear solvers. The goal of the machine learning acceleration is to reduce the number of iterations required by the nonlinear solver by adjusting the value of the relaxation factor to the complexity/physics of the system. A set of dimensionless parameters is used to train and control the machine learning. In this way, a simple two-dimensional layered reservoir can be used for training while still exploring a large portion of the dimensionless parameter space. As a result, the training process is simplified, and the machine learning model can be applied to any type of reservoir models.

We demonstrate that the presented technique dramatically reduces the number of nonlinear iterations without sacrificing the quality of the results, even for models that are far more complex than the training case. The average reduction in the number of nonlinear iterations obtained due to the presented method is 24% and the reduction in runtime is 37%. It is worth noting that the optimum value of the relaxation factor is not known a-priori and it is problem specific. Hence, having an acceleration that adapts itself to the complexity/physics of the system throughout the numerical simulation is extremely valuable and has driven several publications in multiple fields.

The method presented here provides an easy way to deal with nonlinear system of equations that does not necessitate as much effort as a custom nonlinear solver while producing outstanding results. We believe that the machine learning acceleration is not limited to the multiphase porous media flow

but extendable to any other system that can be studied based on dimensionless numbers, and that a relaxation technique can be used to stabilize the nonlinear solver.

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MS07 / 405

Reliable and efficient error estimates for nonlinear flow processes using linear iterative schemes

Author: Koondi Mitra¹

Co-author: Martin Vohralik²

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Nonlinear advection-diffusion-reaction equations are used to model complex flow processes such as multiphase flow and flow through porous media/biological systems. When discretized in time, such equations result in a sequence of nonlinear degenerate elliptic problems which require linear iterative schemes to solve. The linear iterates can be used to provide upper/lower bounds to the error, and to separate the error contributions due to linearization and discretization. However, the nonlinearity and degeneracy (referring to the loss of ellipticity of the problem) impede the construction of sharp error bounds in the standard framework.

In this work, using the internal structure of different linear iterative schemes, we derive reliable, fully computable, and efficient error bounds for the finite element solution of the nonlinear elliptic problem which originates from the time-discretization of a wide range of parabolic equations. For obtaining sharp bounds, a pseudo-norm is introduced which is invoked by the linear operator associated with the iterative scheme. The equivalence between a standard norm and the pseudo-norms is shown. An orthogonality relation is derived equating the error with a linearization component and a discretization component. This equality relation is then used to bound from above and below the error, using computable residual-based a-posteriori estimators. Numerical results for different types of equations and iterative schemes are presented that demonstrate the effectivity of the estimators.

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References:

1 Mitra, K. & Vohralik, M. (2021). "A posteriori error estimates for the Richards equation". HAL Preprint, hal-03328944.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS09 / 406

FEATURES OF THE PORE SCALE REACTIVE FLOW WITH COMPLEX CATALYTIC REACTIONS

Authors: Pavel Toktaliev¹; Oleg Iliev^{None}

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Most of the papers discussing pore scale simulation of reactive flow consider synthetic 2D geometry and/or simple reactions. On macroscale the engineers mostly use heuristically derived equations, for which the area of applicability is not clearly defined. Studies on the size of the Representative Elementary Volume, REV, are rarely presented for reactive flow, with effective coefficients computed as a function of the solution of microscale cell problems. A reason for this is the fact that pore scale simulation is a computationally intensive problem, especially in the case of complex reactions, and there is a lack of efficient algorithms for such problems.

A related question is when the upscaling of reactive flow through thin porous media (e.g., membranes) is possible. While there are a lot of discussions when this can be done for single phase flow depending on the pore size distribution, there is a lack of understanding in the case of passive and reactive transport through thin heterogeneous porous media. In 1 it was shown that a particular problem –reactive flow through real catalytic filter (converter), can not be upscaled, and only pore scale simulations can help to understand the performance of the filter in this particular case. Obviously, for other micro geometry or other process parameters upscaling might be possible.

In many applications the complicated chemical reactions are handled via coupling a transport solver to a proper software tool for chemistry, e.g., such as ChemKin, Cantera end etc. The practice, however, shows that such simulations are very time consuming, and often are subject of severe time step restrictions

In the case of complex catalytic reactions the question about REV is much more difficult due to the presence of different reaction time scales. Our goal is to investigate reactive flow in catalytic filters on real and realistic geometry and in the case of complex reactions. The first step toward achieving this goal is to develop efficient algorithms for pore scale simulation in the case of complex reactions. Our current results on this task are the subject of this presentation.

We are developing an integrated solver for transport and reactions. Different coupled and splitting approaches are investigated, together with adopting proper methods for stiff ODEs when needed. Results from numerical simulation of reactive flow in catalytic porous converter on real and realistic geometries for different flow and reaction regimes are presented and discussed.

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References:

1 R. Greiner, T. Prill, O. Iliev, B.A.A.L. van Setten, M. Votsmeier. Tomography based simulation of reactive flow at the microscale: Particulate filters with wall integrated catalyst. *Chemical Engineering Journal*, 378, 2019, 121919

Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS06-A / 407

Jaynes Statistical Mechanics Applied to Multiphase Flow in Porous Media

Author: Alex Hansen¹

Co-authors: eirik flekkøy²; Per Arne Slotte³; Santanu Sinha⁴

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Jaynes statistical mechanics 1 is a generalization of statistical mechanics for thermal systems based on the ideas of Boltzmann. Jaynes bases his approach on the Shannon interpretation of entropy as a measure of what is known about the system at hand. By optimizing the entropy while taking into account the knowledge one has as constraints, such as conserved quantities, it is possible to determine the probability distribution of states for the system.

We implement the Jaynes approach to statistical mechanics for immiscible two-phase flow in porous media under steady state conditions. We determine the probability distribution for the fluid configurations from which macroscopic averages and fluctuations may be found.

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1 E. T. Jaynes, Information theory and statistical mechanics, Phys. Rev. 106, 620 (1957).

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Participation:

Unsure

MS13 / 408

A New Precise Correlation for Permeability Estimation of Tight Carbonate Rocks Using Mercury Intrusion Porosimetry (MIP) Data

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There has been a long-standing concern with the estimation of permeability, particularly in tight carbonate reservoirs. So far, scholars have proposed several empirical correlations for permeability assessment, but the need for a correlation to provide reliable predictions for tight carbonate reservoirs is still felt. In this study, we aim to present a correlation for permeability estimation, based on the results of mercury intrusion porosimetry (MIP) tests and that improves the reliability of the estimation in comparison to regularly-used existing correlations. For this purpose, an extended series of regression analyses, on MIP data of 75 tight carbonate rock samples (selected from a pool of 250 rock samples due to their small pore throat sizes), was performed to find a promising relationship between permeability and the porosity, pore throat sizes of rocks, and a newly-defined dimensionless threshold capillary pressure (P_{dt}) coefficient. In tight carbonate rocks, the pore throat size range falls below 1 μm , and those corresponding to lower mercury saturations act as predictors. Among them, we used pore throat radii corresponding to a mercury saturation of 10% (r_{10}) as the optimum radii in our correlation, and MIP data of 25 rock samples were used to validate the suggested equation. We demonstrate the superiority of the suggested equation against other regularly-used empirical equations in the permeability estimation of dense carbonate rocks. Thus, this equation can be utilized to accurately predict the rock permeability of dense reservoirs using easily accessible data obtained from tests performed on inexpensive drill cuttings.

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References:

- 1 Rezaee R, Saeedi A, Clennell B. Tight gas sands permeability estimation from mercury injection capillary pressure and nuclear magnetic resonance data. J Pet Sci Eng 2012;88:92–9.
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- [3] Razavifar M, Mukhametdinova A, Nikoee E, Burukhin A, Rezaei A, Cheremisin A, et al. Rock Porous Structure Characterization: A Critical Assessment of Various State-of-the-Art Techniques. Transp Porous Media 2021;136:431–56.

[4] Saki M, Siahpoush S, Khaz'ali AR. A new generalized equation for estimation of sandstone and carbonate permeability from mercury intrusion porosimetry data n.d.

[5] Rezaei A, Abdollahi H, Derikvand Z, Hemmati-Sarapardeh A, Mosavi A, Nabipour N. Insights into the Effects of Pore Size Distribution on the Flowing Behavior of Carbonate Rocks: Linking a Nano-Based Enhanced Oil Recovery Method to Rock Typing. *Nanomaterials* 2020;10:972.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 409

Geochemical studies of CO₂-Brine-Rock interaction at surface and subsurface conditions during geological storage of carbon dioxide

Author: Edigwe Jude¹

Co-authors: Mardin Abdalqadir¹; Sina Rezaei-Gomari²

¹ Teesside University

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To support effective geological CO₂ capturing and storage design and operations, the dissolution and precipitation of the CO₂-Brine-rock system were simulated to investigate the chemical interactions within the system concerning the effect resulted from change in their thermodynamics properties. Geochemical models were built using PHREEQC software to represent surface, injectivity and subsurface conditions. Brine rich in magnesium and calcium ions (Mg²⁺ and Ca²⁺) collected from desalination plant were reacted with CO₂ and supercritical CO₂ (scCO₂) to form carbonates. The initial model created are CO₂ + Brine and scCO₂ + Brine reaction buffered with NaOH, also, their reaction with formation water as well as their interaction in formation rock were equally modelled. The chemistry of the aqueous solutions for the models are then investigated in terms of CO₂ (mol/kg) dissolution, specific conductance (μS/cm, °C), Density (g/cm³), Pe (redox parameter), and pH with respect to changes in temperature, pressure, CO₂ Concentration, and ion concentration (Mg²⁺ and Ca²⁺) at surface and subsurface conditions.

The results show that, scCO₂ increases the reactivity of the aqueous species as well as enhances the dissolution of components to form insoluble carbonate minerals. Base pH 8 reduction was observed in all case but more in scCO₂, Also Pe was uniform at 4 in surface condition, but fluctuation was observed as CO₂ reacts in aquifer with a range from 0 –12, and -0.2 –4 for scCO₂ reaction in aquifer. At high temperature specific conductance increase by more than 50% in surface condition compared to pressure, pH and CO₂ concentration. The fluid chemistry showed that the concentration Ca, Mg and K increase with time due to the dissolution of rock minerals such as K-Feldspar, Calcite etc. On the other hand, the release concentration of Al, Si and Fe ions decrease with time due to the precipitation of secondary minerals such as Dawsonite, Muscovite, Clinocllore, Kaolinite, Magnetite, Gibbsite and others.

The order of dissolution and precipitation of the reacting components using calcite as a case study was observed with the Kinetic model of PHREEQC which predicted the dissolution of calcite for 50 years. Calcite dissolves in less than one year at high temperature above 80°C/230atm and dissolve gradually to precipitate secondary minerals within 50 years at temperature below 80°C. The precipitation of secondary minerals confirms the chemical reactivity of the aquifer to precipitate minerals that can serve as an impermeable seal for long term confinement of CO₂.

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Time Block B (14:00-17:00 CET)

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MS13 / 411

Electrochemical Actuation in Nanoporous Silicon

Authors: manuel Brinker¹; Patrick Huber²

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² *Hamburg University of Technology and Deutsches Elektronen-Synchrotron DESY*

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Porous silicon provides a scaffold structure to study the confinement related effects of soft matter. We investigate the electro-sorption of electrolyte anions and the electrochemical behaviour of nanoporous silicon in acidic electrolytes. The silicon-electrolyte interface acts as a capacitor which allows the accumulation of electrolyte anions in a chemical double layer by an applied voltage, whose characteristics can be measured by cyclic voltammetry. The surface stresses that are caused to the monolithic porous silicon membrane by such an accumulation lead to a macroscopic strain which can be determined in-situ with a laser beam-bending setup. Comparing nanoporous silicon with a planar silicon surface yields insights on the observed electrocapillarity - in particular with respect to the importance of oxide formation and wall roughness on the single-nanopore scale.¹

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1 Brinker, M., & Huber, P. (2021). Wafer-Scale Electroactive Nanoporous Silicon: Large and Fully Reversible Electrochemo-Mechanical Actuation in Aqueous Electrolytes. *Advanced Materials*, 2105923.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS06-B / 412

Measuring fluid-solid interfacial area during multiphase flow in a porous medium at different wetting and flow conditions

Authors: Deepshikha Singh¹; Jyoti Phirani²

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² *University of Strathclyde*

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Wetting a porous solid with a fluid is one of the most fundamental phenomena governing the multiphase flow in a porous medium for applications such as CO₂ or H₂ storage in geological reservoirs or oil and gas reservoirs. Quantifying wettability using contact angle is limiting due to the scale and heterogeneity of these reservoirs. Capturing the effect of flow and surface roughness while measuring the contact angle is difficult. In this study, we demonstrate a tracer method to directly measure the wetted area of the solid by a liquid during multiphase flow in a sand-pack. The wetted area is a function of the contact angle; therefore, measuring the wetted area can quantify the wettability of the porous solid. We use multiphase flow experiments in the sand-pack at different wetting conditions of the sand tested by floatation test and capillary rise experiments. We do tracers tests at different fluid phase saturations (i) organic phase is at residual saturation (ii) both the organic and the aqueous phases are moving. When the organic phase is at the residual saturation for water-wet sand, we observe that increasing the flow rate does not change the residual saturation significantly. However, the contact area of the aqueous phase with the porous solid increases with an increase in the water flow rate. This is because of the increased capillary number and different pore-scale fluid distributions at rising water flow rates. For oil-wet sand, we observe that the water saturation increases with the flow rate; however, the water-solid contact area first decreases and then increases when we increase the water flow rate. This is because of the considerable alteration in matrix dissolution at various water-flow rates. In other words, the topology of individual trapped oil globules changes at different water flow rates. When both phases move, we see that the contact area and phase saturations are correlated. We obtain a monotonic increasing behaviour of the water-saturation and water-solid interfacial area, increasing the water flow rate in the porous medium during all wetting conditions.

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India

References:

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Schlüter, S., Berg, S., Rücker, M., Armstrong, R. T., Vogel, H. J., Hilfer, R., & Wildenschild, D. (2016). Pore-scale displacement mechanisms as a source of hysteresis for two-phase flow in porous media. *Water Resources Research*, 52(3), 2194-2205.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 414

Effects of porous media morphology on two-phase fluid displacement and distribution

Authors: Harris Rabbani¹; Nima Shokri²; Tannaz Pak³¹ *Texas A&M University at Qatar*² *Hamburg University of Technology*³ *Teesside University***Corresponding Authors:** t.pak@tees.ac.uk, nima.shokri@tuhh.de, harris.rabbani@qatar.tamu.edu

The Effects of pore-space morphology on multiphase fluid displacement in porous media has been studied extensively in literature (1-3). The general understanding is that, among other factors, pore-space morphology controls the type and importance of pore-scale events that occur during multiphase fluid displacement and hence governs the final fluid saturation distribution. In this research we performed direct numerical simulation using OpenFoam to investigate the influence of erosion and dilation of grains on the dynamics of immiscible displacement. Erosion and dilation operations were progressively performed on the original model. These morphological operations modify the objects (here grains) present in an image by shrinking or growing them in a specific direction. For erosion, a set number of pixels are removed from the object boundaries (open pore space) while for dilation a set number of pixels are added to the object boundaries (tighter pore space). Using erosion/dilation operations one can design porous structures that are similarly interconnected (i.e. have similar skeletons) but display controlled differences in pore and pore-throat size distributions. Our results show that during the drainage, for the dilated models, i.e. the tighter structures, water displacement is more uniform with no single dominant preferential flow pathway. On the contrary, water displacement is less efficient within the eroded models. Moreover, we observed retraction of interface after breakthrough in eroded models which was not visible in dilated models.

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References:

1. Rabbani, H. S., Or, D., Liu, Y., Lai, C. Y., Lu, N. B., Datta, S. S., ... & Shokri, N. (2018). Suppressing viscous fingering in structured porous media. *Proceedings of the National Academy of Sciences*, 115(19), 4833-4838.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 415

The Influence of Imaging Contrast Agents on Emulsification under Flow Conditions

Author: Ahmad Kharrat¹**Co-authors:** Mostafa Borji²; Bianca Brandstätter¹; Holger Ott¹¹ *Montanuniversität Leoben*² *Montanuniversität Leoben***Corresponding Authors:** bianca.brandstaetter@unileoben.ac.at, holger.ott@unileoben.ac.at, mostafa.borji@ugent.be, ahmad.kharrat@unileoben.ac.at

X-ray and optical contrast agents are widely used in porous media research in order to image fluid displacement processes. The field of application is wide and reaches from microfluidics (optical and fluorescence microscopy) to core floods and in the latter form the continuum (medical CT) to the pore scale (micro CT). In all these applications, the contrast is increasing with the increasing concentration of the contrast agent, and some applications require relatively high agent concentrations for the required sensitivity. However, contrast agents are chemicals that may influence fluid properties, fluid-fluid and rock fluid interactions.

The present study deals with surfactant and alkaline flooding on the pore scale. In this frame, we are concerned about the influence of x-ray, optical and fluorescence contrast agents on the fluid-phase behavior, respectively, on the formation of emulsion phases. For this, we test common contrast agents at different concentrations for both crude oil and synthetic oil systems. For x-ray contrast, compounds with heavy elements are required, such as CsCl (Cesium chloride), KI (potassium iodide) for water doping, or Iododecane, Bromoheptane for oil phase doping. In the present study, we focus on CsCl and Iododecan. On the other hand, optical contrast between transparent oil and water phase can be reached by Sudan and Eosin or by fluorescent salt under fluorescence light.

For minimizing the influence of doping agents on the phase behavior of the intended fluid systems, we perfumed a series of classical phase behavior experiments and experiments under porous-media-flow conditions. As porous media, 2D microfluidics as well as 3D porous glass was used. The resulting emulsion phases were detected by optical (optical and fluorescence microscopy) and x-ray (medical and micro CT) means. In the presentation, we discuss the results of the study in terms of agent concentrations and the resulting emulsion phases, respectively, the reliability of experimental results.

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS03 / 417

Multiphysics of Fractured Reservoirs in a Unified Modeling Environment

Author: Nancy Bannach¹

Co-authors: Ed Gonzalez²; Tycho van Noorden³; Sonja Weinbrecht¹

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Modeling flow, transport, and mechanics in naturally fractured reservoirs is a challenging task. On the one hand, the properties of such reservoirs can only be described on the basis of limited measurement data and these are therefore also subject to uncertainties. On the other hand, a computer model should still be able to represent the typical characteristics.

One approach to tackle the uncertainties in fractured reservoirs is using discrete fracture network (DFN) modeling. In this process, the properties of the fractures such as position, orientation, shape, and aperture width are described with the help of statistical distribution functions and represented in the computer model. The underlying equations are then solved on the generated fracture set(s) (which are realization(s) of the DFN model) and, if required, also in the surrounding matrix.

We present a holistic approach to multiphysics modeling of fractured reservoirs, where the geometric representation, the physical processes, the postprocessing, and evaluation take place in the single simulation environment of COMSOL Multiphysics®. Using the example of fractured reservoir flow, we demonstrate how the software can be used to generate discrete fracture networks, with fracture distribution, size, orientation, and aperture following different distribution functions such as power law and Fisher distribution. In the next step, we show how the physical effects, such as flow and heat transport, can be considered. Interactions with the surrounding matrix are also accounted for. After solving and evaluating the results, we briefly discuss the current limitations and future development tasks within this approach. The advantage of the underlying implementation is that it can be extended and thus adapted to a variety of tasks in the field of modeling fractured reservoirs and fractured porous media in general.

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Participation:

Online

Poster / 418

Wettability Restoration of Reservoir Rocks: A Comparison between Static and Different Dynamic Methods

Author: Amin Rezaei¹

Co-author: Yves Méheust¹

¹ Univ Rennes, CNRS, Geosciences Rennes, UMR 6118)35042 Rennes Cedex, France

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The wettability of reservoir rocks affects oil recovery, relative reservoir fluid flow, the capillary pressure, and the electrical characteristics of the formation, by strongly impacting the spatial distribution of fluid phases in the pore space. We investigate the effect of different aging methods on wettability restoration of strongly water-wet carbonate core plugs having similar petrophysical properties. The standard aging method, used in many core analysis laboratories, consists in immersing plugs in a small amount of crude oil for approximately 20-30 days at reservoir temperature. Here, we test wettability restoration processes following two dynamic aging procedures: i) constant flooding of crude oil for different aging times (0.03 cm³/s for 48 h and 96 h), and ii) constant aging time (72 h) using various flooding rates (0.03, 0.05, and 0.1 cm³/s), both at 80 °C. To this end, three rock samples with similar petrophysical properties, aged following the different aging methods, are used in unsteady-state oil-water relative permeability measurements. The outcomes of these core flooding experiments reveal a shift in the crossing point of oil-water relative permeability curves for each plug. The changes in oil-water crossing point saturations are thus used as a proxy for wettability changes; they are recorded in water saturations of almost 53% to 67% indicating wettability changes from mixed-wet to oil-wet state. Bases on that proxy, the static aging method is observed to be less successful than the dynamic aging methods. Furthermore, for the constant aging period dynamic method, there is an ideal crude oil injection rate that is most effective at changing the wettability in terms of the injected pore volumes that are needed and the achieved wetting preference.

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References:

- 1 Anderson WG. Wettability literature survey-part 1: rock/oil/brine interactions and the effects of core handling on wettability. *J Pet Technol* 1986;38:1–125.
- [2] Derikvand Z, Rezaei A, Parsaei R, Riazi M, Torabi F. A mechanistic experimental study on the combined effect of Mg²⁺, Ca²⁺, and SO₄²⁻ ions and a cationic surfactant in improving the surface properties of oil/water/rock system. *Colloids Surfaces A Physicochem Eng Asp* 2019:124327.
- [3] Rezaei A, Khodabakhshi A, Esmaeili A, Razavifar M. Effects of initial wettability and different surfactant-silica nanoparticles flooding scenarios on oil-recovery from carbonate rocks. *Petroleum* 2021.
- [4] Fernø MA, Torsvik M, Haugland S, Graue A. Dynamic laboratory wettability alteration. *Energy & Fuels* 2010;24:3950–8.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS23 / 419

Modeling of the Darcy-Brinkman Equation Indicates Possibility of Deterministic Chaotic Behavior for Flow in Fractured-Porous

Media

Authors: Boris Faybishenko¹; Jens Birkholzer¹

¹ *Lawrence Berkeley National Laboratory*

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The goal of the presentation is to demonstrate examples of modeling of the Darcy-Brinkman (DB) equation, which can be used to describe nonlinear dynamical flow in fractured-porous media. The DB equation is presented as a surrogate system of four ordinary differential equations, including a kinetic component related to fluid velocity, pressure, and a gravitational potential. The results of modeling demonstrate the transition of the system from steady state to periodic and then to aperiodic, which exhibit oscillatory deterministic chaotic or random behavior. The results of simulations are illustrated using 2D and 3D phase-space (PSA) and pseudo-phase space attractors (PPSA). The PSAs are plotted from the time series of system variables. The PPSAs are calculated and plotted using the time lags determined from the mutual information function. Depending on input parameters, the attractors become either a closed loop or strange attractors. The state of the system is characterized using a set of nonlinear dynamics parameters—global and local embedding dimensions, a correlation dimension, an information dimension, and a spectrum of Lyapunov exponents. The system complexity is characterized based on calculations of the Kolmogorov-Sinai entropy. The Granger causality test is used to assess a null hypothesis of independence of time series variables. The results of simulations show high sensitivity to initial conditions and model parameters, which are typical for deterministic chaotic behavior. The solutions of the DB equation are important for developing hypotheses and directing experimental and modeling research to improve our understanding of sub-surface flow and transport processes and interactions in fractured-porous media, relating to various environmental scientific and practical problems.

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Time Block C (18:00-21:00 CET)

Participation:

Online

MS06-B / 420

Evolution of partially miscible ganglia in porous media: A pore-network approach

Authors: Yashar Mehmani¹; Ke Xu²

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² *Peking University*

Corresponding Authors: kexu1989@pku.edu.cn, yzm5192@psu.edu

Non-wetting bubbles trapped inside porous solids are common to many applications including geologic CO₂ storage, design of optimal components for fuel cells and electrolyzers, and cleanup of non-aqueous pollutant liquids from groundwater aquifers. Their evolution is dictated, almost entirely, by the complex geometry of the pore space to which the bubbles' morphology must conform. As bubbles grow/shrink in size, they undergo a series of events such as pore-invasion, pore-retraction, snap-off, dislocation, fragmentation, and coalescence with other bubbles in the system. And if partially miscible, the bubbles can dissolve in the surrounding wetting phase and exchange mass with one another; a process known as Ostwald ripening. To engineer such systems, it is important to understand how the volume, surface area, curvature, and topology of bubbles co-evolve, and whether one can be predicted from a knowledge of the others. In this work, we present a pore network model that is capable of simulating the evolution of a population of trapped bubbles inside a heterogeneous porous material. Its novelty lies in that bubbles can span multiple pores, called ganglia, a limitation that has mired prior modeling attempts. After validating the model against microfluidic, direct simulation, and analytical results of the literature, we use it to understand growth-shrinkage cycles of ganglia inside complex porous microstructures. The outcomes generalize theoretical results derived previously by the authors for 2D homogeneous domains.

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Time Block C (18:00-21:00 CET)

Participation:

Online

MS10 / 421

A Hybrid Multiscale Pore Network Modeling Method Applied to Complex Carbonate Rocks

Authors: Viswasanthi Chandra¹; Gwenole Tallec^{None}; Arsalan Zolfaghari²

¹ King Abdullah University of Science and Technology (KAUST)

² Application Specialist

Corresponding Authors: viswasanthi.chandra@kaust.edu.sa, gwenole.taltec@thermofisher.com, arsalan.zolfaghari@thermofisher.com

Accurate modeling of multiphase flow in geological porous media is a critical component of a wide range of energy and environmental science applications, including production of oil and gas, geological sequestration of CO₂ and evaluating geothermal systems. This is particularly challenging in carbonate rocks, due to their inherently complex pore systems, associated with multi-scale depositional and diagenetic heterogeneities, varying in a broad range of length scales. A significant portion of carbonate pore space is comprised of microporosity (pore size less than 10 microns), and there is an urgent need for pore network modeling methods that can account for the impact of micropores and the connectivity between micro- and macro-pores on the digital rock properties. Traditional pore

network modeling and simulation methods that rely on single resolution images fail to adequately capture all these relevant length scales, due to computational limitations. In this work, we present a hybrid/multiscale Pore Network model that enables the integration of micro- and macro-scale imagery derived from micro-CT and SEM for predicting static and dynamic petrophysical properties. We used multiple heterogeneous carbonate samples, including standard core plugs from a prolific reservoir in the Arab-D Formation of Saudi Arabia, which are representative of the main lithofacies associations. We applied state-of-the-art image processing workflow that allowed integrated image analysis of different modalities (micro-CT and SEM) and multiple resolutions (ranging from 30 μm to $<1 \mu\text{m}$). Multiple segmentation methods were tested on the micro-CT and SEM images and converged into an automated segmentation routine using Deep Learning models, which enabled us to easily replicate the segmentation work for similar samples. High resolution micro-CT data was used to obtain 3D pore type distribution that accounted for unresolved pore volume, that was subsequently imaged using SEM. Process-Based (PB) modeling approach was used to derive 3D pore space models from the SEM images. The resulting micro-scale pore type models were then used as input in our multiscale Pore Network model to be combined with the macro-scale 3D pore network. The multiscale Pore Network model was used to compute effective rock properties such as porosity, permeability, relative permeability, capillary pressure, and resistivity index. Experimentally measured porosity, permeability and mercury-air primary drainage and oil-water imbibition capillary pressure curves were used to verify the multiscale Pore Network model. Evidently the micropores and pore throats in the studied samples significantly contribute to flow and electrical properties, and our method captured this multi-scale pore effect on rock properties more effectively compared to traditional PNM workflows.

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References:

A Multi-Scale Imaging and Modeling Workflow for Tight Rocks, L. C. Ruspini, G. Lindkvist, S. Bakke, L. Alberts, A. M. Carnerup, and P. E. Øren, FEI Company

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS15 / 422

Digital twin of a laboratory-scale porous medium

Authors: Benyamine Benali^{None}; Jakub Both¹; Martin Ferno¹; Eivind Fond²; Kjetil Johannessen²; Eirik Keilegavlen¹; Trond Kvamsdal³; Jan Martin Nordbotten¹; Adil Rasheed³

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Physics-based modeling of a reservoir can suffer from several uncertainties as in the constitutive modeling, the choice of model parameters, or geometrical representation of the physical asset, just to mention a few. Yet, it allows for explicitly incorporating fundamental principles of physics, as conservation laws. On the other hand, data (as long as available and sufficient) may assist in tuning constitutive models and close the gap between predictions and the true physics.

In this work, we investigate to what degree hybrid modeling of a physical porous medium can result in accurate flow predictions. For this, we execute flow experiments in the FluidFlower 1, a laboratory-scale rig filled with different layers of homogeneous sands, equipped with several pressure sensors, and allowing for high-precision tracking tracer flow experiments from the outside via a glass screen. On the other hand, corresponding simulations are performed using PorePy [2], an open-source physics-based finite volume simulator tailored to multiphysics problems in complex geometries. In order to bring data and physics together, the concept of Hybrid Analysis and Modeling [3] is introduced, correcting the physics-based simulations essentially by learning the residual using machine learning. We discuss how much or little sparse and/or dense data affects the final prediction abilities, eventually potentially enabling real-time integration of reservoir flow, simulation, and control with experimental operational parameters.

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References:

1 FluidFlower webpage, <https://fluidflower.w.uib.no/>

[2] Keilegavlen, E., Berge, R., Fumagalli, A., Staronni, M., Stefansson, I., Varela, J. and Berre, I., 2021. Porepy: An open-source software for simulation of multiphysics processes in fractured porous media. *Computational Geosciences*, 25(1), pp.243-265.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS05 / 423

Engineering biofilm hydraulic resistance on the microscale

Authors: Eleonora Secchi¹; Dorothee Luise Kurz^{None}; Cameron Boggon²; Sam Charlton²

¹ *ETH Zürich*

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Bacterial biofilms are amongst the most successful modes of life in the terrestrial environment and ubiquitous within porous systems, such as soils and membrane interfaces (1). The bacteria within a biofilm are bound together by self-secreted extracellular polymeric substances (EPS), yielding a natural gel-like structure (2). EPS provides a protective shield and structural architecture to constituent

cells of the biofilm, which shapes internal mass transport within the biofilm and flow field of the colonized porous media (3). The interplay between biofilm formation and flow leads to the formation of preferential flow pathways and significant increases in membrane hydraulic resistance, as investigated in macroscale experimental systems (4, 5). However, the complex multiphase interaction between biofilm proliferation and flow within irregular porous media make the deduction of scalable physical relationships challenging. Consequently, a mechanistic understanding linking EPS composition, biofilm morphogenesis and porosity with hydraulic resistance is still missing (6).

In this work, we investigate the time evolution of biofilm morphology and hydraulic resistance as a function of flow conditions and EPS composition. We grow the model bacterium *Bacillus subtilis* in two types of microfluidic channel and use a library of EPS mutants devoid of polysaccharide (EPS-O), protein (TasA) or hydrophobin (BslA) to modulate EPS composition. Firstly, we grow and characterize the biofilm during its morphogenesis in a novel microfluidic platform where the biofilm is grown on a cellulose nanofibril (CNF) membrane barrier. The CNF platform allowed precise measurement of single colony biofilm hydraulic resistance as a function of pressure driven flow and EPS composition, whilst retaining full optical access. To validate the scalability of our findings, we use an unconfined microfluidic geometry, a model 2D porous media, which increases the biofilm volume by approximately two orders of magnitude. We measure hydraulic resistance and apply advanced optical visualization techniques to quantify biofilm morphogenesis and internal transport. This study allowed us to quantify how flow and EPS composition shape the hydraulic resistance of biofilm at the micro and meso scale. The relationships derived from these studies enhance our understanding of how we can engineer biofilms to tune their hydraulic resistance.

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References:

1. H.-C. Flemming, et al., Biofilms: an emergent form of bacterial life. *Nat Rev Micro* 14, 563–575 (2016).
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6. P. Desmond, et al., Controlling the hydraulic resistance of membrane biofilms by engineering biofilm physical structure. *Water Res.* 210, 118031 (2022).

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS10 / 424

NEW INSIGHTS IN POROUS MEDIA CHARACTERIZATION: SPECTRAL COMPUTED TOMOGRAPHY

Authors: Wesley De Boever^{None}; Marijn Boone¹; Denis Van Loo²; Marek Dosbaba²

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1. Introduction

Micro-CT can be used to study the structure of samples from a centimeter to micrometer scale. One of the main limitations in this, however, is the inability to perform true material identification without prior knowledge, as contrast inside a micro-CT scan is mainly caused by the atomic number of the sample. Also density, used x-ray energy, the x-ray spectrum and the used detector have influence on the achieved grey values and contrast in a dataset. We present integration of an energy-sensitive spectral detector inside laboratory-based micro-CT scanners: the TESCAN PolyDET.

2. Materials and Methods

Using the TESCAN UniTOM XL, both traditional (attenuation-based) and spectral tomography and reconstruction were performed. Spectral measurements were acquired using the mounted TESCAN PolyDET. This way, not only the attenuated intensity of the X-ray beam when travelling through samples could be measured, but the entire energy spectrum (20-160 keV) of the X-ray beam was measured by the TESCAN PolyDET. Measurements were performed on various types of samples, from simple plastic specimen as proof of concept to economically important samples such as batteries and raw materials for the mining industry.

3. Results and Conclusion

In this work we show the first results of the method for the investigation of porous media. The most obvious use of a spectral detector enhances micro-CT with EDS-like capabilities for mineral identification. Spectral imaging can positively identify gold grains inside an ore sample, even without prior knowledge or when gold grains are so small that they are masked by the partial-volume-effect of traditional micro-CT. It is also positive to differentiate multiple important ore materials inside rock specimen, or to do rapid screening of different types of limestones and sandstones, important for energy storage solutions. The information obtained can later be used to calculate more indirect properties, such as relative saturation inside the measured porous media. More advanced analytical capabilities can be used to get true contrast between materials –independent of the X-ray energy used to scan them, get more insights into density differences between materials or perform dual-energy CT scans in just one scan –without any assumptions. Spectral CT can also diminish or remove any artefacts originating from the polychromatic nature of the X-ray beam used in micro-CT, of which beam hardening is the best known. All results show the large potential of spectral CT in enhancing attenuation-based micro-CT and providing new and unique insights in all types of materials.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 425**Modeling digital twins of grain-based reservoir rocks****Author:** Arne Jacob¹**Co-authors:** Christian Hinz ¹; Jens-Oliver Schwarz ¹; Andreas Wiegmann ¹¹ *Math2Market GmbH***Corresponding Authors:** christian.hinz@math2market.de, andreas.wiegmann@math2market.de, arne.jacob@math2market.de, jens-oliver.schwarz@math2market.de

The key to accelerate research and production in the energy industry resides in the efficient and generally applicable determination of physical properties of reservoir rocks. Here, we present recent advancements in the generation of statistical digital twins of reservoir rocks, in a workflow that may commonly be applied to any grain-based sample. Digital twins and the modeling of reservoir rocks have become an increasingly powerful tool in numerical simulations applied to digital core analysis in recent years. Indeed, the digital twins of reservoir rocks can be used for further non-destructive digital measurements, reducing costs and resource usage.

Here, we generate digital models of reservoir rocks in a voxel-based geometry at dimensions of at least 1000^3 voxels, with the aim of precisely and accurately replicating the rock and the pore geometry. The generated digital twin is then ready for further applications in the range of digital core analysis since the physical parameters of the original rock sample are represented with fidelity in the modeled digital twin.

This approach is validated via analysis, modeling, and property prediction on the basis of a digital rock core sample. We determine the grain-size distribution of a 3D geometry obtained from the scanned images of a Doddington sandstone and subsequently, generate a statistical 3D digital twin of the rock structure. The absolute permeability is computed and compared for both 3D geometries and validates the approach within sufficient accuracy. We thereby demonstrate the applicability of this workflow to further reservoir rocks by means of a high performance approach.

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References:

Andrew, M., Bijeljic, B., and Blunt, M., "Doddington Sandstone." Digital Rocks Portal, Digital Rocks Portal, 30 April 2020, <http://www.digitalrocksportal.org/projects/290> Accessed 27 Dec. 2021.

Andrew, M., Bijeljic, B., and Blunt, M.J., Pore-scale imaging of trapped supercritical carbon dioxide in sandstones and carbonates. International Journal of Greenhouse Gas Control. 2014

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS06-B / 426

Liquid relative permeability through foam-filled porous media

Authors: Olivier PITOIS¹; Margaux Ceccaldi¹; Vincent Langlois¹; Marielle Guéguen²; Daniel Grande³; Sébastien Vincent-Bonnieu⁴

¹ *Université Gustave Eiffel, Lab. Navier*

² *Université Gustave Eiffel, Lab. CPDM*

³ *Institut de chimie et des Matériaux Paris-Est*

⁴ *ESA*

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In the context of soil remediation or oil extraction, foam flooding is useful to mitigate effects due to permeability contrast within the soil layers. For some applications, the liquid relative permeability of the foam-filled porous medium is a crucial parameter to control the liquid flow rate at which active substances or nutrients (for bacteria) can be delivered deep into the medium. In pioneer works and in more recent studies, it was concluded that the presence of foam lamellae does not change the liquid (water) relative permeability with respect to the foam-free porous medium at same liquid saturation larger than 20%. Here, we are interested in the liquid relative permeability of foam-filled porous media within the range of low liquid saturations, i.e. 5%-20%. Our goal is to demonstrate that there are situations where the characteristics of the foam trapped into the porosity has significant impact on liquid permeability.

We used two surfactants, alkyl polyglucosides (APG) and saponin, and we produced well-controlled liquid foams in terms of bubble diameter and liquid volume fraction. It is shown that the dimensionless bulk permeability (liquid permeability divided by squared bubble diameter) for APG foam is about 5 times larger than for saponin foam at same liquid fraction, which is explained by the respective intrinsic viscosities of the liquid-air interfaces.

Model porous media made of packed spherical grains were prepared and then filled with the controlled foam. Particular attention was paid to ensure that the bubbles were not destroyed during the filling step, which allowed to have foam-filled porous media with controlled parameters, namely the bubble-to-grain size ratio r and the liquid saturation.

We show that the liquid relative permeability of such foam-filled porous samples is non-monotonous for saponin foams as a function of r and exhibits an optimal permeability value. For APG foams, the relative permeability increases significantly with r . When plotting the ratio of the relative permeabilities APG/saponin as a function of r , two regimes are revealed: (1) for $r \leq 0.25$, the ratio is equal to the ratio measured for the bulk foams; (2) for larger r values this ratio is increased by one order of magnitude. This behavior can be explained by the configurations of the bubbles into the pores: the latter are filled with foam for small r values, while each pore contains about one bubble for r values close to 0.35. For such high r values the liquid is distributed in the form of foam liquid bridges, which are reminiscent of the classical pendular liquid bridges, but here they are connected together by parietal liquid channels formed by the foam on the surface of the grains. For APG foams, significant permeability is ensured thanks to that particular geometrical configuration.

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Time Block B (14:00-17:00 CET)

Participation:

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MS06-A / 427

Hysteresis in Contact Angle and Interfacial Tension: Implications on Multiphase Flow

Author: Qi Liu¹**Co-authors:** Marcelo Benitez¹; Carlos Santamarina¹¹ KAUST**Corresponding Authors:** qi.liu@kaust.edu.sa, carlos.santamarina@kaust.edu.sa, marcelo.benitez@kaust.edu.sa

Multiphase fluids are common in the subsurface and affect a wide range of natural and engineering process from infrastructure performance above unsaturated soils, to contaminant transport, environmental remediation, oil and gas recovery, and CO₂ geological sequestration. The capillary pressure $P_c = \sigma \cos \theta / r$ between two immiscible fluids is proportional to the interfacial tension σ , the contact angle θ and the interface curvature r . Both contact angle and interfacial tension may show significant hysteresis.

Instead of a single thermodynamic contact angle predicted by Young's equation, fluid-liquid-mineral interfaces exhibit contact angles that can vary between the asymptotic advancing θ_A and receding θ_R contact angles. Typical explanations involve surface roughness and chemical inhomogeneity; yet, contact angle hysteresis is observed even on smooth, homogeneous surfaces. The normal component $\sigma \sin \theta$ of the fluid-liquid surface tension underscores the attractive interaction between the solid surface and the contact line where the three phases meet. Experimental results show that contact line adhesion is highest under static conditions and decreases to the kinetic adhesion during sliding, causing the stick-slip motion of the fluid-liquid interface. Consequently, DI water, brine, surfactant solutions and nanofluid droplets resting on smooth and homogeneous silicon wafers and quartz glass substrates exhibit distinct advancing and receding behaviors. In particular, surfactant molecules and nanoparticles adsorbed at interfaces enhance contact pinning, alter the contact line behavior during advancing and receding and result in unique contact angle hysteresis.

The presence of surface-active species such as ions, surfactants and colloidal particles changes the interfacial tension. The Gibbs adsorption isotherm relates the interfacial tension to surface excess concentration relative to the bulk concentration under thermodynamic equilibrium. However, a migrating fluid-fluid interface is continuously evolving as it traverses interconnected pores through converging and diverging cross-sections. Interfacial tension hysteresis induced by surfactants, nanoparticles and asphaltene in crude oil exhibit distinct interfacial tension hysteresis patterns that reflect the properties of adsorbed species, and both the strain and strain rate the fluid-liquid interface experiences.

Experiments and pore network analyses show that contact angle hysteresis and interfacial tension hysteresis work collectively to affect the migration of fluid-fluid interfaces across a pore constriction, invasion patterns and the resultant distribution of phases.

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MS09 / 429

Image-based reconstruction of multiscale porous structures and coarsening of microporosity regions

Authors: bowen shi¹; Han Jiang²; li zhang²; Bo Guo³; Chao-Zhong Qin²¹ *Chongqing university*² *Chongqing University*³ *University of Arizona***Corresponding Authors:** 20202001035@cqu.edu.cn, chaozhong.qin@cqu.edu.cn, boguo@arizona.edu, lizhang1@email.arizona.edu, hanjiang@cqu.edu.cn

A number of geological and industrial materials present multiscale porous structures, such as Estailades limestones, tight sandstones, and catalyst layers of some electrochemical devices (Gao et al., 2019; Mehmani and Balhoff, 2015; Bultreys et al., 2016). In the context of a digital rock of multiscale porous structures, we may resolve macropores by the μ CT imaging technique, while unresolved regions will be termed as microporosity. Flow and transport in the macropores can be solved by either a pore-network model or a direct numerical simulation model. A Darcy-scale model is used for the microporosity. Furthermore, material properties in the microporosity may be obtained by the FIB-SEM technique. This sort of multiscale numerical framework has been seen in the literature (Guo et al., 2018; Zhang et al., 2021). However, computational efforts pertaining to the Darcy-scale modeling could be prohibitive, when tens of millions of voxels of microporosity are present in a digital rock. In this work, we propose a convolution-based method to conduct multilevel coarsening of microporosity, while keeping high-resolution domain interfaces between macropores and microporosity. We have developed our in-house code, and set up test cases of compressible single-phase flow in a digital rock of multiscale porous structures. The macropores are solved by the pore-network model, and the microporosity is solved by the single-phase Darcy model (Qin et al., 2021). We will show that alongside the developed coarsening technique, our hybrid model is pretty robust, which not only considerably reduce computational efforts, but also well predict multiscale flow and transport phenomena.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Unsure

MS13 / 432

Impact of salt on sorption isotherms of water in nanoporous media**Authors:** HUGO BELLEZZA^{None}; Mark Busch¹; Stella Gries¹; Juan Sanchez¹; Patrick Huber¹; Olivier Vincent²¹ *Institute for Materials and X-Ray Physics*² *CNRS***Corresponding Authors:** hugobellezza68@gmail.com, olivier.vincent@univ-lyon1.fr, patrick.huber@tuhh.de, juan.sanchez@tuhh.de, stella.gries@tuhh.de, mark.busch@tuhh.de

Salt water is ubiquitous in nature (e.g. geomaterials, soil, clouds formation) and in technology (e.g. desalination, concrete weathering, heritage conservation). In most of these situations, salt water is confined within a porous medium, often with pores down to the nanometer scale: for example, crystallization and dissolution cycles induced by humidity changes are known to induce structural damage to building materials, artwork, etc 1. And yet, these processes are not well characterized, especially when pores are in the nanometer range [2]. Here, we investigate the response of the salt water confined in several porous silicon and alumina samples (average pore diameter from 3 nm to 20 nm) to humidity cycles. We performed sorption isotherms where we monitored optically water content in the porous medium. We systematically characterized how the salt concentration impacts the shape of the isotherms and compared these results to a minimal model coupling solution thermodynamics to capillarity, nucleation and confinement effects [3]. We also probed the appearance of the crystal and its structure by X-ray diffraction.

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1 Robert J. Flatt et al. “Chemo-mechanics of salt damage in stone”. en. In: Nature Communications 5.1 (Sept. 2014). Bandiera abtest: a Cg type: Nature Research Journals Number: 1 Primary atype: Research Publisher: Nature Publishing Group Subject term: Chemical physics;Geophysics Subject term id: chemical-physics;geophysics, p. 4823. issn: 2041-1723. doi: 10.1038/ncomms5823.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS09 / 433

Analysis of Stokes-Brinkman modeling for solute/particle transport in a domain with microporous regions

Authors: Bin Wang¹; Karsten Thompson^{None}; Richard Hughes¹

¹ Louisiana State University

Corresponding Authors: rghughes@lsu.edu, binwang.0213@gmail.com, karsten@lsu.edu

Microporosity is present in many natural porous media. It can also be an intentionally designed component in manmade porous materials. Its impact on transport depends on various factors including the properties of the microporosity, the amount and placement within the main porous structure, and the type and regime of the transport process being considered. Modeling transport with microporosity is challenging because of the differences in spatial and temporal length scales that govern the transport, and numerous methods have been studied for modeling these systems. One method that can be used for pore-scale modeling is the Stokes-Brinkman Equation, which enables direct modeling of viscous flow in the well-defined “macro” part of the pore structure, while assuming a Darcy-like flow in the microporous regions. This approach is useful if the microscale pore structure is not fully resolved or if direct modeling requires excessive computational demands. While significant research has been performed on matching boundary conditions and assigning the effective viscosity parameter for fluid flow and permeability modeling, relatively little work is published about the potential use of the Stokes-Brinkman equation for mass transport of solutes or nanoparticles.

In this work we present a micromodel design that contains macro and microporosity, and is being used for both physical and computational experiments. The problems we are studying involve two particular scenarios: changes in advected mass transport behavior due to its capture or delay in microporous regions, and the elution of mass that originates or has been captured in microporous regions. These situations are relevant in a number of practical applications.

We show solute/particle transport simulations within this domain that are being used to study physical behavior and quantify the ability of the Stokes-Brinkman equation to capture the correct solute mass transport behavior. The Stokes-Brinkman results are compared with direct numerical simulations that capture the detailed transport within both macro and microporosity. We first compare the methods for the case of fluid flow and permeability estimation, showing that traditional empirical equations (for microporosity permeability) give significant error for our particular micromodel geometry but that these errors can be reduced to essentially zero by extracting the correct microscale

permeabilities from DNS and choosing an appropriate effective viscosity term. More importantly, we show that the same corrections for permeability and effective viscosity do not address the error in solute transport that is observed when comparing Stokes-Brinkman versus DNS. Additional parameter adjustments are analyzed to help determine what factors can be used to improve models of solute transport.

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Time Block B (14:00-17:00 CET)

Participation:

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Poster / 434

Use of semi-automatic deep learning algorithms for the segmentation and classification of cavities in carbonate fault rocks

Authors: Eva Wellmann¹; Joyce Schmatz¹; Mingze Jiang¹; Jop Klaver¹; Anastasia Hoffmann¹

¹ *MaP - Microstructure and Pores GmbH*

Corresponding Authors: eva@m-a-p.expert, anastasia@m-a-p.expert, jop@m-a-p.expert, joyce@m-a-p.expert, mingze@m-a-p.expert

Accurate knowledge of pore space in fault zones in stratified carbonate and marl sequences is important because fault zones play an important role in reservoir properties (e.g. Agosta et al., 2010, Caine et al., 1996). However, estimating pore space in these structures is difficult due to their heterogeneity, and sampling is also complicated due to the often non-cohesive properties of fault rocks and the gouge. Here we briefly review sampling and processing methods and discuss automated analysis approaches using deep learning algorithms to analyse microscopic and CT images. We have developed a semi-automated tool for facies analysis of fault rocks, with particular emphasis on mineral phase porosity and automatic identification and segmentation of fractures.

Orientated transfer sample were taken from a limestone quarry in Ittlingen, Bavaria in Germany. We used transfer preparations perpendicular to the fault plane to obtain, large (45x60x20 cm) samples which offers the opportunity to obtain samples from the fault zone including the damage zone and fault core with known orientation. Subsamples of the transfer preparations were measured by using scanning electron microscopy in combination with broad ion beam polishing. At the macro-scale CT imaging was used to obtain the fracture networks and spatial distribution of the different building blocks of the fault zone.

We mainly use image data from backscattered electron and energy dispersive X-ray spectroscopy measurements and develop a tool for rock facies segmentation with superpixel algorithms (e.g. Stutz et al., 2018). The tool also enables automatic segmentation of mineral phases based on a customisable decision tree (Jiang et al., 2021) after superpixel generation. We then analyse the void space using secondary electron images with a trained deep learning model (Klaver et al., 2021) based on a U-Net structure. To distinguish between fractures and pores, a decision tree was created based on the shape of the segmented pores, e.g. eccentricity, circularity, aspect ratio and size.

Initial results show that the semi-automated tool provides a simple and fast way to determine the distribution of mineral phases and that the trained deep-learning algorithm for pore segmentation has an accuracy of about 98 % for two different fault facies. By iteratively integrating the training data into the existing model, the results are continuously improved. In future work, we aim to train the deep-learning algorithms to analyse and classify multiple fault facies and minimise the manual labour and expertise required to automatically segment and classify pores and fractures in faults in carbonates

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Klaver, J., Schmatz, J., Wang, R., Jiang, M., Kleipool, L.M., Cilona, A., and Urai, J.L. [2021] Automated Carbonate Reservoir Pore and Fracture Classification by Multiscale Imaging and Deep Learning. In, 2021:1–5. European Association of Geoscientists & Engineers. <https://doi.org/10.3997/2214-4609.202011981>

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 435

Design of a model for the prediction of petrophysical properties from microstructural image data

Authors: Mingze Jiang¹; Joyce Schmatz¹; Eva Wellmann¹; Jop Klaver²

¹ MaP - Microstructure and Pores GmbH

² MaP - Microstructure and Pores GmbH

Corresponding Authors: mingze@m-a-p.expert, jop@m-a-p.expert, eva@m-a-p.expert, joyce@m-a-p.expert

We present the design of a prototype for the prediction of permeability from 2D microstructural image data. Fault rocks of a normal fault in a Jurassic limestone-marl sequence in northern Bavaria, Germany, are analyzed for the algorithmic integration of microstructural data (light microscopy and scanning electron microscopy) with petrophysical measurement results (including He pycnometry

and MICP derived permeability).

It is assumed that the rock microstructure is directly related to the petrophysical properties - such as permeability - of the rocks (Schmatz et al., 2017, Saxena et al., 2017). The good comparability in carbonates of e.g. He porosity with BIB-SEM porosity (Broad-Ion-Beam-Polishing in combination with SEM, Norbistrath, 2015) and pore space connectivity from mercury porosimetry and LMI-BIB-SEM (Liquid-Metal-Injection, Klaver et al., 2021) shows the empirical relationship between volume measurements and image information.

With the help of deep learning algorithms, quantitative data on the porosity, permeability and mineralogical composition of the rock samples are analysed and linked. The step is first performed on homogeneous samples. The trained algorithm will first be tested on a test data set and finally compared with the simulation results (e.g., Kottwitz et al. 2021). Subsequently, the analyses of the different fault rock facies will be combined and again integrated with the corresponding simulation results.

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Klaver, J., Schmatz, J., Wang, R., Jiang, M., Kleipool, L.M., Cilona, A., and Urai, J.L. (2021) Automated Carbonate Reservoir Pore and Fracture Classification by Multiscale Imaging and Deep Learning."In , 2021:1–5. European Association of Geoscientists & Engineers.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS22 / 436

Additive Manufacturing of open porous structures: correlation of laboratory testing to simulations for application related properties

Authors: Robert Otto¹; Uliana Soellner²; Stefan Boschert²; Christoph Kiener²; Knut Sorby³

¹ *Siemens AG & NTNU Trondheim*

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³ *NTNU Trondheim*

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Additive manufacturing (AM) is well known for its high customizability and freedom of form but can also be utilized to produce open porous structures. Those structures are widely known for being advantageous to mixing and heat transfer applications, as they combine high surface areas with a stochastic cross-linked network of channels. Thus, good mixing of flowing through media is achieved as well.

This study investigates the possibilities especially enabled by laser-based powder bed fusion (PBF-LB) to create and design porous structures with pre-defined properties. The current state of the art of manufacturing functional structures will be explained, while perusing recent complements. Consequently, a novel manufacturing-parameter-based way of designing functional structures will be utilized. Various open porous samples will be created, showing the comprehensive range of achievable variations. Samples will be evaluated for application-related properties in laboratory tests, whereby direction-dependency will be considered as well.

To improve future application and to finally come to the situation of creating materials with pre-defined properties a Digital Twin of the material will be created. As a first step to realize this vision, the results of laboratory testing will be correlated to simulations. 3D-imaging will be applied to generate a digital twin of selected open porosities. Predictive simulation models can be built based on the first mathematical, testing and digital analyses of porous samples. By means of simulation models, the thermodynamic and fluid mechanical properties of porosities are further investigated for practical applications.

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Poster / 437

Effect of physicochemical properties and structural heterogeneity on reactive transport in saturated porous media

Authors: Jianying Shang¹; Jinhui Tong²; Xiaofan Yang²; Xueying Li²; Yuanyuan Liu³

¹ *China Agricultural University*

² *Beijing Normal University*

³ Nanjing University

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Physicochemical properties serve as crucial indicators on reactive solute transport and soil structure evolution in porous media, meanwhile structural heterogeneity of soil significantly alters physicochemical properties via redirecting solute transport path. Key biogeochemical processes such as precipitation–dissolution (PD) is essential to reactive solute transport in porous media, yet their relation with soil physicochemical properties and how they are influenced by soil heterogeneity remains unknown for years. This study took the PD process of Ca^{2+} and CO_3^{2-} ($\text{Ca}^{2+} + \text{CO}_3^{2-} \rightleftharpoons \text{CaCO}_3$) as an example to study the reactive solute transport behavior with different physicochemical conditions in heterogeneous media by a series of column experiments and numerical simulations. In the meantime, X-ray computed tomography (XCT) and morphological measurement (via ImageJ) were applied to investigate the effects of PD process on structural heterogeneity. Results demonstrate that the salinity, acidity, and flow rates in homogeneous columns significantly altered the reaction rate of PD process, leading to immediate hydraulic conductivity variation, and thus converted reactive transport behavior. Preferential flow paths in heterogeneous columns could lead to early breakthroughs and thereby promoted the transport of calcium carbonate (CaCO_3) in saturated porous media. XCT images revealed that more Ca^{2+} precipitated on flat and concave surface, forming a round coat outside grain particles. The CaCO_3 precipitates could also narrow or even block pore throat, and thus decrease pore connectivity. Our study provided essential experimental data for predictive modeling of Ca^{2+} reactive transport as well as new insights into the changes in soil structural heterogeneity and transport properties during the PD process.

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MS02 / 438

Hydro-mechanical coupling to uncover stability and permeability of coated biopore on the pore-scale: the way to improve larger-scale modelling

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¹ ZALF

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Exudates and finer particles often coat the surface of biopores, increasing mechanical stability and altering the physico-chemical properties (e.g. wettability or sorption) of the surrounding. Consequently, the pore region of the biopore surface governs the macropore-matrix mass exchange processes during preferential flow in the soil macropores. However, the relationships between mechanical and hydraulic properties of coated biopore regions are not fully understood nor expressed by numerical models. Correlations between soil hydraulic and mechanical properties could perhaps be established by quantifying the water flow in defined pore structures of the biopore. In this contribution we develop a model-based approach for studying coupled hydro-mechanical properties of biopore walls and the effects of clay-organic coatings. The technical challenge was first to develop a one-way coupling (i.e., structural impact on fluid flow) between discrete element method (DEM) and a Stokes solver to perform hydro-mechanical simulations of a coated biopore structure. The presented one-way coupling method between DEM and Stokes solver provided data for quantitative analysis of coupled hydro-mechanical properties of the biopore structure. A relationship between Young's modulus and permeability depending on the coating cohesion could be established. This model-based approach could be extended to describe hydro-mechanical properties of dynamic and more complex soil structures. All in all, our findings pave the way to a better understanding of preferential flow and matrix domains and we discuss important implications to improve continuum-scale models based on pore-scale simulations –the necessary step to produce reliable models of all soil processes and functions.

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Participation:

In person

MS18 / 440

Transport of Contaminant Slices under Unfavorable Viscosity Ratio in Porous Media with Dead-End Pores

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Less cleanup efficiency or sweep efficiency is a significant challenge in a variety of applications such as groundwater remediation, CO₂ sequestration, hydrogen geological storage, and enhanced oil recovery. Two key factors in the miscible displacements are the viscous fingering (VF) and fluid retention. The VF happens when a less-viscous fluid displaces a more-viscous one. While leading to large unswept areas by miscible VF, it is widely believed in swept areas the contaminant can be 100% cleaned up. This is however not true, especially considering the fluid retention, which however cannot be captured by previous studies in the VF research community. Here, we employ a fundamentally different model to investigate the transport and retention of contaminant slices in porous media with non-negligible dead-end pores. We show by highly accurate numerical simulation the

impact of dead-end pores on VF dynamics and temporal and spatial distribution of contaminant slices. Our research shows that porous medium not only acts as a medium for fluids to transport but also first acts as a sink and then a source of contaminant in newly swept areas. Furthermore, the local mass transfer between well-connected and dead-end pores substantially modifies VF dynamics and distribution of contaminant slices. We also find the maximum uncleaned contaminant in swept areas is 9-15 times higher than the classical models, when 40% dead-end pore volume is considered in porous media. Our research challenges the traditional viewpoint that miscible displacements can 100% clean up contaminant. It provides new insights into the roles of porous media and allows better characterization of contaminant transport, retention, and cleanup in aquifer system.

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MS18 / 441

Regeneration of granular activated carbon by microwave (MW) irradiation and its application in a novel in situ regenerating permeable reactive barrier (PRB) approach (MW-PRB)

Author: Pietro Paolo Falciglia¹

Co-authors: Erica Gagliano¹; Guido De Guidi¹; Stefano Romano²; Paolo Roccaro¹; Federico Vagliasindi¹

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Permeable reactive barrier (PRB) is considered one of the most effective in-situ alternatives for the remediation of contaminated groundwater and Granular Activated Carbon (GAC) a very performable material used in PRB systems. PRB reduced longevity due to a GAC saturation is the major problem affecting full-scale treatments (Ghaeminia and Mokhtarani, 2018). Landfill disposal of exhausted GAC is considered a further problem, which can also lead to secondary contamination paths. The investigation of in situ regenerating PRB to extend its longevity is a frontier and active research field. This approach may include the use of barriers coupled with other process or regenerating technologies in order to enhance PRB longevity.

Microwave (MW) heating is a growing interest issue in several energy and environmental applications. It is based on the ability of some dielectric materials in converting the MW energy into a very large and rapid heat production. Then, the excellent MW-absorbing features of GACs can enhance their thermal regeneration by MW irradiation (Falciglia et al., 2018). The present study evaluates the novel concept of PRB coupled with MWs (MW-PRB) as in situ regenerating technology. Experimental batch and column tests were carried out to assess the potentiality of the MW-PRB system as

combined treatment for Cesium (Cs) impacted groundwater.

Batch experiments investigated the effects of 10 adsorption-MW regeneration cycles under different MW irradiation conditions. Column tests were carried investigating different irradiation times (5-15 min, power 300 W) using a custom-made bench-scale setup. It is mainly made up of a Pyrex glass column (50 mm inner and 450 mm high) filled with a commercial GAC and inserted in a MW oven cavity equipped with a MW generator (1 kW) for column irradiation. The system was feed with a peristaltic pump using a Cs-contaminated solution to simulate the groundwater dynamics. Effluents were collected at set intervals for Cs concentration analysis before and after the regeneration phases. Batch test results showed a very rapid increase in GAC temperature up to over 650 °C, confirming the GAC strong ability to convert MW power into heat due to GAC excellent dielectric properties. Physical tests showed that GAC pore volume and specific surface area do not significantly change with the number of regeneration cycles. GAC regeneration ability was shown to increase over multi-cycle regeneration with a maximum value of ~110% (5th cycle). The final GAC weight loss of ~7% further demonstrates GAC life span preservation during MW irradiation.

Results from column tests confirm that GAC can be regenerated by MW also in dynamic condition, due to sublimation/vaporization and vapour stripping Cs removal mechanisms and that the regeneration process strictly depends on the irradiation time. The breakthrough curves after the regeneration phases demonstrate significant benefits from MW irradiation proving the feasibility of the proposed MW-PRB concept and providing essential data to guide its scaling-up application.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS18 / 444

Fungi-enhanced in-situ bioremediation of NAPL: A microfluidics study

Author: Sang Lee^{None}

Co-authors: Marcel Moura¹; Peter Kang²

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² *University of Minnesota*

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Non-aqueous phase liquid (NAPL) trapped in stagnant regions such as dead-end fractures and rock matrix are hard to remediate because they are inaccessible by groundwater flow. Recent studies showed the potential of bioremediation technologies that utilize the chemotactic motility of bacteria [1-3]. However, such methods rely on diffusion and dissolution of contaminants from NAPL to an aqueous phase which is slow and limited by the oil-water interfacial area. Hyphae of fungi are known to generate a tremendous amount of turgor pressure (~ 10 bar) on its tip [4] and produce surfactants [5] that allow them to navigate through small pores and air-water interfaces in porous media. In addition, biosurfactants alter the balance of the capillary forces at the oil-water interfaces in-situ, opening new flow pathways with immediate impact on the NAPL removal. However, to the best of our knowledge, there has been no direct visualization of fungal hyphae's penetration into oil-water interfaces, and its implication on the bioremediation of NAPL has been unclear.

This study reports striking results showing the active removal of NAPL by fungi using microfluidic experiments. Naphthalene-degrading fungus isolated from a local coal-tar contaminated site was injected into the PDMS microfluidic chip with a flow channel surrounded by NAPL-saturated low porosity regions. Vegetable oil with 10 g/L of naphthalene was used as the model NAPL, and fungal suspension in minimal salt medium (M10) was injected into the chip using a syringe pump. Then, the growth of the fungus and the change of oil-water interfaces were recorded through a scientific CMOS camera at the pore scale. Our results showed the active removal of NAPL by fungi. Fungi hyphae effectively penetrated through water-oil interfaces and significantly enhanced the oil removal from low porosity regions compared to the control case where a sterile medium was injected. Moreover, we observed that the growth of fungi induced flow instability which dramatically mobilized the trapped NAPL phase. In this contribution, we will further discuss the detailed mechanisms behind the effective removal of NAPL by fungi.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

Phase-wise Conservative and Physics Preserving Algorithms for Porous Media Flow

Author: Shuyu Sun¹

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Flow in geological porous media is central to a wide range of natural and industrial processes, including geologic CO₂ sequestration, enhanced oil recovery, and water infiltration into soil. Petroleum engineers use reservoir simulation models to manage existing petroleum fields and to develop new oil and gas reservoirs, while environmental scientists use subsurface flow and transport models to investigate and compare for example various schemes to inject and store CO₂ in subsurface geological formations, such as depleted reservoirs and deep saline aquifers. One basic requirement for accurate modeling and simulation of multiphase flow is to have the predicted physical quantities sit within a physically meaningful range. For example, the predicated saturation should sit between 0 and 1 while the predicated molar concentration should sit between 0 and the maximum value allowed by the equation of state. Unfortunately, popular simulation methods used in petroleum industries do not preserve physical bounds. A commonly used fix to this problem is to simply apply a cut-off operator. However, this cut-off practice does not only destroy the local mass conservation but it also damages the global mass conservation, which seriously ruins the numerical accuracy and physical interpretability of the simulation results. Another major issue with common algorithms for two-phase flow, especially common semi-implicit algorithms, is that they are (locally) conservative to just one phase only, not all phases.

In this talk we present our work on both fully implicit and semi-implicit algorithms for two-phase and multi-phase flow in porous media with capillary pressure. Our proposed algorithms are locally mass conservative for all phases. They are able to accurately reproduce the discontinuity of saturation due to different capillary pressure functions, and the computed total velocity is continuous in the normal direction. Moreover, the new schemes are unbiased with regard to the phases and the saturations of all phases are bounds-preserving (if the time step size is smaller than a certain value for the semi-implicit algorithms). We also present some interesting examples to demonstrate the efficiency and robustness of the new algorithms. The semi-implicit algorithms are based on our novel splitting of variables, and the fully implicit algorithms are based on the two nonlinear preconditioner of active-set reduced-space method and nonlinear elimination, as well as the linear preconditioner of overlapping additive Schwarz type domain decomposition. The semi-implicit part of this presentation is based on our joint work with Huangxin Chen (Xiamen University), Jisheng Kou (Shaoxing University), Xiaolin Fan (Guizhou Normal University), and Tao Zhang (KAUST), and the fully implicit part is based on our joint work with Haijian Yang (Hunan University), Chao Yang (Beijing University), and Yiteng Li (KAUST).

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Time Block A (09:00-12:00 CET)

Participation:

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MS09 / 446

Comparison of the Generalized Network Model to Direct Numerical Simulation for Two-Phase Flow

Author: Luke Giudici¹

Co-authors: Ali Qaseminejad Raeini²; Takashi Akai³; Martin Blunt⁴; Branko Bijeljic¹

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A thorough understanding of pore-scale modelling techniques is essential to flow through permeable media research. We compare two phase-flow simulations from the generalized network model (GNM) [Raeini et al, 2017, 2018] with a recently developed lattice-Boltzmann model (LBM) [Akai et al, 2018, 2020] for drainage and waterflooding in two samples—a synthetic beadpack and a micro-CT imaged Bentheimer sandstone—under water-wet, mixed-wet and oil-wet conditions. Macroscopic capillary pressure analysis reveals good agreement between the two models, and experiments, at intermediate saturations but shows large discrepancy at the end-points. At a resolution typically used in research settings, the LBM is unable to capture the effect of layer flow which manifests as abnormally large initial water and residual oil saturations. Critically, pore-by-pore analysis shows that the absence of layer flow limits displacement to invasion-percolation in mixed-wet systems. The GNM is able to capture the effect of layers, and exhibits predictions closer to experimental observations in water and mixed-wet Bentheimer sandstones. Overall, we present a workflow for the comparison of pore-network models with direct numerical simulation of multi-phase flow. We demonstrate that the GNM is an attractive option for cost and time-effective predictions of two-phase flow, and show that care must be taken when selecting pore-scale models.

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Akai, T., B. Bijeljic, and M. J. Blunt (2018). Wetting boundary condition for the color-gradient lattice Boltzmann method: Validation with analytical and experimental data. *Advances in Water Resources* 116 (April), 56-66.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS14 / 447

MCMC Convergence Studies for Flow Problems with Multiscale Sampling**Authors:** Alsadig Ali^{None}; Abdullah Al-Mamun¹; Felipe Pereira²; Arunasalam Rahunathan^{None}¹ *United International University*² *Mathematical Sciences Department, The University of Texas at Dallas, Richardson, TX, USA***Corresponding Authors:** arahunathan@centralstate.edu, alsadig.ali@utdallas.edu, luisfelipe.pereira@utdallas.edu, mamun3213ssh@gmail.com

We use subsurface characterization to describe porous media properties, such as permeability and porosity. One of the main challenges in the characterization is that we need to deal with a large dimension of the stochastic space. It is a common practice to apply a dimensional reduction method, such as a Karhunen-Loeve (KL) expansion, to the prior distribution in a Bayesian framework to make the characterization computationally tractable. Owing to the large variability of the properties in the subsurface formations, it is worth localizing the sampling strategy. This strategy permits us to capture the local variability of rock properties more accurately. In this talk, we mainly introduce the concept of multiscale sampling to localize the search in the stochastic space. In the Bayesian framework, we combine the new multiscale algorithm with a preconditioned Markov Chain Monte Carlo (MCMC) algorithm. The new sampling algorithm decomposes the stochastic space in orthogonal complement subspaces, through a one-to-one mapping to a non-overlapping domain decomposition of the permeability field. A Gibbs sampler is used for the localized search. In that search, the KL expansion is applied locally at the subdomain level. The proposed sampling algorithm is applied for the solution of an inverse elliptic problem. Using PSRF and MPSRF convergence diagnostics, we show that the new algorithm clearly improves the convergence rate of the preconditioned MCMC algorithm.

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Time Block C (18:00-21:00 CET)

Participation:

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MS15 / 448

Fitting correlation-based and neural-network-based relative permeability models to a large dataset of forced and spontaneous imbibition experiments

Author: Helton Magno Ciriaco¹

Co-authors: Hamid M. Nick²; Ali Akbar Eftekhari¹

¹ *Technical University of Denmark*

² *DTU*

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Estimating multiphase flow properties from Special Core scale Analysis (SCAL) has been extensively applied to obtain multiphase flow parameters representing the reservoir scale. Core flooding experimental data can also be used to investigate the mechanisms of more complex multiphase flow systems such as modified salinity water flooding, which has been shown to increase the oil recovery in chalk formations. However, the complexity of physicochemical phenomena cannot be captured by core flooding experiments; thus, the available models and tools which are based on input from core flooding experiments create uncertainties unless the models are tuned to many core flooding experiments, which is expensive and time-consuming. Moreover, the core flooding experiments only cover a narrow range of saturation changes. Spontaneous imbibition tests, which are usually cheaper, can serve as a complementary source of data for obtaining multiphase flow parameters; however, simulating a spontaneous imbibition test requires a model that links the diffusion of ions to the core and to/from the water film between the oil and formation water, how these ions modify the wettability of the system and alter the mobility of the phases. Furthermore, unlike the viscous-force-driven core flooding experiments that can be simulated with a 1D model, the SI test requires a 2D or 3D model which can be computationally expensive when used with an optimization algorithm for parameter estimation. We develop a numerical tool that is capable of estimating multiphase flow parameters for modified salinity water flooding using a combination of core flooding and spontaneous imbibition data. Our model is capable of capturing all the rock-fluid interactions and can be run in a reasonable computational time. First, we address the modelling of the reactive flow problem, focusing on the surface interactions between the brine and chalk formation, and the implications of the physicochemical phenomena that can alter the flow properties. We use surface complexation models to describe the ionic interactions at the oil/brine/chalk interfaces. We also use kinetic and equilibrium models to describe the dissolution of chalk. We use an empirical parameter linking the surface reactions to the relative permeability and capillary pressure model parameters. Then, we discuss a solution to the inverse problem of the model described, which can obtain parameters using a large database of in-house and literature experimental data. Our model can accurately and rapidly estimate the relative permeability and capillary pressure curves by fitting a reactive multiphase flow model to the measurements from core flooding and spontaneous imbibition experiments. Additionally, we replace the correlation-based relative permeability curves with a neural network (NN) in the multiphase reactive flow model to create a physics-informed neural network model. We fit the model to our large database of experimental data and compare the NN-based model with the correlation-based relative permeability curves. Our results indicate that a machine learning tool that combines the governing physics equations and a large set of experimental data can predict with accuracy the multiphase flow properties at a reduced running time that reasonably matches with the expected trend of relative permeability curves.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

Poster / 449

Investigation of different clay activation techniques to capture and store carbon dioxide (CO₂)

Author: Cindy Chomba¹

Co-authors: Mardin Abdalqadir¹; Sina Rezaei-Gomari²

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Global warming due to greenhouse gases has been a major concern over the years. CO₂ is among the most common greenhouse gases that has been released in significant quantities and hence the demand for its reduction. Recently, adsorption technology in particular clay minerals has drawn attention as a low cost, environment friendly means of carbon capture. The major drawback in adsorption technology is designing a biodegradable adsorbent with large CO₂ uptake and adequate adsorption kinetics. Due to its natural abundance and high stability, this study focuses on natural clay minerals such as: Kaolinite, Montmorillonite and Illite as potential adsorbents for carbon capture. The effectiveness of proposed adsorbents is investigated at different conditions to optimize their capacity for CO₂ uptake. Therefore, this work, investigates the impact of chemical activation of clay minerals using acidic and amine solutions on their CO₂ adsorption capacity. Moreover, the effect of operating parameters such as temperature and reaction time with and without use of microwave are also included in this study.

The clay materials are activated by nitric acid and 3-aminopropyltriethoxysilane (APTES) solutions at elevated temperature from 25 to 70°C and as well as in microwave under 30 seconds and 1 minute. The materials are then characterized for their surface morphology, functional group interactions, surface area determination, and pore volume calculation by SEM, FTIR, BET and Image J software, respectively.

The results show that montmorillonite had the best adsorption capacity than kaolinite and illite before and after activation. The clay minerals also displayed an increase in surface area and pore

volume and subsequently adsorption capacity. Kaolinite and illite were more resistant to acid attacks however, there is an improvement in pore size when the microwave is used thus implying reaction time may influence CO₂ adsorption capacity. Increasing activation temperatures from 25 to 70°C resulted in a change of adsorbent structure and behaviour. In conclusion, microwave assisted clay activation at ambient conditions could be a competitive adsorbent in CO₂ capture technologies where the surface area and pore volume of clays increased by 10%.

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Participation:

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MS16 / 450

A Review on Polymer Adsorption in Carbonate and Sandstone Reservoirs

Author: Anoo Sebastian^{None}

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Of the innumerable EOR techniques, Polymer flooding is one of the most effective methods which aids oil recovery (Khalilinezhad et al., 2019; Lamas et al., 2021) by increasing the viscosity of water (Chang, 1978; Saboorian-Jooybari et al., 2016; Panthi et al., 2016b; Mohsenatabar Firozjahi and Saghafi, 2020; Lu et al., 2021) hence lowering the water-oil mobility ratio (Jennings RR et al., 1971; Dano et al., 2019), thus improving the volumetric sweep efficiency (Sandiford, 1964; Rashidi et al., 2009; Han et al., 2014; Yoo et al., 2020; Lamas et al., 2021). Polymer flooding has been widely used over the years in the case of sandstone reservoirs with lower temperatures, low salinity, and high permeabilities (Zhang and Seright, 2014; Panthi et al., 2016a; Oluwaseun Taiwo et al., 2019; Yoo et al., 2020; Bera et al., 2020; Zhu et al., 2020). However, its application is limited in the case of carbonates reservoirs due to complex heterogeneity, low permeability values less than 100mD (Saberhosseini et al., 2019; Khalilinezhad et al., 2021; Mahmoodpour et al., 2021), higher reservoir temperature, i.e., above 850C, high salinity above 100,000ppm (Lu et al., 2014; Das et al., 2020) and hardness over 1,000ppm (Diab and Al-Shalabi, 2019; Abalkhail et al., 2020; Mogensen and Masalmeh, 2020).

The success of a polymer flooding project depends on the efficient transport and propagation of polymer slug through the reservoir. As polymer solution flow through the porous media, interactions happen between the rock surface and the polymer molecules, which causes these polymer molecules to be retained on to the rock surface (Huh et al., 1990; Rashidi et al., 2009; Gaillard et al., 2014; Alfazazi et al., 2020), thus resulting the injected fluid to be deprived of polymer molecules and causing the reduction in viscosity (Zamani et al., 2017; Skauge et al., 2018; Zhang et al., 2021) and further reducing the efficiency of the polymer flooding (Riahinezhad et al., 2017; Al-Hajri et al., 2018; Liang et al., 2019). Polymer retention can be caused due to polymer adsorption onto the rock surface, mechanical entrapment of polymer molecules in the tiny pores of the porous media, and hydrodynamic retention due to varying flow rates (Sorbie, 1991; Al-Hajri et al., 2018; Sugar et al., 2020). A higher amount of polymer adsorption can cause a delayed polymer propagation resulting delay in the oil displacement. The significant economic impact due to the delayed polymer propagation

caused by the polymers being permanently lost to the porous rock resulted in increased consumption of chemicals and increased injection period. Some pores of reservoir rocks are relatively small, which restricts the entry of large size polymer molecules. The bulk of these pores through which polymers cannot penetrate is known as inaccessible pore volume. Further, due to this inaccessible pore volume, a polymer solution will sweep through less pore volume in a porous medium; thus, there will be an early breakthrough of polymer solution. There are many factors affecting polymer adsorption including polymer type, polymer concentration, salinity, presence of oil and type of rock surface.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Dynamic X-ray micro-CT measurements of tablet disintegration

Authors: Jan Dewanckele¹; Wesley De Boever¹; Shumaiya Ferdoush²; Pedro Martins²; Marcial Gonzalez³

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Dynamic X-ray micro-CT was used to get a better mechanistic understanding of the disintegration process of pharmaceutical solid dosage forms (tablets or capsules). Dosage forms are the predominant form to control active pharmaceutical ingredients to a patient and typically consist out of compacted powder with added excipients. In order to deliver the active pharmaceutical ingredients to the patients, the compacted tablet needs to mechanically break up into smaller particles. Therefore, the admixture of excipients is essential as it controls the process of the drug release in the body and assures a high product quality. As a result, solid dosage forms are complex structures with high heterogeneities on different length scales. In order to simultaneously study the penetration of the water inside of the tablet, the disintegration and swelling, one needs to non-destructively and in full 3D visualize the process.

The tablet was compacted in a 6 mm die at a predetermined thickness to control the maximum in-die relative density (0.8) at Purdue University (Prof. Gonzalez Research Group). The formulation used was: MMC (89%) + APAP (9%) + MgSt (1%) + Cab-O-Sil (1%). MMC or MicroCrystalline Cellulose is widely used in pharmaceuticals, primarily as binder in oral tablets. The tablet was afterwards placed in the TESCAN UniTOM HR on a styrofoam sample holder with a syringe pump attached. The pump added water at an injection rate of 2ml/min to the styrofoam. As a results, the water was absorbed by the tablet through capillary uptake at the bottom. This complete in-situ set up was mounted on the rotation stage of the TESCAN UniTOM HR and powered through the slipping of the system. By doing so, an endless, uninterrupted rotation of the complete in-situ set up was possible as fluid cable tangling was bypassed.

In order to capture the fast, mechanical dynamics of the disintegration process, a high temporal resolution was needed. The total time for complete disintegration of the tablet was 7 minutes. In the experiment, 100 uninterrupted tomograms at a temporal resolution of 4 seconds (200 projections/360°, 20 ms exposure time) per rotation could be obtained while water was absorbed inside the tablet. The voxel size of the scan was 13 µm, small enough to visualize the deformation mechanics inside of the sample.

The resulted reconstructed volumes clearly demonstrate the disintegration pattern of the samples. A crack forms at the bottom of the sample, opening upwards during the water absorption. The water front itself in not uniform throughout the complete sample and shows a faster absorption on the boundaries of the sample. Micro-cracks are developing throughout the sample, some of them filled with liquid while others remain dry. A more thorough investigation, including image analysis, is required to fully understand the behavior of the sample, but the principal disintegration mechanisms are captured throughout the process.

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MS09 / 453

Memory, energy dissipation and hysteresis of two-phase flows**Authors:** Ran Holtzman¹; Marco Dentz²; Ramon Planet³; Jordi Ortin⁴¹ *Coventry University*² *IDAEA-CSIC*³ *University of Barcelona, Spain*⁴ *Universitat de Barcelona***Corresponding Authors:** marco.dentz@csic.es, jordi.ortin@ub.edu, ramon.planet@gmail.com, rholtzman4@gmail.com

Memory, hysteresis, and energy dissipation are related concepts that appear in nonequilibrium disordered systems, but the links between their microscopic origins and the resulting macroscopic properties remain elusive. Using the return-point memory of cyclic macroscopic trajectories, we formulate an accurate thermodynamic characterization of quasistatically-driven dissipative systems with multiple metastable states. We use this framework to quantify the energy dissipated in fluid-fluid displacements in disordered media. Our simulations highlight the importance of correlations between individual microscopic interfacial jumps, resulting in an overall collective hysteretic and dissipative behavior. This cooperative mechanism is absent from classical compartment models. Comparison to experiments provides interesting insights into the role of viscous dissipation in slowly driven systems.

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MS16 / 454

Absorption of surfactants on porous media: Method development and Numerical prediction of surfactant distribution

Authors: Amber Louwhoff¹; Mirthe Mampaey¹; Jasper van den Hoek¹; Jeroen Schell¹; Chris Smit¹; Helder Salvador¹; Nicolae Tomozeiu¹; Herman Wijshoff¹

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Media composition and structure play a fundamental role in the absorption of liquids into its porous media. Enhancing the absorption behaviour of such substrates is crucial for the printing industry to develop faster processes, better print quality and improving print durability. Absorption can among other be improved by tailoring the printing liquid. A common way to achieve this is by lowering the surface energy of interfaces by using surfactants in the ink composition. In this work we tackle the study of the influence of surfactants into porous media by developing a measurement method to extract surfactant concentration along the thickness of the paper and the developing of a numerical model that computes transport equations of surfactant during liquid uptake into capillaries

Microtomes are commonly used method to extract thin slices from porous media that can further be analysed. However, the usage of such method demands an extremely skilled operator and the accuracy of a microtome can often become a limiting factor. As an improvement on method development of the microtome method, a milling device is developed that can extract slices from several types of media very precisely. Subsequently, the composition of a water-surfactant mixture along the paper thickness was measured, using Karl Fischer titration to determine water content, and quantifying surfactants concentration using a Liquid Chromatography - Mass Spectrometry setup.

For modelling liquid uptake into porous media Darcy's law together with the continuum equation for incompressible flow was used to model the absorption process, and an advection-diffusion-adsorption equation was used to compute the surfactant concentrations. The influence of surfactants on the absorption rate was modelled using the Sheludko approximation as an equation of state which correlates the concentration at the interface to a change in solid-liquid surface energy. This model clearly shows that pore diameter, adsorption/desorption rate of surfactants into the solid interfaces and maximum surfactant concentration at solid interfaces are the predominant parameters that control absorption phenomena.

Combining both developments we can to show that there are fundamental differences between the absorption depth of surfactants on different porous media. This indicates that there is fundamental interaction between surfactants and the media which that can be further investigated using the developed model. This work clearly shows that depending on the surfactant interaction with the porous structure and the physical properties of both the porous medium and the surfactants we can have a situation where surfactants are transported along the wetting front or we can have a situation where the wetting front is depleted of all surfactants.

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MS23 / 456

Field-scale Modeling of CO₂ Injection into Highly Reactive Rocks

Authors: Tom Postma¹; Karl Bandilla¹; Michael Celia¹

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Injection of anthropogenic carbon dioxide into deep geological formations requires one or more trapping mechanisms to keep the CO₂ contained in the injection formation. The most stable of these trapping mechanisms is mineral trapping where the injected carbon is ultimately trapped in solid form via precipitation of carbonates. While mineral trapping in most sedimentary formations is extremely slow and not of practical relevance, injection into highly reactive rocks like flood basalts may result in substantial mineral trapping on shorter time scales. Laboratory and small-scale field experiments show very fast reaction time scales, on the order of months to years. To understand how such systems will behave at large spatial scales, consistent with practical field-scale injection operations, we have developed a field-scale model for CO₂ injection and migration that includes mineral reactions. The model assumes the injection takes place in a deep saline aquifer and uses a vertically integrated set of governing equations, based on a vertical equilibrium assumption for the buoyant two-phase flow system. The model includes CO₂ dissolution into the aqueous phase with an associated upscaled representation of convective mixing in the brine, residual CO₂ saturations that lead to capillary trapping of separate-phase CO₂, a set of reactions both within the aqueous phase and involving the rock matrix, and calculation of porosity changes associated with the mineral reactions. The model allows for many different scenarios to be investigated. Simulation results show how mineral reactions that proceed rapidly at small spatial scales are tempered by mass-transfer limitations between different regions in the vertical equilibrium model. Results also provide quantification of porosity changes with associated implications for possible pore clogging due to carbonate precipitation. Advantages and disadvantages can also be identified for different injection strategies including comparison between injection of separate-phase CO₂ and injection of an aqueous phase pre-saturated with dissolved CO₂.

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MS03 / 457

An Uncertainty Quantification Workflow for Naturally Fractured Reservoirs using Proxy Modelling based on Poro-mechanically Informed Flow Diagnostics Simulations

Authors: Lesly Gutierrez Sosa¹; Sebastian Geiger^{None}; Florian Doster^{None}

¹ Heriot Watt University

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Carrying out uncertainty quantification and robust optimisation workflows for naturally fractured reservoirs (NFR) is very challenging because exploring and capturing the full range of geological and mechanical uncertainties requires a large number of numerical simulations and hence computationally intensive. Specifically, the integration of poro-mechanical effects in full-field reservoir simulation studies is still limited, mainly because of high computational cost. As a result, poro-mechanical effects are often ignored in uncertainty quantification and optimisation workflows, which may result in inadequate reservoir performance forecasts. Computationally efficient poro-mechanical screening methods are therefore important to identify if poro-mechanics could impact reservoir dynamics and identify individual models from a model ensemble for more detailed full-physics reservoir simulations.

Here we introduce a new methodology that extends traditional uncertainty quantification workflows, through the use of poro-mechanical informed flow diagnostics and proxy models. This approach provides first-order approximations of the complex interactions between poro-mechanics and hydrodynamics using existing steady-state dual-porosity flow diagnostics and coupled dual-continuum poro-mechanics. The calculations are computationally efficient and allow us to quickly quantify their impact of poro-mechanics on reservoir dynamics and further enable us to select representative reservoir models that capture the uncertainty quantified in a reservoir model ensemble. These representative models can then be used in further, more detailed and computationally intensive full-physics coupled reservoir simulations. The proposed poro-mechanical screening hence provides an efficient complement to traditional reservoir simulation and uncertainty quantification workflows and enable us to assess a broader range of geological, petrophysical and mechanical uncertainties.

Using a series of case studies based on a fractured carbonate reservoir analogue, we demonstrate how (1) uncertainty quantification workflows can be improved by considering different hydrodynamical-poro-mechanical scenarios, (2) how bias in the uncertainty estimation can be reduced by carrying out by thousands Monte Carlo realisations using ANN-based proxy models, and (3) how cluster analysis can be performed to identify a suitable set of representative models from a much larger model ensemble without reducing uncertainty in reservoir performance predictions. The proposed framework has been implemented using the open-source MATLAB Reservoir Simulation Toolbox MRST and was linked to a commercial reservoir simulation package to carry out the experimental design, construct the proxy model, and perform the sensitivity and uncertainty analysis.

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MS12 / 458

Study on Microscopic Imbibition process in Variable Diameter Capillary Tubes

Authors: Lihua Shi¹; Shiqing Cheng¹; Yuwen Chang²; Binchi Hou³

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Spontaneous imbibition plays an important role in water injection development of tight reservoirs. At present, few research focused on micro-imbibition law considering capillary diameter change in liquid-liquid system. In this study, based on Poiseuille's law and imbibition theory, the theoretical formula of spontaneous imbibition in variable diameter capillary under liquid-liquid system was derived. A new theoretical model of imbibition considering capillary structure and viscosity ratio was established, and the imbibition behavior of liquid-liquid system in multi-stage expanding-shrinking capillary was revealed. It was found that the capillary geometry is the main factor affecting the imbibition process of the variable diameter section. The end time of liquid imbibition is much longer than that in gas-liquid system. With the increase of the variable diameter section, the imbibition curve presents a convex curve. The viscosity ratio has a great influence on the end time of imbibition in liquid-liquid system. In gas-liquid system, the increase of gas phase viscosity has little influence on the end time of imbibition, and it is better to fit the previous numerical simulation and analytical results. On this basis, the multi-stage expansion-shrinkage equivalent capillary model is obtained. Compared with the traditional BCLW imbibition model, the prediction deviation is smaller, the coincidence rate is higher. The model can quickly and accurately predict the imbibition process in the variable diameter capillary, and provide a theoretical basis for optimizing the water injection development strategy of tight reservoirs.

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Time Block C (18:00-21:00 CET)

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MS23 / 459

From streamlines to discrete fracture modelling of multi-phase flow and deformation in fractured porous media

Authors: Rainer Helmig¹; Bernd Flemisch¹; Holger Class¹; Dennis Glaeser¹

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One of the most important problems related to the modeling of fluid flow in natural porous media is accounting for their heterogeneous structure, which occurs on various spatial scales. A typical and widespread example of heterogeneous porous media is fractured rocks. While the volume of the fractures is negligible, their presence significantly alters the mechanical and hydraulic properties of the porous medium. Accurate simulations of fluid flow in fractured geological formations are very important in applications such as the exploitation of petroleum, groundwater or geothermal reservoirs or the design of waste-disposal facilities. An emerging field of application is related to the geological storage of, for example, green gas. The description of complex flow and transport processes including deformation-dependent fracture apertures is necessary. Mathematical models of fluid flow in fractured media can be broadly divided into discrete fracture models, where the fractures are represented explicitly on the numerical grid, and multi-continuum models, where the fracture network and the porous matrix are represented as overlapped continua, each characterized by its own set of hydraulic parameters. In the discrete fracture models, the fractures are often represented as elements of reduced dimensionality, i.e. 1D elements in a 2D matrix or 2D elements in a 3D matrix. Existing models for fracture-matrix systems are usually available for the simulation of flow and transport processes without fracture deformation. To overcome the above-mentioned challenges, the focus of this presentation is on the development of a hybrid-dimensional model for multi-phase flow in fractured poro-elastic media. The results are discussed in terms of the physical relevance of the observed phenomena as a quantitative assessment would require detailed experimental data.

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1. Gläser, D.; Schneider, M.; Flemisch, B.; Helmig, R. (2022): Comparison of cell-and vertex-centered finite-volume schemes for flow in fractured porous media. *Journal of Computational Physics*, 448, 110715. DOI: 10.1016/j.jcp.2021.110715.
2. Gläser, D.; Flemisch, B.; Helmig, R.; Class, H. (2019): A hybrid-dimensional discrete fracture model for non-isothermal two-phase flow in fractured porous media. In *GEM-International Journal on Geomathematics* 10 (1), p. 5. DOI: 10.1007/s13137-019-0116-8.
3. Gläser, D.; Helmig, R.; Flemisch, B.; Class, H. (2017): A discrete fracture model for two-phase flow in fractured porous media. In *Advances in Water Resources* 110, pp. 335–348. DOI: 10.1016/j.advwatres.2017.10.031.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS06-A / 460

Pore-scale imaging of hydrogen in porous media

Authors: Yihuai Zhang^{None}; Branko Bijeljic¹; Martin Blunt²

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Green hydrogen geological storage and production is a strategy for mitigating greenhouse gas emissions and climate change. However, there is still a lack of serious mechanisms research of how hydrogen trapping and migrations in the porous media of the rock when considered the buoyancy effect can not be ignored. Through a series of microCT in situ two-phase drainage and imbibition experiments on a sandstone sample, we demonstrate that the pore-scale phase configurations, curvatures, and contact angles are different for hydrogen compared to other traditional gas (e.g. nitrogen). In addition, we found that hydrogen is less wetting gas, and its buoyancy forces can be higher than the capillary forces, where the capillary trapping mechanisms will be invalid.

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References:

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Time Block B (14:00-17:00 CET)

Participation:

In person

MS10 / 461

Time and spatial resolved X-ray imaging of wicking in interlaced yarns

Author: Robert Fischer^{None}

Co-authors: Dominique Derome ¹; Christian Schlepuetz ²; Rene Rossi ³; Jan Carmeliet ⁴

¹ *Universite de Sherbrooke*

² *PSI*

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Understanding wicking dynamics in textiles is challenging due to the complex pore structure of yarns as well as of the interfaces between interlaced yarns. Time-resolved synchrotron X-ray tomographic microscopy (XTM) is performed at the TOMCAT beamline of the Swiss Light Source of Paul Scherrer Institute in Switzerland. Full high-quality tomographic scans of 5.5 mm height with voxel size 2.75 µm are performed at 2.5 Hz.

XTM reveals the pore structure of the yarns and the interface zone at the yarn contact. In addition, the evolution of the water configuration is documented with high temporal and spatial accuracy. Segmentation of the pore space shows that yarns contain long elongated pores connected laterally with a small number of throats, while the pore space at the interface zone shows a saddle shaped waffle structure originating of the contact of two orthogonally stacked yarns consisting of parallel fibers. Free energy analysis shows that such a pore structure does not enhance flow due to the occurrence of minima in capillary pressure.

Analysis of the XTM data shows an irregular wicking process characterized by two distinct periods: fast pore filling events followed by long time delays between different pore-to-pore transitions 1. As a result, the wicking process does not follow classical square root of time behavior as predicted by Washburn equation. For the interlaced yarns, we observe that some samples even show very much longer time delays during flow through the interfaces at yarn-to-yarn contacts, while other do not show delays. Therefore, we determine the free energy evolution, determined from the change in interface areas, both water-air area and water-fiber area, as obtained from the images at each time step. The capillary pressure is obtained as the partial derivative of free energy to the water filled pore volume, also determined from the images. We find that wicking is delayed at the pore-to-pore and yarn-to-yarn transitions when experiencing a minimum in capillary pressure. The occurrence of a minimum in capillary pressure is explained by the particular pore structure at the contacts. We also determine the resistance from the volume flux and capillary pressure assuming Darcy's law, finding that no extra resistance exists at the contacts. Excluding extra flow resistance as origin for the delays at the contacts makes us conclude that the delays are originating from the occurrence of minima in capillary pressure due to particular pore structure arrangements at the contacts.

As a consequence, heterogeneity in fiber arrangements at the contacts may prevent the occurrence of minima in capillary pressure and delays, as observed for some samples. As a practical implication for the development of wicking enhancing fabrics, irregular pore structures should be preferred and yarns with equally sized circular filaments, as used in the present study, be avoided.

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1 R. Fischer et al, 10.1103/PhysRevE.103.053101

Time Block Preference:

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Participation:

In person

MS18 / 462

Laboratory scale demonstration of cationic organics removal by graphene oxide nanosheets injection in porous media

Authors: Carlo Bianco¹; Ali Beryani¹; Alessandro Casasso¹; Rajandrea Sethi¹; Tiziana Tosco¹

¹ Politecnico di Torino

Corresponding Authors: rajandrea.sethi@polito.it, alessandro.casasso@polito.it, tiziana.tosco@polito.it, ali.beryani@polito.it, carlo.bianco@polito.it

Graphene oxide nanoparticles (GONPs) are promising materials for the adsorption of a broad set of environmentally relevant contaminants, such as organic aromatic compounds, heavy metals, dye molecules, pharmaceuticals (Iqbal and Abdala, 2013; Zhou et al., 2016). Moreover, thanks to their small size, GONPs can be injected in the subsurface and effectively migrate within groundwater (Beryani et al 2020). Therefore, due to its high sorption capacity and high subsurface mobility, this material has a good potential for being employed as a remediation agent for enhanced in-situ soil washing of secondary sources of groundwater contamination (i.e. the controlled recirculation of a washing GO suspension via injection/extraction wells).

In this study, the capability of GONPs to remove organic contaminants was characterized at the laboratory scale. Methylene blue (MB) was opted as a model molecule representative of these contaminants of concern, which could be absorbed by GONPs in aquatic environments. MB is a common aromatic, water soluble, cationic dye which has been reported as a major pollutant of water resources because of its carcinogenicity and other health adverse effects on aquatic organisms and humans. Additionally, MB removal processes can be representative of other contaminants removal procedures since electrostatic interactions, π - π stacking and hydrogen bonds are the most effective phenomena governing all adsorption processes.

Laboratory tests included batch tests, aimed at assessing the capability of GO to adsorb MB, and column desorption tests, aimed at evaluating the efficacy of GO as a washing agent to remediate MB-contaminated sand columns.

The adsorption experiments demonstrated that GO is highly effective in the rapid adsorption of MB. The results indicated a maximum sorption capacity of 1.6 mgMB/mgGO in moderately alkaline conditions. This is an extremely interesting removal efficiency in view of a technical application in water purification.

The desorption experiments, which were performed injecting a 50 mg/L GO suspension into a sand column artificially contaminated with MB, showed a high potential of GO nanosheets to accelerate the removal of MB from contaminated sand compared with the use of deionized water only. The GO-flushing allowed to recover more than 25.8% of the adsorbed MB after only 3 pore volumes and 42.4% after 10 pore volumes. Only 8.1% and 8.3% of MB was instead recovered after the same water injection times. The results open positive perspectives for the potential application of GO for groundwater reclamation purposes. In particular, a GO-assisted soil flushing can be envisioned. In this way, fast desorption of contaminants strongly adsorbed on the aquifer solid matrix can be promoted, thus allowing for the treatment of secondary sources of contamination.

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Iqbal, M.Z., Abdala, A.A. "Oil spill cleanup using graphene." *Environ Sci Pollut Res* 20, 3271–3279 (2013). <https://doi.org/10.1007/s11356-012-1257-6>

Zhou DD, Jiang XH, Lu Y, Fan W, Huo MX, Crittenden JC. "Cotransport of graphene oxide and Cu(II) through saturated porous media." *Science of The Total Environment* (2016); 550: 717-726.

Beryani, A., Alavi Moghaddam, M.R., Tosco, T., Bianco, C., Hosseini, S.M., Kowsari, E., Sethi, R. "Key factors affecting graphene oxide transport in saturated porous media" *Science of the Total Environment*, (2020) 698, art. no. 134224.

Beryani, A., Bianco, C., Casasso, A., Sethi, R., Tosco, T. "Exploring the potential of graphene oxide nanosheets for porous media decontamination from cationic dyes" *Journal of Hazardous Materials*, (2022) ISSN 0304-3894, <https://doi.org/10.1016/j.jhazmat.2021.127468>.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS06-A / 463

Extension and Uncertainty Modeling of Imbibition Processes using the Morphological Method –a Reality Check**Author:** Pit Arnold¹**Co-authors:** Mario Dragovits¹; Fatime Zekiri²; Sven Linden³; Holger Ott⁴¹ *Montanuniversität Leoben*² *OMV Exploration & Production GmbH*³ *Math2Market GmbH*⁴ *Montanuniversität Leoben***Corresponding Authors:** sven.linden@math2market.de, holger.ott@unileoben.ac.at, mario.dragovits@gmail.com, fatime.zekiri@omv.com, pit.arnold@unileoben.ac.at

A prime target of Digital Rock Physics is to compute multi-phase flow saturation functions in a time-effective and cost-competitive way. Traditional approaches for flow simulations in porous media may be split into full-physics direct numerical simulations and pore network modeling. Associated with high computational demand and scale limitations, full-physics direct numerical simulations, such as e.g. Lattice Boltzmann, are not suited for uncertainty modeling. It requires the simulation of many scenarios to explore the uncertainty range, e.g. with a Monte Carlo type of sampling. However, there are hybrid methods such as the morphological method, a geometry-based approach to model the two-phase fluid distribution in the pore space, combined with single-phase direct flow simulations on the actual pore structure, the digital twin. This approach is still computationally favorable.

Good agreements for drainage capillary pressure sets of water wet systems have already been found in the past. However, the method lacks capabilities when modeling the complementary imbibition processes, particularly the forced imbibition part, which was missing so far. To overcome the wetting state limitation, we introduced multiple contact angles and a turn of material wetting state. Further, we combine an imbibition and drainage operation in order to extend the imbibition process to the forced imbibition branch.

To achieve a realistic description and model uncertainty, we studied the impact of contact angle distribution and its spatial variation in combination with a turn of the wetting state of material after the drainage process. By the developed approach, full-scale capillary pressure and relative permeability saturation functions were calculated and varied in a physically meaningful way. Comparison to experimental data (Berg et al. 2016) showed good agreement of the relative permeabilities. Additional computation of topological measurements gave further insight into the uniqueness of the results.

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<https://doi.org/10.1016/j.advwatres.2016.01.010>

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS12 / 464

Experimental Research of Spontaneous Water Imbibition in Oil-Saturated Reservoirs with Ultra-low Permeability

Authors: Hailong Dang¹; Hanqiao Jiang¹; Binchi Hou²

¹ *China University of Petroleum, Beijing*

² *Shaanxi Yanchang Petroleum (Group)*

Corresponding Authors: houbinchi1015@163.com, danghailong71@126.com, jianghanqiao@163.com

Spontaneous water imbibition (SWI) in porous media is of great importance in many industries. It is useful to predict the oil production in the fractured reservoirs developed by water flooding or associated with aquifers. The objective of this study is to investigate the combined effects of interfacial tension (IFT), salinity, and wettability on spontaneous Imbibition of water in ultra-low permeability rocks saturated with oil and the related mechanisms. Rock plugs with permeabilities ranged from 0.01 to 5 md were sampled from Yanchang Oilfield, China. A series of experiments on SWI have been conducted in these rock samples after cleaning, drying, and saturating with simulated oil at different IFT, salinity, and wettability conditions. The tests were done at room temperatures but the ratio of the oil-water viscosity in the experiments was equal to those at the reservoir conditions. Surfactants were used to alter the interfacial tension, and wettability. The experimental data of oil recovery by SWI under different conditions were then analyzed using different methods, including Li-Horne imbibition-model. The combined effects of IFT, salinity, and wettability on the oil recovery by SWI in ultra-low permeability rocks have been obtained experimentally. The results demonstrate that brine could imbibe into the oil-saturated rock with an ultra-low permeability of about 0.01 md at a relatively fast rate beyond our expectation. The oil recovery by SWI increased with the decrease in interfacial tension, contact angle, and brine salinity. The water imbibition rate is inversely proportional to the oil recovery, which follows the Li-Horne imbibition model. A mathematical model has been utilized to predict the oil recovery by considering almost all of the parameters involved in the spontaneous water imbibition. It is worth to further study the mechanisms of SWI imbibition in ultra-low permeability rocks, including the fluid flow in nanometer pores.

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MS13 / 465

Water confined in salt crusts: insights from molecular simulations

Author: Simon Gravelle¹

Co-authors: Sabina Haber-Pohlmeier²; Alexander Schlaich¹; Christian Holm¹

¹ *Institute for Computational Physics*

² *Institut für Wasser und Umweltsystemmodellierung*

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The evaporation of water from a bare soil can be accompanied by the formation of a layer of crystallized salt. This salt crust forms an additional porous layer that affects the evaporation of water in a counter-intuitive way: depending on the conditions (i.e. depending on the pore size of the crust, soil-crust connection, external atmospheric conditions), the crust can hinder or enhance the net flow of water. To better understand the transport properties of water through porous salt crusts, we use molecular simulations and explore the behavior of water confined by three types of solid surfaces: NaCl, Na₂SO₄, and charged silica. We measure NMR relaxation times T₁ and T₂, extract their values for different degrees of confinement, relative humidity, and surface rugosity, and discuss their relation with the structure of water near solid interfaces. Then, using non-equilibrium molecular dynamics, we study the transport properties of water at the salt interface. Our results show that at low humidity, transport through salt crust is likely to be dominated by a thin layer of water of a few molecules at the salt wall.

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Poster / 466

Decontamination-induced contaminant redistribution in porous media

Author: Emily Butler^{None}

Co-authors: Francesco Paolo Conto¹; Merlin Aragon Etzold²; Stuart Dalziel¹; Joel Daou³; Julien Landel³

¹ *University of Cambridge*

² *DAMTP, University of Cambridge*

³ *University of Manchester*

Corresponding Authors: julien.landel@manchester.ac.uk, fpc25@cam.ac.uk, emily.butler@manchester.ac.uk, s.dalziel@damtp.cam.ac.uk, joel.daou@manchester.ac.uk, mae38@cam.ac.uk

The cleaning of porous media is ubiquitous and the difficulties associated with cleaning such materials are numerous. Surface contamination may ingress inside the pore space and become inaccessible to a cleaning flow. This makes it very difficult to monitor the levels of contamination throughout the medium and determine whether cleaning has been successful. The addition of a surface washing flow can also encourage spreading of contaminant over the surface of porous material. These problems are exacerbated in a military or industrial context since leaving hazardous residual contamination inside the porous medium can pose significant risks to human health and the environment.

To explore the decontamination process in porous media, we propose a simple two-dimensional model for a washing flow over the surface of a wet porous medium contaminated by a drop of a single-species contaminant. We impose a single-phase unidirectional flow through the porous medium and model the washing flow using a linear shear velocity profile. At the interface, we assume that the flow fields match by definition so that interfacial boundary conditions for the velocity are not required. We construct a coupled mass transport problem to monitor the concentration of contaminant in both the washing flow and the porous medium. In both phases, we assume that mass transfer is governed by advection and diffusion processes with the addition of dispersion effects in the porous medium. We focus our analysis on asymptotic regimes that exhibit contaminant redistribution in the porous medium and consider how the efficiency of the decontamination process can be improved by variation of the problem's dimensionless parameters. We also present comparisons with numerical simulations performed in COMSOL to validate our analytical model.

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MS17 / 467

Acute observations into multifractal characteristics of bituminous coals by Qualitative analytics

Authors: Paul Naveen¹; Debjeet Mondal²

¹ Pandit Deendayal Energy University Gandhinagar

² Central Mine Planning and Design Institute Limited

Corresponding Authors: debjeet.mandal@coalindia.in, paul.naveen@spt.pdpu.ac.in

Adopting FESEM and AFM imaging technology, a concatenation of 2-D and 3-D nano-scale investigations are comported on the types of pore-cleat constituents inherent to CBM and CO₂-ECBM producibility. A finely dispersed mineral material is ascertained within the organic coal matrix. The latter may influence the differing pore geometries and capillaries featuring characteristic lengths varying from nanometers to microns. A significant portion of gas producibility appears to be associated with these inter-connected large scale nanopores within the matrix. This investigation finds its implications on optimal producibility of CBM and CO₂-ECBM processes. Thermodynamics of fluid-rock interactions in these pores are very diverse. Gas transportation in these conduits is rarefied due to the mineral phase pore walls and indicate a tendency of density profile across the damped oscillations. This arises the complications about the gas producibility predictions, under the insitu conditions, the fraction of gas considered to be as adsorbed phase and accurate estimation of gas adsorption capacity by the use of volumetric measurements. Also, density contrast between the adsorbed/free phase in mineral material for accurate gas producibility.

To emphasize on these complications associated with gas transportation, we attempted to integrate the volumetrics of adsorbed/free gas phases with multifractal characteristics of a high proliferous bituminous coal. The outcomes of the investigations yield a gas producibility because of corrected pore volumetrics that is affected as a result of average adsorbed/ free gas density. In addition, we address the complications associated with the thermodynamic phase transitions of gas in mineral conduits using dynamic simulations engrossing gas transportation in ink-bottle neck pores of diverse diameters. Investigations indicate that the gas density profiles across these pores reveal that density of adsorbed phase is 1.85 –2.5 times lower than that of the bulk methane considering only molecular diffusion constraints. These investigations create a new paradigm in a pore volumetric adjustment in particular to gas transportation in bituminous coals. At an outset, employing the typical parametric values, we repeated the evaluation for various bituminous samples and asserted that 16-20% decrease in the estimation of adsorbed/free gas sorption by volumetric measurements. A significant proportion of mineral material is abstracted by the adsorbed phase which is proved with multifractal characteristics of coal pore geometries and capillaries which is disregarded in sorbed volume consumption, unintentionally overestimating the gas producibility. This methodology can be adopted for evaluating the unconventional resource producibility for various basins in compliance to CBM and CO₂-ECBM processes.

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MS14 / 468

Simultaneous Uncertainty Analysis for SCAL Data Interpretation

Author: Omidreza Amrollahinasab¹

Co-authors: Siroos AzizMohammadi¹; Holger Ott¹

¹ *Montanuniversität Leoben*

Corresponding Authors: holger.ott@unileoben.ac.at, omidreza.ir@gmail.com, siroos.azizmohammadi@unileoben.ac.at

Relative permeability and capillary pressure saturation functions are key uncertainties to characterize multiphase flow in porous media. Therefore, typically a lot of resources are spent on measuring these key functions for various operations. Despite the effort and time, it is not yet common practice to forward simulate or numerically match SCAL data to reliably extract relative permeability and capillary pressure with a realistic estimation of the errors. In this paper, we present a MATLAB-MRST based SCAL interpretation tool for simultaneous history matching and uncertainty analysis of SCAL data sets from different experiments using Markov chain Monte Carlo (MCMC) methods. We focus on the most common and difficult to interpret experimental methods namely steady state and unsteady state relative permeability, and centrifuge capillary pressure experiments. The simulator was benchmarked against a synthetic dataset and applied to a comprehensive SCAL data set of primary drainage in a carbonate rock type. We propose a point-by-point construction of the saturation functions to overcome the limitations of the saturation function parametrizations (e.g., Corey) and deliver a more comprehensive sensitivity and uncertainty analysis. The reliability of the interpretation is assessed by a variation of the experimental samples, and then analyzing how the interpretation of the SCAL datasets fits into the results. Thereby, we attach importance to the uncertainty analysis, which is important for an honest evaluation of the reservoir performance.

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Poster / 469

Montecarlo simulations of gas transportation in multifractal shale reservoirs

Authors: Paul Naveen¹; Debjeet Mondal²

¹ *Pandit Deendayal Energy University Gandhinagar*

² *Central Mine Planning and Design Institute Limited*

Corresponding Authors: debjeet.mandal@coalindia.in, paul.naveen@spt.pdpu.ac.in

The oil or gas producing shales are ultra-tight source rock predominantly containing organic rich consolidated formation of clay-sized particles. The clay content severely limits the fluid flow within the shale matrix. It is, therefore, necessary to understand the organic content, level of thermal

maturity, mineral composition, natural fractures, shale porosity, pore structure and permeability, adsorption characteristics to determine production potential potentiality of undiscovered shale resources. Shale reservoirs are multiscale pore structures because of which exactly predict of the fluid flow mechanisms through the medium, the governing factor to exploit the resource become highly challenging. In this work, we have made an attempt to study the shale fractals, which describe the pore distribution and implemented the Monte Carlo technique to predict the rarefied fluid flow through the shale formation. A probabilistic model is developed by analysing various parameters which intervene in the fluid flow during dynamic conditions. Each parameter's respective impact of risk and uncertainty in prediction and forecasting models are thoroughly evaluated. In addition, fluid flow at insitu conditions is characterised by solving partial order differential equations viz., unsteady-state flow equation for slightly compressible fluids. By examining the sensitivity analyses for the influential parameters, the model is more optimised to obtain more certainty in evaluating the shale reservoirs.

Evaluating and predicting the accurate fluid flow heuristics for various shale samples at laboratory scale becomes increasingly exorbitant due to long lab hours and experimental errors. Computational approach finds its advantages if it captures the variability and complexity of the flow controlling constraints in shale porous media. Though researchers have worked in illustrating the flow mechanisms adopting effective medium theory, stochastic approach, however it is still persisting to be the arduous task to characterise the surface irregularities and microstructure heterogeneities in the shales. Hybrid of fractal analyses and montecarlo simulation considering microstructure scaling lacunarity provides an effective way to characterize the complex pore structures in shale and can bridge microscale structures and macroscale transport properties. The developed probabilistic model analyses various parameters which intervene in the fluid flow during dynamic conditions. Each parameter's respective impact of risk and uncertainty in prediction and forecasting models are thoroughly evaluated. In addition, fluid flow at insitu conditions is characterised by solving partial order differential equations viz., unsteady-state flow equation for slightly compressible fluids. By examining the sensitivity analyses for the influential parameters, the model is more optimised to obtain more certainty in evaluating the shale reservoirs.

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MS15 / 470

Improving the Performance of Reactive Transport Simulations using Artificial Neural Networks

Authors: Ersan Demirer¹; Emilie Coene²; Aitor Iraola Galarza¹; Albert Nardi³; Elena Abarca³; Andrés Idiart¹; Giorgio de Paola⁴; Noelia Rodríguez-Morillas⁴

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Reactive transport models (RTM), which couple geochemical reactions with solute, water and heat transport, are extensively used in a broad range of geoscientific applications related to e.g. Oil & Gas, Carbon Capture & Storage, Mining and Nuclear Waste Management. Despite being powerful tools, RTM often require significantly large computational times, which means that massively parallel high-performance computing equipment and codes are needed for direct numerical solutions in realistic applications. Thus, increasing efforts are currently being made to improve the computational performance of available reactive transport codes. In this contribution, we present a modelling framework using Artificial Neural Networks (ANN) that provides a substantial reduction of the computational burden of reactive transport simulations.

Typical reactive transport simulations involve recursive calculations of chemical reactions at each element and time step of the spatio-temporal discretization of the model domain. These calculations, which might be considerably slow, are sometimes redundant as they might be based on a very similar set of input values. In this work, an ANN is trained to calculate calcite replacement by dolomite with data obtained with PhreeqC, a widely used geochemical simulator. Several training strategies are tested to obtain the best trained ANN. It is shown that the ANN, if trained correctly, can provide considerable accuracy, typically in the range of tolerances required by RTM, and dramatically improves the performance of chemical calculations.

Subsequently, we use the trained ANN in conjunction with Comsol Multiphysics to carry out reactive transport simulations in a three-dimensional highly coupled system: the hydrothermal dolomitization of a fractured carbonate reservoir 1. This realistic test case is used to evaluate the performance of the proposed modelling tool in comparison with that of a more traditional reactive transport code. The overall conclusion of this study is that the Machine Learning approach presented here results in a speed up of one order of magnitude as compared to traditional reactive transport, while providing accurate results. This makes the proposed algorithm potentially appealing for the simulation of large-scale complex geochemical systems.

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References:

1 Abarca, E., Idiart, A., Grandia, F., Rodríguez-Morillas, N., Pellán, C., Zen, M., Ait-Ettajer, T., & Fontanelli, L. (2019). 3D reactive transport modeling of porosity evolution in a carbonate reservoir through dolomitization. *Chemical Geology* 513, 184–199.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS19 / 471

Pore-network modeling of the two-phase flow and transport in the MPL-GDL double layer: model validation and exploration of

optimal pore structures

Authors: Wenqian Zhang¹; Sidian Chen¹; John Xu^{None}; Chao-Zhong Qin²; Bo Guo¹

¹ *University of Arizona*

² *Chongqing University*

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Proton exchange membrane fuel cells are promising energy devices that involve complex two-phase flow and transport in multiple porous layers. During fuel cell operation, oxygen in the flow channel diffuses through a porous cathode gas diffusion layer (GDL) and a microporous layer (MPL) to the catalyst layer, where the oxygen reduction reaction takes place. The water generated via oxygen reduction reaction is then drained out through the MPL-GDL in the other direction. Water flooding—a problem that commonly occurs in fuel cells—impedes oxygen transport and limits the cell's current density. Therefore, how to better manage water in the MPL-GDL double layer to achieve a greater oxygen diffusivity becomes a critical issue. However, the primary factors controlling the two-phase flow and transport dynamics in the MPL-GDL especially regarding the main features of an optimal pore structure of MPL remain not understood.

To address this knowledge gap, we develop a pore-network modeling framework to represent the two-phase flow and transport—including both liquid water percolation and oxygen diffusion—in the MPL-GDL double layer. We employ water percolation and flow-through experiments conducted on multiple MPL-GDL products to validate our numerical simulations covering a wide range of pore structures and experimental conditions. Using the validated pore-network model, we then conduct a set of comprehensive numerical experiments to evaluate performance of different pore structures of the MPL with a focus on improving water management and oxygen transport in the MPL-GDL double layer.

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Poster / 472

Digital Rock Physics as a Tool for Upscaling Cores Petrophysical Properties from Pore to Continuum Scale

Authors: Mohamed Mahrous¹; Enzo Curti¹; Sergey Churakov¹; Nikolaos Prasianakis¹

¹ *Paul Scherrer Institute*

Corresponding Authors: nikolaos.prasianakis@psi.ch, sergey.churakov@psi.ch, enzo.curti@psi.ch, m.mahrous91@gmail.com

Reactive transport modeling is a powerful numerical tool to assess the spatiotemporal evolution of chemical reactions occurring in porous media across different scales (pore, core, and field scales). The geostatistical information required to initialize the petrophysical fields for core-scale reactive transport modeling is often missing and thus need to be assumed. The objective of this work is to acquire geostatistical information for Indiana limestones cores. This is done using digital rock physics, as follows; First, the whole-core porosity and permeability of 8 Indiana limestone cores (cm-scale) were measured in the laboratory. The cores were then scanned using micro-Computed Tomography (μ CT). From the resulting 3D reconstructions (shown in figure 1), a Representative Elementary Volume (REV) analysis was performed to determine the minimum representative grid cell size within the core. Then, the 3D reconstructions were divided into grid cells of REV size. On each of the discretized grid cells, pore scale 3D calculations were performed at the micrometer scale to compute the rock petrophysical properties which are relevant to reactive transport modeling, namely, porosity, permeability, and reactive surface area (shown in figure 2). The frequency distributions of each property, as well as the porosity-permeability and the porosity-reactive surface area relationships, were plotted and approximated with empirical relationships. Also, the petrophysical properties spatial correlation model is found, and the correlation lengths are calculated. The results obtained aim at reducing the uncertainties associated with petrophysical initialization of core-scale reactive transport simulations of carbonate rocks in general, and Indiana limestones in particular. This work also highlights the application of Digital Rock Physics as a promising tool to bridge the gap between pore-scale and continuum-scale simulations.

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Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS11 / 473

On the Challenges of Pore Scale Models to Capture Minerals Precipitation and Dissolution in microfluidic setups: A Combined Computational-Lab-on-a-Chip Approach

Authors: Mohamed Mahrous¹; Jenna Poonoosamy²; Enzo Curti¹; Sergey Churakov¹; Nikolaos Prasianakis¹

¹ Paul Scherrer Institute

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Minerals precipitation and dissolution dominate and control a large number of geochemical processes in porous media. The precipitation/dissolution reactions alter the pore space and its connectivity in a way that has a complex feedback on the solutes transport. Pore-scale reactive transport

models provide the numerical framework to understand and predict such interactions. While incorporation of minerals dissolution into pore-scale reactive transport models has been extensively studied in the past¹, incorporation of minerals precipitation is still scarce and lacks experimental validation^[2]. This can be explained by the fact that precipitation is more fundamentally complex process compared to dissolution. Precipitation involves creation of a new mineral phase via nucleation, which is a purely molecular phenomenon occurring at a scale much smaller than the pore-level resolution. This in turn represents a challenge for pore scale models to accurately predict minerals precipitation, and more investigations are still needed.

In this work, we investigate mineral precipitation processes by combining lab-on-a-chip experimental investigations with pore-scale modeling. The experiments are a set of microfluidics in which Celestine mineral precipitate^[3]. The computational model is a pore-scale multi-component model incorporating fluid flow, solutes transport, aqueous speciation, nucleation modelled at a sub-voxel level, and crystals growth and dissolution. In the developed model, the Lattice Boltzmann Method (LBM) was used to model fluid flow and solute transport, while the nucleation effects are incorporated using the classical nucleation theory, and chemical reactions were modeled using the Law of Mass Action (LMA). Coupling between the chemical reactions and solutes transport is done using a sequential non-iterative approach (SNIA). Reactive transport simulations were accelerated using machine learning techniques ^[4]. During the experiments, the spatiotemporal evolution of the precipitating/dissolving crystals were monitored using optical microscopy. This allowed direct comparison between the modeling and the experimental results in the following aspects: induction time, location of the first crystallite, crystal shape, crystal orientation, and crystal growth/dissolution rates. Our results highlight that computational and experimental microfluidics is a promising tool to unravel the coupled physiochemical processes occurring in geological porous media. Several experimental observations were successfully reproduced such as the flow and concentration fields, precipitation induction times, and reaction rate at crystal-fluid interfaces. However, it still remains challenging to predict the exact location of the first crystallite and the number of critical nuclei which will form into crystals.

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References:

- 1 Molins, Sergi, et al. "Simulation of mineral dissolution at the pore scale with evolving fluid-solid interfaces: Review of approaches and benchmark problem set." *Computational Geosciences* (2020): 1-34.
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS10 / 474

Novel maximum entropy algorithm for multiscale pore network reconstruction and extension.

Authors: Rustem Sirazov¹; Aleksey Khlyupin²; Kirill Gerke³; Aleksei Samarin⁴

¹ *Shmidt Institute of Physics of the Earth (UIPE RAS)*

² *Moscow Institute of Physics and Technology*

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Macroscopic porous materials properties depend on a number of porous media parameters such as porosity, connectivity, pore and throat size distributions, etc. Pore Network Models (PNM) provide a fast and convenient way to estimate those macroscopic parameters by representing a porous medium as a graph [1]. Classical Pore Network extraction methods in literature represent obtaining pore network structure directly from the three-dimensional micro-CT image of porous media. This approach works well on small-scale geometries with a fast increase of required computational power for larger scales. That is where probabilistic models of Pore Network generation are the main tool used [2]. Those methods lose some important information about restored pore space structure. The difference in internal porous media structure at the same time can drastically change macroscopic porous materials properties such as permeability tensor of a sample.

A new approach to generating complex point structures is inspired by recent advances in gradient descent methods for maximum entropy models [3]. Using this approach, we can preserve information about pore location patterns and the relative position of different pores in this pattern. Using an advanced interpore connection generation algorithm allows us to restore information about the relationship between different pore scales.

The main goal of the work is to build a fast reliable method to generate a statistical pore network. One of the main features of the proposed algorithm is the ability to increase the analyzed sample size based on statistical features of a smaller sample (pore network extension). We reconstruct samples of carbonate, sandstone, and ceramics from PNM extracted from micro-CT images and compare statistical and hydrodynamic properties for original PNM and reconstruction. Comparison of our state-of-the-art algorithm with classical algorithms [1,4,5,6] shows a noticeable improvement in reconstruction accuracy in the number of porous media.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS09 / 475

Investigating compressible gas flow through porous media considering the choked condition and shockwave formation for Pulse-Pressure Decay test: A Computational Fluid Dynamics (CFD) approach

Authors: Ali Nabizadeh¹; Jingsheng Ma²; Steven McDougall²

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It is well known that when compressible gas expands through a porous system, the flow may be choked at geometrically constricted paths, to limit mass flow rate if inlet and outlet pressure ratio exceeds a critical gas-specific limit, while induces shockwaves along with sharp variations in fluid thermophysical properties. Modelling such flow behaviours and their impacts in time on a porous system is challenging but necessary to design short and long-term operations for geo-energy engineering such as hydrogen storage and carbon capture and storage.

In this work, we model transient flow behaviours of compressible gas in a system which comprises three sequentially connected components: an upstream gas reservoir, a cylindrical pore channel with a throat-forming uniformly wavy radius profile, and a downstream reservoir. Higher pressured gas expands from the upstream reservoir through the channel into the downstream reservoir. The latter two are initialised with the same and lower pressure. This mimics the well-known Pressure Pulse Decay (PPD) setup, for measuring the permeability of tight porous samples containing fractures. We investigate flow choking and shockwaves occurrences across the channel along the time till the upstream and downstream pressure difference is small, for several configurations of initial upstream and downstream pressures and channel radius profiles.

We examined the changes of Mach number and pressures at time and found that choking and shockwaves occur prominently at an early time for cases where the initial pressure difference is large. The Mach number and pressure magnitudes decrease with the decrease of pressure difference. For some cases, the Mach number, at the furthest downstream throat, rather unexpectedly, remains above one even when the pressure difference is always diminishing. In addition, the impact of the choking on the pressure decay of the upstream reservoir and pressure build-up at the downstream is being analysed against counterpart cases where a wavy channel is replaced with a straight channel with an equivalent radius. The results of this work will be reported.

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Time Block B (14:00-17:00 CET)

Participation:

Online

MS01 / 476

Supercritical Adsorption of CO₂ and CH₄ on Shales and Surrogate Porous Media

Author: Humera Ansari^{None}**Co-authors:** JP Martin Trusler¹; Geoffrey Maitland¹; Ronny Pini¹¹ Imperial College London**Corresponding Authors:** g.maitland@imperial.ac.uk, r.pini@imperial.ac.uk, m.trusler@imperial.ac.uk, hsa210@ic.ac.uk

Low natural gas recovery factors from shale reservoirs have stimulated interest in Enhanced Shale Gas Recovery (ESGR) using CO₂ injection. This process seeks to exploit the preferential adsorption of CO₂ in shale's nanometric pores, so as to enhance desorption of CH₄ and to promote geological sequestration of CO₂. To facilitate the design of this process, an integrated experimental and modelling workflow was developed and deployed on shale samples from the Longmaxi (China), Marcellus (USA) and Bowland (UK) formations to achieve the following: (i) high-resolution textural characterisation, (ii) supercritical adsorption measurements with CO₂ and CH₄, and (iii) their description by a novel mathematical model that predicts adsorption in chemically and morphologically heterogeneous materials. The results show that CO₂ adsorbs more than CH₄ at all pressures (2–3 times) and that both adsorption capacities and textural properties are strongly influenced by the shale mineralogy. The model developed in this work is based on the lattice Density Functional Theory and describes adsorption systems featuring both slit and cylindrical pores and accounts for the presence of energetically distinct organic- and clay-rich pore surfaces. The workflow was calibrated on three model adsorbents (micro/mesoporous carbon 1 and source clays [2]) that have been used in this study as surrogates for the organic- and clay-rich fractions of shale, respectively. As such, the model is used in a predictive fashion to describe supercritical adsorption, only requiring knowledge of the shale's composition. The adsorption data have been used as input to an equilibrium-based ESGR proxy reservoir model, which uses the concept of Pressure Swing Adsorption, and was deployed to demonstrate that a cyclic CO₂ injection operation, including three stages (Injection/Soak/Production), may be required to achieve sufficient recovery and secure CO₂ storage [3]. The results indicate that competitive adsorption and partial pressure both influence enhanced recovery and reveal a trade-off between CH₄ production and CO₂ sequestration. The practical workflow presented in this work can be used to quantify accurately the Gas-in-Place and CO₂ storage potential of shale reservoirs at subsurface conditions and design an optimal CO₂-ESGR process.

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References:

1 H. Ansari, L. Joss, J. Hwang, JPM. Trusler, G. Maitland, R. Pini, *Microporous and Mesoporous Materials*. 308 (2020) 110537.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS01 / 478

Coupled Geochemical-geomechanical Processes in CO₂ Storage Reservoirs

Authors: Zhuofan Shi¹; Lauren Beckingham¹; Jack Montgomery¹; Charlotte Garing²

¹ *Auburn University*

² *University of Georgia*

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Geologic CO₂ sequestration is a promising means of reducing atmospheric CO₂ emissions. At the interface between the scCO₂ and formation brine, CO₂ will dissolve into formation brine, lowering formation pH and creating conditions favorable for mineral reactions. These reactions may alter the porosity, permeability, and stiffness of the formation, impacting injectivity and reservoir security. However, the rate, extent, and impacts of mineral trapping on formation properties is not well understood. The objectives of this work are to experimentally measure mineral dissolution rates and changes in porosity, permeability, and stiffness in core samples mimicking CO₂ sequestration systems. We conducted core flood experiments in a custom-built triaxial core holder with in-situ acoustic measurement capabilities at temperature of 50 °C and pressure of 100 bar. Representative reservoir rocks, here sandstone samples with high porosity and permeability, were tested in this study. During the experiments, the aqueous effluent samples were periodically collected, and their composition were measured using ICP-MS. Ion concentrations were used to infer column scale mineral dissolution rates and the evolution of mineral volume fractions. The pressure at the core inlet and outlet were continuously monitored and used to infer changes in the permeability of the core sample as reactions progress. Changes in the material stiffness was measured using acoustic wave velocities. These changes in stiffness can be correlated to changes in the mineral volume fractions and degradation of sample cementation. Before and after the experiments, 3D images of the core samples were captured via X-ray Computed Tomography to determine the changes in porosity. Reactive transport and geomechanical simulations were developed based on the experimental system. Reactive transport simulations were performed to seek to match the observed ion concentrations. Geomechanical simulations were performed to examine the effects of changes in the mineral volume fractions on the material stiffness and compare these with the measured changes from the experiments.

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Time Block C (18:00-21:00 CET)

Participation:

Online

MS06-B / 479

Numerical Simulation of Multi-phase Flow in Porous Media with a Phase-field Method

Authors: Lukas Maier¹; Manuel Hopp-Hirschler¹; Ulrich Nieken¹¹ *Institute of Chemical Process Engineering, University of Stuttgart***Corresponding Authors:** manuel.hopp-hirschler@icvt.uni-stuttgart.de, ulrich.nieken@icvt.uni-stuttgart.de, lukas.maier@icvt.uni-stuttgart.de

Multiphase flows in porous media are central to many applications in the chemical industry, such as coating, infiltration of resin in composites, and reactive gas-liquid flows in gas diffusion electrodes. To improve these processes, a deep understanding of flow phenomena is crucial. Therefore, detailed simulation of multiphase flows is of great importance.

In this contribution, we present a Cahn-Hilliard phase field model coupled with the Navier-Stokes equation to simulate two-phase flow. This relatively new approach is characterized by a diffusive representation of the interface. Because of the diffusive interface, it is possible to use continuum mechanics methods with Eulerian formulation to simulate the interfacial flow without explicitly tracking the interface, making the model suitable for a wide range of software.

The focus of this contribution is on the validation and application of the phase field model in context of multi phase flow in porous media. Comparisons with experiments are rare and usually involve steady-state or very simple interfacial phenomena. In addition to some basic wetting phenomena, such as capillary rise in a thin channel and the spreading of a droplet on a flat surface, we compare our simulation with an experimental dynamic drainage process in a micromodel [2]. The capillary finger formation observed in the experiment is very well reproduced by our simulation. This shows the great potential of the method for modeling multiphase flows in porous media.

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References:

- 1 Jacqmin, D. (1999). Calculation of Two-Phase Navier–Stokes Flows Using Phase-Field Modeling. *Journal of Computational Physics*, 155(1), 96–127. <https://doi.org/10.1006/JCPH.1999.6332>
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 480

Groundwater contamination in the north-east of the UK: Exploring and projecting pollution trends using the Environment Agency data archives

Author: Nouha Samlani¹

Co-authors: Akanji Lateef²; Zia Ush Shamszaman¹; Tannaz Pak¹

¹ Teesside University

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In England and Wales, groundwater provides around a third of public water sources (British Geological Survey, 1998). However, the intense industrialised past of the country has caused significant pollution in some of its important aquifers. The northeast area of England, where groundwater contribution is estimated to be 20% to public supply per region (British Geological Survey, 2019), stands out as one of the most industrialised areas in England. Indeed, the area hosts a multitude of eventual pollution sources such as metallurgical industries, closed coal mines and agricultural fields.

Since the 1974 Water Act, a particular focus has been put on groundwater quality degradation and the risk of pollution (Downing, 1993). In this context, a water quality archive published by the Environmental Agency of the UK presents a regular record of a wide range of parameters from physico-chemical parameters to organic and inorganic pollutants, monitored in millions of sampling points in groundwater and rivers, ponds, or sewage discharges. It is, therefore, a rich source of data to characterise and describe the evolution of different kinds of pollutants across England. However, just a few studies have investigated specific pollution risks based on this dataset and almost all of them are limited to surface water.

To fill this gap, we characterize the present state of pollution in this study and evaluate future quality trends in the groundwater of the northeast of England (Northumbria and Yorkshire). Analysing the two-decade-long open-access part of this dataset can shed light on major pollutants affecting the region's aquifers. Furthermore, hotspots and critical areas will be identified in a tentative way to understand the origins and extent of the contamination deploying spatial statistics.

In order to go beyond traditional analytics consisting of just the description and diagnosis, deep learning algorithms fed with more than 2500 samples per parameter are deployed for predictive analysis. This will in turn allow the generation of new insights concerning the evolution and the fate of pollutants in the areas of interest.

To conclude, this work, on the one hand, updates the state of groundwaters within the northeast of England; on the other hand, it demonstrates the use of machine learning in groundwater management, particularly groundwater quality monitoring.

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References:

Downing, R. A. (1993). Groundwater resources, their development and management in the UK: a historical perspective. *Quarterly Journal of Engineering Geology and Hydrogeology*, 26(4), 335–358. <https://doi.org/10.1144/GSL.QJEGH.1993.026.004.09>

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS18 / 481

Long-term retention and leaching of PFAS in the vadose zone: controlling processes, mathematical formulation, and practical modeling approaches

Author: Bo Guo¹

¹ *University of Arizona*

Corresponding Author: boguo@arizona.edu

PFAS are emergent contaminants of which the fate and transport in the environment remain poorly understood. A growing body of site investigations have demonstrated that vadose zones serve as significant long-term sources of PFAS to contaminate groundwater. Quantifying PFAS leaching in the vadose zone and mass discharge to groundwater is therefore critical for characterizing, managing, and mitigating long-term contamination risks. As surfactants, adsorption at air–water and solid–water interfaces leads to complex retention of PFAS in soils. These interfacial behaviors depend strongly on the chemical properties of PFAS such as chain length and functional groups. Concomitantly, PFAS present in pore water can modify surface tension and in turn impact variably saturated flow, which further complicates the fate and transport of PFAS in the vadose zone.

In this talk, I will give an overview of our recent mathematical and numerical modeling studies that aim to understand and quantify the primary processes that control the long-term leaching of PFAS. A few years ago, we have developed a full-process mathematical model that represents a set of PFAS-specific transport processes including concentration-dependent capillary pressure, and rate-limited and nonlinear adsorption at the air–water and solid–water interfaces. The full-process model has been employed to quantify the impact of a variety of factors on long-term PFAS leaching in the vadose zone including surfactant-induced flow, rate-limited and nonlinear air-water interfacial adsorption, PFAS chain length and functional group, pore water chemistry, and subsurface heterogeneity. Insights from the comprehensive analyses then allow us to develop a simplified model with a focus on the primary processes that dominantly control PFAS leaching. We derive new analytical solutions for the simplified model and validate them by application to miscible-displacement experiments under a wide range of conditions and by comparisons to the full-process model under both experimental and field conditions applicable to PFAS-contamination sites. Overall, the simplified analytical model appears to provide an efficient and accurate screening-type tool for quantifying long-term PFAS leaching in the vadose zone.

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References:

Guo, B., Zeng, J. and Brusseau, M.L., 2020. A Mathematical Model for the Release, Transport, and Retention of Per- and Polyfluoroalkyl Substances (PFAS) in the Vadose Zone. *Water resources research*, 56(2), p.e2019WR026667.

Zeng, J. and Guo, B., 2021. Multidimensional simulation of PFAS transport and leaching in the vadose zone: Impact of surfactant-induced flow and subsurface heterogeneities. *Advances in Water Resources*, 155, p.104015.

Zeng, J., Brusseau, M.L. and Guo, B., 2021. Model validation and analyses of parameter sensitivity and uncertainty for modeling long-term retention and leaching of PFAS in the vadose zone. *Journal of Hydrology*, 603, p.127172.

Guo, B., Zeng, J., Brusseau, M.L. and Zhang, Y., 2022. A screening model for quantifying PFAS leaching in the vadose zone and mass discharge to groundwater. *Advances in Water Resources*, p.104102.

Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS05 / 482

A novel platform for monitoring and imaging bacterial biofilm growth in complex structures

Authors: Christos Papadopoulos¹; Laurent Malaquin²; Julie Foncy³; Yohan Davit¹

¹ *Institut de Mécanique des Fluides de Toulouse (IMFT), Université de Toulouse, CNRS, 31400 Toulouse, France*

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Biofilms are complex microbial communities that grow primarily on solid surfaces where the microorganisms are nested in a self-secreted polymer matrix. Recent experimental studies have aimed at understanding the mechanisms that control the development of biofilms in porous media, including architectural plasticity [1], ecological interactions in connected structures [2] or bio-clogging [3]. These mechanisms cannot be easily studied due to the structural complexity and the opacity of the 3D porous structure but also due to the multiplicity of coupled factors that control biofilm, such as nutrient/oxygen availability, flow rate, communications and shear stress [4]. Improved quantification of the physical aspects of biofilm growth is essential in unravelling the mechanisms of biofilm formation in porous materials and progress towards new biotechnologies.

In order to get an insight into how fluid flow, transport phenomena and biofilms interact within heterogeneous structures, we have devised a versatile, micro-scale, 3D-printed micro-bioreactor for the precise measurement of several parameters of such systems that would allow for controlled and reproducible studies of biofilms in 3D porous systems. We have also developed a novel approach to 3D imaging of biofilms in such systems using X-ray micro-tomography using functionalized gold nanoparticles as a contrast agent.

Preliminary results of *P. aeruginosa* biofilm development at room temperature show a permanent regime after about 3 days with persistent temporal fluctuations in the pressure drop and oxygen consumption. This suggests that biofilm growth in porous media under flow is a dynamic process resulting from an equilibrium between competing mechanisms such as bacterial growth and biofilm detachment due to hydrodynamic stresses. This is confirmed by direct optical absorption measurements of the biofilm detachment events at the outlet of the bioreactor. Complementary to the biofilm development measurements, the x-ray tomography scans showed that the spatial distribution of biofilm within the porous medium is heterogeneous, with most of the biomass being concentrated at the inlet of the bioreactor and regions within the porous medium that are completely inaccessible to the main flow due to pore clogging.

Our experimental setup, with the 3D-printed micro-bioreactor being in the heart of it, provides an adjustable, versatile experimental workbench for the study of the growth and detachment dynamics of biofilms in porous media under controlled conditions over long periods of time. The combination with X-ray tomography imaging provided an insight on how physical (flowrate, shear stress) and chemical (oxygen, nutrient availability) parameters of the system affect the biofilm's spatial distribution. A better understanding of biofilm growth dynamics in the mesoscale could potentially unlock novel biotechnologies [5,6].

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References:

- (1) Coyte, K. Z.; Tabuteau, H.; Gaffney, E. A.; Foster, K. R.; Durham, W. M. Microbial Competition in Porous Environments Can Select against Rapid Biofilm Growth. *Proc. Natl. Acad. Sci.* 2017, 114 (2), E161–E170. <https://doi.org/10.1073/pnas.1525228113>.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS02 / 483

Modeling colloid remobilization during temporal variation in ionic strength in porous media

Author: Sai Rama Krishna Yerramilli¹

Co-author: Seetha N¹

¹ *Indian Institute of Technology Hyderabad*

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Infiltration of surface water into the subsurface through rainfall events and irrigation activities causes temporal variability in the groundwater flow and chemistry. As a result, the colloids that were previously deposited onto the grain surfaces get remobilized thereby causing recontamination

of groundwater. Understanding colloid remobilization during perturbations in flow and chemistry is essential to estimate the travel distances of colloidal contaminants and to protect drinking water wells from contamination. In this study, laboratory soil column experiments were performed to understand the effect of temporal variation of ionic strength on colloid release in saturated porous media. The deposited colloids were remobilized through a step-decrease in ionic strength. Colloid release was observed only when the ionic strength became smaller than a critical concentration. Colloid release curves exhibited sharp peaks followed by extended tailing. A one-dimensional mathematical model accounting for ionic strength-dependent release was found to fit the observed breakthrough curves reasonably well.

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MS07 / 484

Thermodynamics-Informed Neural Network for Phase Equilibrium in Subsurface Reservoirs

Authors: tao zhang¹; Shuyu Sun²

¹ King Abdullah University of Science and Technology

² King Abdullah University of Science and Technology (KAUST)

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Multi-phase multi-component flows are the key problems needing to be solved in the study of subsurface geological formation and fluid flows, which are essentially required in the understanding and description of complicated heat and mass transfer behaviors commonly seen in oil and gas reservoirs. A large number of chemical species have been detected in the reservoir fluids, which challenges the conventional computational multi-phase fluid dynamic simulation using empirical formulas. The number of phases existing in the fluid mixture, as well as the phase partitioning information of each component, play an important role in the multi-component multi-phase model and simulation to keep the thermodynamic consistency and physical meaningfulness. Flash calculation, the main approach to obtain these information, including overall density, chemical composition and the total phase numbers at equilibrium, has shown its inevitability in energy discovery and recovery, especially when the concept of Enhanced Oil Recovery (EOR) is discussed. Recently we demonstrated that the deep neural network models, while preserving high accuracy, are more than two hundred times faster than the conventional flash algorithms for multicomponent mixtures. Previous machine learning methods assume a fixed number of components in the fluid mixture, which makes such models to have very limited practical usefulness. In this work, we propose to develop self-adaptive deep learning methods for general flash calculations, which can automatically determine the total number of phases existing in the multicomponent fluid mixture and related thermodynamic properties at equilibrium. Our preliminary work showed that, for example, the deep learning model with the

8-component Eagle Ford oil flash calculation results as training data accurately predicts the phase equilibrium properties of a 14-component Eagle Ford fluid mixture.

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MS06-A / 485

Dynamic Behaviours of Foam Flooding assisted by Newtonian and non-Newtonian Viscosifying Agents in Porous Media

Authors: Seyed Mojtaba Hosseini-Nasab¹; Martin Taal²; Mohammad Rezaee³; Pacelli Zitha⁴

¹ School of Chemical, Oil and Gas Engineering

² Flour Company, Amsterdam

³ Amirkabir University of Technology, Department of Petroleum Engineering

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One of the main reasons for Enhanced Oil Recovery (EOR) are that to mobilize oil left in the reservoir after primary recovery (depletion by pressure difference solely) and water flooding. However, it might be necessary to expand the infrastructure for certain EOR projects as more wells are required or a different well pattern is necessary. The objective of this study is to investigate the generation and stability of foam generated by Newtonian and non-Newtonian viscosifying agents. The shear rate inside the core was calculated based on literature, which was combined with viscometric measurements in order to form four pairs of equal apparent viscosity. These four pairs then were the subject of core flood experiments. The differences and overlap within the core flooding experiments with foam generated by Newtonian and non-Newtonian fluids were observed, by examining the mobility reduction factor in transient and steady-state conditions as well as by calculation of the gas fraction present in the core. The main conclusion is that glycerol can be used in core flood experiments and reach the same mobility reduction factor as polymer solutions with the same apparent viscosity, as long as the viscosity of the injected solution is reasonably low. Furthermore, it even showed to reach the maximum mobility reduction factor faster than the foam generated by polymer solution. However, for more viscous solutions with higher glycerol concentrations strong foam could not be generated in these series of experiments which shows an advantage of polymer over glycerol.

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MS15 / 486

A Full Order, Reduced Order and Machine Learning Model Pipeline for Efficient Prediction of Reactive Flows

Author: Oleg Iliev¹

¹ *Fraunhofer ITWM*

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This is a joint work with P. Gavrilenko, D.Fokina, P. Toktaliev (Fraunhofer ITWM), M. Ohlberger, F. Schindler (University of Muenster), B. Haasdonk, T. Wenzel, M. Youssef (University of Stuttgart) and I.Oseledets (Skoltech).

Reactive transport in porous media in connection with catalytic reactions is the basis for many industrial processes and systems, such as fuel cells, photovoltaic cells or catalytic filters. The modeling and simulation of the processes can help in optimizing the design of catalytic components, parameter identification, development of digital twins, etc., but is currently limited by the fact that such simulations lead to large amounts of data, are time-consuming and depend on a large number of parameters. The development of solution approaches for the prediction of the chemical conversion rate using modern data-based methods is essential in order to achieve fast, reliable predictive models. Various method classes are required for this. In addition to the experimental data, fully resolved simulations are necessary. It is important to note that while the reactions occur at microscale, the observations are usually carried out at macroscale. The simulations at microscale are usually too expensive to generate a large set of training data. Therefore, model order reduction is crucial for acceleration as it can produce large amounts of training data. In this talk projection based model order reduction of pore scale linear reactive flow with different flow regimes, is considered. Advection-diffusion-reaction problem for a concentration c is considered, with appropriate initial and boundary conditions, for varying flow fields u as well as Damkholer and Peclet numbers $Da, Pe > 0$. While the approximation by discretization schemes and model order reduction (by e.g. Reduced Basis methods) of such problems is well understood, the characteristics of the underlying flow, and thus the solution manifold, may differ significantly if Damkhler and Peclet numbers change by several orders of magnitude. We thus consider practical implications of strongly varying Damkhler and Peclet numbers on stable and accurate reduced order models for such problems, which are then used for generating training data within the collaborative BMBF-funded project on Machine Learning and Model Order Reduction to Predict the Efficiency of Catalytic Filters (ML-MORE).

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References:**Time Block Preference:**

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MS09 / 487

An image-based hybrid pore network-continuum modeling framework for fluid flow and transport in multiscale porous media

Authors: Li Zhang¹; Bo Guo¹; Chao-Zhong Qin²; Yongqiang Xiong^{None}¹ *University of Arizona*² *Chongqing University***Corresponding Authors:** lizhang1@email.arizona.edu, boguo@arizona.edu, chaozhong.qin@cqu.edu.cn, xiongyq@gig.ac.cn

Hydrocarbon transport in unconventional reservoir rocks remains poorly understood due to the presence of a wide range of pore sizes (from sub-nanometer to micrometers) and their complex spatial connectivity. In the present work, we combine hyper-resolution imaging techniques and image-based modeling to develop a novel hybrid pore network-continuum modeling framework for the flow and transport processes in the multiscale pore domains. The hybrid framework treats the smaller pores (i.e., pores below the image resolution) as a continuum using models described by the Darcy equation and explicitly represents the flow and transport processes in the larger pores (i.e., pores that are resolved in the images) using a computationally efficient pore network model. We validate the new framework via comparisons to direct numerical simulations (DNS) for several scenarios including steady-state single-phase flow, solute transport, and transient compressible single-phase flow. The results demonstrate that the new hybrid model accurately predicts the overall flow and transport process and the mass transfer between the pore network and the subresolution continuum domains, while being much more computationally efficient than the DNS methods.

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References:Guo, B., Ma, L. and Tchelepi, H.A., 2018. Image-based micro-continuum model for gas flow in organic-rich shale rock. *Advances in Water Resources*, 122, pp.70-84.Guo, B., Mehmani, Y. and Tchelepi, H.A., 2019. Multiscale formulation of pore-scale compressible Darcy-Stokes flow. *Journal of Computational Physics*, 397, p.108849.**Time Block Preference:**

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 488**Adsorption of methylene blue from solution using pomegranate and orange peels powder****Author:** Asma Jedidi^{None}**Co-authors:** Manuel Marcoux ; Sana Dardouri ; Jalila Sghaier**Corresponding Authors:** jed-asma@hotmail.fr, manuel.marcoux@imft.fr, jalila.sghaier@enim.rnu.tn, sanadardouri_en@yahoo.fr

The textile industry is the major source of dyes and generates colored wastewater. Colored dye effluents are generally considered to be toxic to the animal and plant life of a particular region and habitat. Moreover, almost all dyes are poorly biodegradable or resistant to environmental conditions and, therefore, create major problems in the treatment of wastewater stemming from the dyeing industry. In this context, numerous organic sorbents have been introduced in recent years to develop technologies aimed at preventing the pollution of soil and water. This work set out to study and compare the effect on the mobility of MB in a soil mixed with two low-cost organic residues (pomegranate and orange peels powder). The efficiency of pomegranate and orange peels powder as a low-cost adsorbent for removing the cationic dye methylene blue MB from silty soil collected from industrial zones in Tunisia has been investigated using batch mode experiments.

Particle size analysis is an essential phase for specifying samples of the soil studied. This analysis allows the determination of the size distribution and the distribution of the particles. The particle sizes are measured using a Microtrac S3500 laser particle size analyzer at the Center for Research and Energy Technology in Borj Cédria (CRTEN) in Tunisia.

Numerical modelisation were conducted under water unsaturated flow in hand-packed soil columns in which soil mixed with sorbents were incorporated as barriers. The effects of contact time have been studied to understand the adsorption behavior of the adsorbent under various conditions. The kinetic results of adsorption obeyed a pseudo-second order model for all adsorbent used in this study. The results revealed that the adsorption of methylene blue on the soil mixed with pomegranate and orange peels powder is feasible.

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References:**Time Block Preference:**

Time Block A (09:00-12:00 CET)

Participation:

In person

MS06-A / 489

PORE-TO-CORE LINKAGES AND UPSCALING FOR GAS INJECTION (CO₂ STORAGE, EOR) IN CARBONATES

Authors: Sojwal Manoorkar^{None}; Senyou An¹; Samuel Krevor²

¹ *University of Manchester, Imperial College London*

² *Imperial College London*

Corresponding Authors: s.krevor@imperial.ac.uk, senyou.an@manchester.ac.uk, s.manoorkar@imperial.ac.uk

The flow in the subsurface is often dominated by heterogeneities with length scales ranging from micrometres to kilometres. Multiphase fluid flow is traditionally modelled using continuum approaches based on Darcy's law and macroscopic properties such as relative permeability, capillary pressure, and residual trapping. These properties are upscaled manifestations of pore-scale capillary dominated fluid dynamics. The presence of heterogeneities affects the representative elementary volume of the rocks which makes it challenging to model the multiphase flow using a continuum framework. Thus, it is crucial to study the pore-scale dynamics in heterogeneous rocks and incorporate them in reservoir characterization to accurately model flow in subsurface carbonate reservoirs.

In this work, we use steady-state core flooding experiments with micro XCT imaging to study the fundamental questions relating to pore-scale fluid dynamics and their upscaled continuum representation. Mixed-wet carbonates and reservoir rocks with heterogeneities are used for the analysis. Whereas most pore-scale flow experiments are performed on mm-scale cores since larger sample size is required to capture rock heterogeneities. Here we perform core floodings with micro XCT imaging using the largest rock sample size (diameter = 1.2 cm and length = 6 cm) where we can still resolve features of the pore-scale fluid dynamics. Also, the linking scales are considered between the heretofore mm scale domain of X-ray imagery and network models and the cm-m scale domain of conventional core analysis petrophysics.

We analyse the fluid distribution throughout imbibition during low capillary number flows to assess the impact of structural heterogeneities and wetting alteration. We evaluate the length scales of heterogeneity in rock flow properties, like capillary pressure characteristics, alongside length scales of wetting alteration by comparing observations of fluid distribution in the rock before and after wetting alteration with crude oil. We identify correlation lengths for the wetting state in relation to correlation length scales of rock pore structure heterogeneity. These are linked to variation in continuum flow properties (capillary pressure, relative permeability). This provides insight into modelling fluid flow in mixed wet rocks at the core scale.

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Online

MS19 / 490

Investigating the effect of triple-phase boundary in zinc-air cathodes utilizing pore network modeling approach

Authors: Niloo Misaghian¹; Mohammad Amin Sadeghi¹; Edward Roberts²; Jeff Gostick¹

¹ *Department of Chemical Engineering, University of Waterloo*

² *Department of Petroleum and Chemical Engineering, University of Calgary*

Corresponding Authors: jeff.gostick@uwaterloo.ca, amin.sadeghi@uwaterloo.ca, etprober@ucalgary.ca, n2misagh@uwaterloo.ca

Zinc-air flow batteries are energy storage devices that have started to receive attention due to their high energy density, and zinc metal being particularly appealing since it's safe and cost effective. Increasing the performance of these electrochemical devices and their useful life will have a substantial economic and operational impact on the development of energy storage projects. Different factors affect these devices' performance including the structure of their porous air electrode and the transport phenomena within the catalyst layer (CL) where the oxygen reduction reaction (ORR) occurs. The ORR takes place at the interface of three phases: catalyst (solid), electrolyte (liquid), and oxygen (gas), the so-called triple phase boundary (TPB). The extent and distribution of the TPB and the electrolyte invasion pattern throughout the CL affect the transport of reactive species and subsequently the performance of air electrode. Therefore, understanding these parameters is a crucial step towards designing and optimizing the CL structure. To investigate the CL porous structure and the TPB at pore scale, a rigorous pore-scale modeling tool is required. Pore network modeling (PNM) is suitable for such investigations due to its low computational cost compared to other modeling options such as continuum-based models, and direct numerical simulations; and more importantly PNMs can easily capture the detailed information on the electrolyte invasion and TPB extent at pore-scale.

In this work a mathematical framework was developed for PNM of the transport phenomena in the CL of the air electrode. The effects of electrolyte invasion pattern, CL's pore size distribution, and TPB extent on the performance of the air electrode were investigated. The PNM results show that in low to intermediate electrolyte saturation (0.1-0.7) as the electrolyte invasion in the CL proceeds, the TPB extent increases and the electrode performance in terms of peak power increases accordingly. In contrast, at saturations greater than 0.7, further invasion by the electrolyte results in reducing the TPB length and reducing its performance in terms of the generated power.

In practice it is possible to alter the electrolyte invasion pattern and the TPB extent by changing the electrode structure. This idea was explored by changing the pore size distribution of the CL in the PNM. The results showed that a narrow pore size distribution provides a higher performance at low saturations whereas a wide pore size distribution provides a higher performance at higher saturations. Although the developed mathematical framework was implemented on synthetic cubic pore network models, it can be applied on extracted networks for other CL samples.

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References:

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T. G. Tranter et al., "Pore Network Modelling of Capillary Transport and Relative Diffusivity in Gas Diffusion Layers with Patterned Wettability," *J. Electrochem. Soc.*, vol. 167, no. 11, p. 114512, 2020, doi: 10.1149/1945-7111/ab9d61.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Unsure

Poster / 492

A molecular dynamics study on CO₂ enhanced shale gas recovery in kerogen nanopores

Authors: Cheng Chen¹; Jun Xia¹; Hamid Bahai¹

¹ *Brunel University London*

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The injection of supercritical CO₂ into shale gas reservoirs, fracturing the reservoir, enhancing shale gas recovery and achieving CO₂ geological storage, is regarded as an optimum scheme in carbon capture, utilisation and storage (CCUS) due to the distinctive physical properties of supercritical CO₂, e.g. a low viscosity, high diffusion coefficient, high adsorption capacity and zero surface tension. A shale reservoir contains inorganic pores such as clay minerals and organic pores like kerogen, among which the gas adsorption characteristics differ dramatically. A deep understanding of the complex transport mechanism of CO₂-CH₄-moistures in kerogen nanopores with diameters < 10 nm is crucial because of the anomalous diffusion phenomenon and nanoconfinement effects in nanoscale. In this study, molecular dynamics with grand canonical Monte Carlo (GCMC) simulation will be performed to study the competitive adsorption of CO₂ and CH₄ with the presence of moistures in kerogen nanopores. Kerogen nanopores are built with six representative molecular structures of different maturity characterised by O/C and H/C ratios. The effects of the pore networks including porosity, pore size, surface area, connectivity and tortuosity will be quantified.

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Time Block B (14:00-17:00 CET)

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In person

MS14 / 493

Quantification of Heterogeneity of Spatially Averaged Generalized sub-Gaussian Random Fields

Author: Matthew Harrison¹**Co-authors:** Mohaddeseh Mousavi Nezhad²; Thomas Hudson¹; Alberto Guadagnini³; Monica Riva³¹ *University of Warwick*² *Associate Professor*³ *Politecnico di Milano***Corresponding Authors:** m.harrison.2@warwick.ac.uk, alberto.guadagnini@polimi.it, m.mousavi-nezhad@warwick.ac.uk, t.hudson.1@warwick.ac.uk, monica.riva@polimi.it

While Gaussian models have been used to describe spatial heterogeneity of hydro-geological attributes, the Generalized sub-Gaussian (GSG) model introduced by Riva et al. (2015) has been shown to be able to capture heavy tailed marginal distributions and simultaneous leptokurtic scaling of increment distributions of a broad range of hydrogeological variables. In this context, it can be noted that the main statistics characterizing the spatial heterogeneity of a given system attribute such as, e.g., permeability, depend on observation scale. A key parameter of the GSG model is a length scale which is proportional to the size of the volume associated with observations and can be characterized through standard inverse approaches. Here, we investigate the dependence of observation scale of the parameters of the GSG model, with specific focus on the way uncertainty propagates across random fields associated with diverse observation scales. We do so by analytically deriving expressions according to which the variance of a (two- or three-dimensional) GSG random field varies as a function of the degree of spatial averaging. Our formulations enable one to estimate the level of heterogeneity (as quantified through the variance) at a given scale, as a result of averaging from a reference scale. Our analytical findings show that the level of heterogeneity in GSG fields (a Gaussian distribution being a special case thereof) is highest at the finest scale and decays towards zero as we increase the spatial averaging volume. As expected, the field becomes homogeneous at the limit of complete spatial averaging. Our model for variance propagation across averaging scales allows efficient estimation of residual heterogeneity retained at larger length scales, thus being of interest when formulating coarse grained hydro-geological flow models. The model is first verified through comparison with results achieved through a Monte-Carlo numerical analysis and it is then applied to a comprehensive dataset composed of more than 2000 air permeability data collected at various observation scales on the surface of a block of Massilon Sandstone sample.

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References:

Riva, M., Neuman, S. P., & Guadagnini, A. (2015). New scaling model for variables and increments with heavy-tailed distributions. *Water Resources Research*, 51(6), 4623-4634.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

Poster / 494

2D Particle Tracking Velocimetry in Multiphase Flow in Porous Media

Authors: Farzan Kazemifar¹; Jason Wong¹; Mingjia Xu¹

¹ *San Jose State University*

Corresponding Authors: mingjia.xu@sjsu.edu, farzan.kazemifar@sjsu.edu, jason.wong01@sjsu.edu

Flow in porous media is ubiquitous in many engineering and natural systems, many of which occur in the geosphere and are intimately linked to energy, environment, and water resources. Transport phenomena in a porous domain is closely linked to the pore-scale velocity structures, thus an important ingredient in development of transport models is having reliable pore-scale experimental velocity data. Presence of a second immiscible fluid phase in the porous medium can profoundly impact flow and transport phenomena. In this work we present results from 2D particle tracking velocimetry (PTV) experiments of multiphase flow in 2D microfabricated porous media, also known as micromodels. Lagrangian particle trajectories in the continuous flowing phase are obtained and velocity and acceleration statistics are presented. The results highlight the similarities and differences between single and multiphase flow. The implications for transport models are discussed.

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Participation:

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MS09 / 495

Parametric study of coolant-injection flow through different pore geometrical patterns for injection flow control in hypersonic flow

Authors: Adriano Cerminara¹; David Adebayo¹; Ahmad Baroutaji¹; Arun Arjunan¹

¹ *University of Wolverhampton*

Corresponding Authors: d.adebayo@wlv.ac.uk, a.arjunan@wlv.ac.uk, a.baroutaji@wlv.ac.uk, a.cerminara@wlv.ac.uk

The control of the flow injected from the porous surface is crucial in transpiration cooling applications suitable for thermal protection systems (TPS) of hypersonic vehicles, where the features of the coolant flow entering the boundary layer can significantly affect the transition to turbulence as well as the turbulent mixing and the wall cooling effectiveness (Cerminara et al., 2020, 2021). The geometry of the porous structure determines the characteristics of the flow through the porous medium as well as those of the flow injected at the surface. As such this work parametrically investigates the flow patterns through the regular porous structure of a triply periodic minimal surface (TPMS) configuration using computational fluid dynamics (CFD) considering key geometrical parameters of the inner pore cells. In particular, a Schwartz-P type TPMS is considered as reference structure, as it was shown to maximise the permeability (and hence the blowing ratio) for a given porosity, due to its lower specific surface in comparison to other TPMS structures, in the study of Jung and Torquato (2005). Deflection angles of the pore channels at the pore intakes are varied to obtain specified values of the velocity components of the outflow at the porous surface. Three different injection directions are considered, namely (i) uniform flow injection at 45-deg inclination angle in the spanwise direction, (ii) flow injection at alternate +/- 45-deg inclination angle (in the spanwise direction) between adjacent pores, (iii) conventional straight 90-deg flow injection. The flow is injected at the same assigned pressure drop for all the configurations. CFD simulations of the internal laminar flow within the periodic porous structure are conducted for the three above-mentioned configurations, considering the same level of porosity (40%), and an analysis of the injected flow features at the surface is conducted, including blowing ratio and injection velocity profiles. Ultimately, the results of this CFD study will inform a model of surface porous injection in high-resolution direct numerical simulations (DNS) of hypersonic turbulent flow over a porous flat plate. This, in turn, will enable accurate analysis of the boundary-layer flow behaviour as well as assessment of the cooling effectiveness for the different configurations, and will inform the additive manufacturing process of porous structures (Arjunan et al., 2020) for TPS applications.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS07 / 498

Solvers for Coupled PDE Problems in Porous Media Science

Author: Arne Naegel¹

¹ *Goethe-University Frankfurt*

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Developing efficient solvers for coupled PDE systems is often a non-trivial task, since one must combine suitable schemes for time integration and linear solvers, which is suitable for HPC systems. In this study, we present a unified solver framework, which combines a linearly-implicit extrapolation scheme with a scalable multigrid solver.

The effectiveness of the approach is demonstrated for different applications in subsurface flow. These include (i) thermohaline flow, in which density depends on temperature and salt concentration, (ii) thermo-hydraulic flow, which features thawing and freezing in permafrost regions, and (iii) density-driven flow in domains with a free groundwater surface. We investigate robustness of the numerical methods, develop suitable error estimators and provide results in an HPC environment.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

MS11 / 500

PIV and Microfluidic Investigation of recirculation induced reaction hot spots in porous media

Author: Michael Chen¹

Co-authors: Sang Lee ; Peter Kang²

¹ *University of Minnesota - Twin Cities*

² *University of Minnesota*

Corresponding Authors: pkkang@umn.edu, chen7007@umn.edu, lee02258@umn.edu

Recirculating flows are increasingly being recognized as a common phenomenon in porous and fractured media. While tracer studies have shown that recirculating zones frequently contribute to anomalous transport observed in breakthrough curves, it is less clear how the recirculating flows may influence mixing and subsequent geochemical reaction. In the case of mineral dissolution, recirculation zones have been found to depress overall reaction as the zones trap fluid which then approaches saturation faster than outside the zones, reducing overall reaction rates.¹ In contrast, recirculating flows have been shown to enhance bimolecular and autocatalytic reactions, where the recirculating flow enhances mixing, thus enhancing overall reaction rates.^[2,3] We have previously shown through microfluidic experiments and direct numerical simulation that a single pore throat can create recirculating flows at moderate to low Re numbers (~20) and creates reaction hot spots (see figure). In that system, the appearance of recirculating flows enhanced both mixing of solutes, however, increasing flow rates simultaneously reduces residence time in the pore throat, thus, a critical Re was observed which maximized reaction that represented a balance between mixing enhancement and pore throat residence time. In this work, we extend these results by presenting first the results of particle imaging velocimetry (PIV) experiments to better understand the nature of flow in our microfluidic experimental system. We then present the results for a bimolecular reaction in a microfluidic channel with a heterogeneous arrangement of pore throats. PIV results show clearly that in the single pore throat system, recirculating flows appear readily at moderate flow rates (Re number) common to porous media, while in multipillar experiments, we show that there is a general enhancement of reaction because solutes which are mixed in an upstream pore throat by recirculating flow have sufficient time to react as they proceed downstream. This work probes how mixing, reaction time scales, and transport time scales interact to influence overall reaction rates in a model porous media. The results of this work form the basis for better understanding how reaction kinetics observed in well mixed experiments are influenced by complex flow structures in porous media.

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1. Deng, H. & Spycher, N. Modeling Reactive Transport Processes in Fractures. *Reviews in Mineralogy and Geochemistry* 85, 49–74 (2019).
2. Lee, S. H. & Kang, P. K. Three-Dimensional Vortex-Induced Reaction Hot Spots at Flow Intersections. *Phys. Rev. Lett.* 124, 144501 (2020).
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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Unsure

MS07 / 501

Population Balance Equation for Porous Media: Upscaled Dynamics and Evolution

Authors: Nicodemo Di Pasquale¹; Matteo Icardi²

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² *University of Nottingham*

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Evolution and dynamics of particles have great importance in environmental, industrial and biological applications. One of the most known way to model their behaviour is through the Population Balance Equation (PBE). The PBE describes the evolution of the size ℓ of a population of particles, $f(\mathbf{x}, \ell; t)$, through the reciprocal interactions of the particles within the population (e.g., collisions) and the interaction of the particles with the environment (e.g., shear-induced breakage). Thanks to its extreme flexibility to account for different mechanisms in different systems, it was applied with great success for several problems in chemical engineering, such as the precipitation of polymer nanoparticles in micro-reactors (Di Pasquale et al., 2012,2013).

Population Balance Equation (PBE) successfully describes particle evolution in different flow conditions (Di Pasquale et al., 2012). However, despite predictive macroscopic models for polydisperse particulate flows are relevant for many Porous Media applications (Municchi and Icardi, 2020; Municchi et al., 2020) such as subsurface (water, oil) reservoirs, industrial filtration, there is still little penetration of the PBE framework into PM community.

Our main goal is to present a general population balance model for particle transport at the pore-scale, which includes the main mechanisms of particle evolution, such as aggregation, breakage and surface deposition. Using dimensional analysis we consider the different terms in the PBE and we propose to split the various mechanisms considered for particle interactions into one- and two-particles processes, defining for each different aggregations and breakage mechanisms a Damköhler number, Da , which, along with the Peclet number, Pe , describes the relative importance of the particle evolution mechanisms with respect the time-scale of the fluid.

In this work, we are also considering fractal aggregates, with fractal dimension ϕ .

One open problem remains the upscaling of the PBE (via volume averaging and homogenisation) to a macroscopic (Darcy-scale) description which requires closures assumptions.

Here, we show how to obtain such closure for some specialised case where we show, for arbitrary periodic geometries, accurate upscaled models in particular for the upscaled breakage and collision frequencies, starting from a non-linear power-law dependence on the local fluid shear rate. This work represents the foundation of a new general framework for multiscale modelling of particulate flows in PM.

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References:

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N. Di Pasquale, D. L. Marchisio, P. Carbone, and A. A. Barresi, *Chem. Eng. Res. Des.* 91, 2275 (2013).
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS06-A / 502

Viscous, gravitational and capillary forces in 3D experiments with a synthetic porous media**Author:** Joachim Falck Brodin¹**Co-authors:** Per Arne Rikvold²; Knut Jorgen Maloy³; Marcel Moura⁴; Mihailo Jankov⁴¹ *PoreLab, Physics Dept., The University of Oslo*² *PoreLab, The Njord Centre, Department of Physics, University of Oslo, Oslo, Norway.*³ *PoreLab, Department of Physics, University of Oslo, Norway*⁴ *PoreLab - University of Oslo***Corresponding Authors:** mihailo.jankov@fys.uio.no, marcelmoura@yahoo.com.br, j.f.brodin@fys.uio.no, maloy@fys.uio.no, prikvold@fsu.edu

We explore the interplay between viscous, gravitational, and capillary forces in flow in porous media, using two different boundary conditions and employing our unique 3D-scanner, based on optical index matching 1. Our findings are considered in comparison with experiments on 2D systems, investigating how the transitions between flow regimes can be captured by a dimensionless fluctuation number, as described in [2,3]. In both cases we look at a more viscous, more dense fluid invading a less viscous, less dense one from above. Gravity here destabilizes the invasion, but this is countered by the viscous pressure drop in the invading fluid. We capture the transition, as a function of flow rate, and find a crossover at $F = 0$ between viscosity-stabilized and gravity-unstable invasion. In the first case (Figure 1), we inject from a point high in a sealed cell, with an outlet at a constant pressure at the bottom. We observe a stabilized, dense invasion body near the inlet, with increasing size and a well-defined spheroid shape as we increase the flow rate. The flow transitions to unstable fingering at a radius corresponding to $F = 0$. In the second case, we present ongoing experiments with the same fluid pair, with the more viscous, more dense fluid now invading from above with a front initialized spanning the full cell cross section. We measure a front width that is a function of the flow rate and investigate if we also here can find a crossover at $F = 0$.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS05 / 503

Microfluidic study of biomass-growth induced changes on hydraulic properties. Investigation of growth characteristics under varying nutrient gas environments.**Authors:** Holger Ott¹; Neda Hassannayebi¹; Boris Jammerneegg^{None}; Patrick Jasek^{None}**Co-authors:** Hannes Konegger ; Frieder Enzmann ; Michael Kersten ²; Andreas Loibner ; Martin Ferno ³¹ *Montanuniversität Leoben*² *Johannes Gutenberg-University Mainz, Germany*³ *University of Bergen***Corresponding Authors:** holger.ott@unileoben.ac.at, hannes.konegger@boku.ac.at, kersten@uni-mainz.de, martin.ferno@uib.no, neda.nayebi@gmail.com, boris.jammerneegg@unileoben.ac.at, patrick.jasek@unileoben.ac.at, enzmann@uni-mainz.de, andreas.loibner@boku.ac.at

Apart from the bacterial instrumentalization for EOR processes, aspiration in utilizing anaerobe archaea representatives for renewable methane synthesis in geological formation exists. In a previous study, the investigation of biomass accumulation in pore-space under saturated flow conditions has shown that bacteria exert a significant change in the hydraulic properties of porous media altering both, porosity and permeability. Via time-lapse imaging different modes of bacterial accumulation, as well as preferential channel formation as a result of the changing velocity field, could be observed. The segmented pictures were used as input for Navier–Stokes–Brinkmann flow simulations in a digital-twin approach to estimate intrinsic biomass permeability. From history matching the experimental data, the average intra-biomass permeability was determined to be 500 ± 200 mD, which indicates a significant contribution to the advective nutrient supply potential. In the following study, an anaerobic culture is utilized to investigate the interaction between a blended hydrogen and carbon dioxide nutrient gas phase, similar to what is considered for synthetic methane production. The metabolic characteristics of a methane-producing species *M.formicicum* were investigated in the presence of nutrient and inert gas at shut-in conditions.

The temporal change in biomass count was captured using a high-resolution camera to establish the link between growth rate and nutrient concentration. The presented results focus on the change in biomass concentration with respect to different gas environments under saturated conditions and investigate the timescale of diffusive nutrient transport and consumption in sub-porous biomass aggregates. These experiments are the next step towards unlocking the potential of hydrogen as an energy carrier for subsurface energy conversion technologies.

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MS10 / 504

Multi-scale Confocal Imaging Approach Applied to Study the Complex Pore Systems in Middle-Eastern Carbonates

Authors: Ahmed Hassan¹; Viswasanthi Chandra²; TADEUSZ PATZEK¹

¹ KAUST

² King Abdullah University of Science and Technology (KAUST)

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Carbonate rocks are well-known to be highly heterogeneous which represents a major challenge for subsurface characterization, which is a critical component of energy and earth science applications including enhanced oil recovery, CO₂ sequestration and geothermal system evaluation. The first step toward establishing realistic model of carbonates is to integrate quantitative analysis of the pore space. Our work focused on capturing the pore-geometry parameters required for pore-network modeling. We used fluorescence confocal laser scanning microscopy (CLSM) for its capabilities in producing high resolution images, down to 0.1 μm , with a sufficient depth of investigation for providing an adequate 3D representation of the carbonates pore-network model.

We imaged etched fluorescent epoxy pore casts using CLSM to produce 3D images to obtain high-quality 3D images that can describe the connectivity of multi-scale pore types, particularly where microporosity connects macro-porosity, and to quantify local porosity and permeability. Thus, we captured the pore space at multiple scales with two objective lenses, 10X air (NA = 0.3), and 20X oil immersion (NA = 0.8), to resolve micro- and macro-pores. The lower NA objective has a wider field of view albeit with a lower resolution, while the higher NA objective enables the imaging of finer, micro-scale features. To register the multi-scale confocal images we used an approach that computes an affine transformation for co-registration of two image datasets using an iterative optimization algorithm (Fig 1). Our goal was to achieve digital registration in order to make use of the high-resolution images to achieve more accurate pore segmentation and estimation of petrophysical properties.

The porosity estimation from the 3D images of the pore space indicated that the lower-resolution objective (10X air) tends to overestimate (+15%) the pore volume. The lack of resolving power of the 10X objective could have impaired the ability of the grayscale confocal images to properly identify microporosity and lead to misinterpretation of the micritic grains. These effects were more pronounced in the permeability estimation. While the higher resolution images, from the 20X objective, proved to capture more accurate petrophysical properties the lower resolution images with the wider field of view are very useful in the qualitative description of the carbonates pore system. Hence, our proposed multi-scale confocal imaging approach can provide a more complete quantitative description of the pore system of carbonates with the ability to highlight the interconnectivity between micro and macro-porosity, and can contribute to improved characterization of micritic carbonate rocks.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 505**Estimating the structure of a spatially layered media from the radial flow experiments with shear-thinning fluids****Authors:** Martin Lanzendörfer¹; Mls Jiří¹¹ Charles University, Prague**Corresponding Authors:** martin.lanzendorfer@natur.cuni.cz, jiri.mls@natur.cuni.cz

We address the possible generalization of the methods for the estimation of effective pore size distributions from the saturated permeability experiments with non-Newtonian fluids. In the standard procedure of the yield-stress fluid method (YSM, see 1) or the later method by Abou Najm & Atallah (see [2]), the flow through the porous sample is one-directional, with both the flux and the hydraulic gradient being constant in space. Based on a suitable set of observations with different fluids and/or hydraulic gradients, a discrete approximation of the distribution of effective pore sizes is computed. Analogously to the flow through parallel capillaries of different radii within the capillary bundle framework, one can describe the flow within parallel layers in a spatially layered porous media. The very same methodology could then estimate the distribution of individual layers.

We are interested in the analogy of these methods that would be based on the experimental observation of radial flows. The radial flow data are far less advantageous for such analysis, since both the flux and the hydraulic gradient vary in space. It is not clear a priori whether the inversion of the effective pore sizes would be possible, especially from the real data that include some measurement error. On the other hand, the method could be of practical importance, e.g., allowing us to estimate the properties of a layered sediment based on single borehole injection data with shear-thinning fluids.

This research is supported by Czech Science Foundation under grant 21-27291S.

1 Rodríguez de Castro, A., Agnaou, M., Ahmadi-Sénichault, A., Omari, A., 2020. Numerical porosimetry: Evaluation and comparison of yield stress fluids method, mercury intrusion porosimetry and pore network modelling approaches. *Computers and Chemical Engineering* 133. <https://doi.org/10.1016/j.compchemeng.2019.1>

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Time Block A (09:00-12:00 CET)

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Online

Poster / 506

Salt precipitation and its impact on rock porosity –An X-ray micro-tomography study

Authors: Pavel Kazakovtsev¹; Nathaly Lopes Archilha²; Nima Shokri³; Tannaz Pak¹

¹ Teesside University

² Brazilian Center for Research in Energy and Materials

³ Hamburg University of Technology

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Saline water evaporation from porous media may result in salt precipitation within the pore system influencing transport properties of porous media (Dashtian et al., 2018). Porosity is one of the key characteristics which could be modified due to salt precipitation. Understanding the nature and extent of porosity reduction as a result of salt crystallization is crucial in understanding transport processes in porous media.

This work studies salt precipitation within four rock samples with significantly different pore systems and compositions. We present the precipitated salt distribution along these samples directly measured using 3D X-ray micro-tomography (micro-CT) imaging technique. The selected samples are Boise sandstone, Silurian Dolomite, Mount Gambier limestone, and Berea sandstone. All samples were initially saturated with Potassium Iodide solution (5 molar concentration) and left to evaporate over the course of 31.5 hours. The evaporation process and salt precipitation are monitored using 3D images obtained with X-ray micro-CT at timestamps of 3 and 31.5 hours after the initial saturation. Images were then segmented to determine the porosity of each sample along the core length. Although a time resolved X-ray micro-CT study (such as Pak et al 2019) may be needed to better understand dynamics of the process, the recorded pore-scale images enabled us to quantify the variation of porosity in natural porous media as a result of drying-induced salt precipitation with a high spatial resolution. Our results reveal the significant impacts of heterogeneity on the spatial distribution of precipitated salt. Additionally, we will discuss the potential consequences of our findings on water evaporation from heterogeneous porous media (Shokri-Kuehni et al. 2017).

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 508**Effects of compaction on pore structure and soil hydraulic properties****Author:** Soheil Safari Anarkouli¹**Co-author:** Martin Lanzendörfer²¹ Charles University² Charles University, Prague**Corresponding Authors:** safarias@natur.cuni.cz, martin.lanzendorfer@natur.cuni.cz

The hydraulic properties of porous media extensively depend on their pore structure as described by the size, arrangement, and connectivity of pores. The current work aims to provide a numerical simulation of the evolution of the pore size distribution (PSD) during oedometric compaction of Zbraslav sand. Apart from the derived unsaturated hydraulic properties, we will be particularly interested in predicting its saturated permeability with respect to non-Newtonian (shear-thinning) fluids.

In this study, we will follow the discrete approach during the sand compaction process introduced by Mahmoodlu et al. 1 and later studies. Discrete element method (DEM) can directly trace the motion of individual particles and explicitly consider the particle–particle interactions without the need of macroscopic constitutive correlations. We will use this method to generate a packing of idealized particles for a certain porosity and particle size distribution, and simulate the movement of grains during the compaction process. It is desirable to derive pore networks from the imaged DEM soil samples and thus establish the relationship between the particle geometric features and the pore characteristics. Subsequently, the extracted pore networks can be used as the input for prediction of hydraulic properties of soil [2].

Further step will be the simulation of the flow of various shear-thinning fluids through the media [3, 4]. We are particularly interested in how the observed variations in pore structure will be represented by the effective PSD obtained by the method introduced by Abou Najm et al. [5], i.e. computed from the observed permeabilities with respect to shear-thinning fluids. Based on this method, we will present the experimental measurement of the effective PSD directly during the oedometric test.

This research is supported by Czech Science Foundation under grant 21-27291S.

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References:

- 1 Mahmoodlu, M. G., Raoof, A., Sweijen, T., & Van Genuchten, M. T. (2016). Effects of sand compaction and mixing on pore structure and the unsaturated soil hydraulic properties. *Vadose Zone Journal*, 15(8).
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS11 / 509

Investigation of the corner flow development in porous media in the absence of main front movement

Author: S.ali ghoreishi¹

Co-author: S. H. Hejazi²

¹ *Interfacial Flow and Porous Media Lab, Chemical and Petroleum Engineering, University of Calgary, Calgary, Canada*

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Understanding multiphase flow in porous media is essential in various fields, including hydrocarbon recovery, natural gas and CO₂ storage, fibre-reinforced composites, and underground water remediation. Capillary snap-off, i. e., breaking up of the fluid interface and forming isolated non-wetting phase ganglia, plays a crucial role in the non-wetting phase trapping and consequently the two-phase distribution. Many studies have focused on the understanding of corner/film flow that drives snap-off in porous media. Various numerical and experimental analyses show that the corner/film flow, as it develops before the breakthrough, tends to be much dominant at lower capillary numbers.

In this study, fluid flow experiments have been performed in 2.5D borosilicate micromodels with the known contact angle of $42 \pm 2^\circ$. The micromodel consists of uniform circular posts with diameters ranging from 1 to 2 mm, creating a throat to pore aspect ratio of 5. The micromodel is horizontally placed to eliminate the gravitational forces and is initially saturated with drakeol 35 (viscosity 178 mPa.s). Oil is linearly displaced by distilled water at rates of 0.1, 1, 5, 10, 20, and 30 $\mu\text{l}/\text{min}$ resulting in the range of capillary numbers from 1.2×10^{-8} to 3.6×10^{-6} . The advancement of the oil-water interface, before and after breakthrough, are recorded using Canon 5DSR camera at 1 frame per minute where the development of corner/film flow is recognized in the form of snapped-off water clusters. Along with recovering known results for displacement before breakthrough where the corner/film flow develops ahead of the main front at low capillary numbers, it is found that the

corner/film flow can also develop after breakthrough in the absence of main frontal advancement. This happens when the fluid displacement is done above a critical capillary number.

A quantitative analysis is performed by measuring the changes in the volume of oil displaced by water, the number of isolated water clusters, and their size distribution. For all capillary numbers, the corner flow, quantified by the volume of displaced oil and number of water clusters, develops for sometimes after breakthrough until it reaches a plateau. It is shown that the corner/film flow development rate is an increasing function of capillary number, mainly due to the higher bulk aqueous phase pressure at increased injection rates. The size of isolated water clusters is almost identical between capillary numbers. A close inspection of displacement images shows that the water clusters mostly form in the smallest pores. In contrast, the prominent pores are mainly saturated with oil and the water flow is limited to their corners. Thus, similar to pre-breakthrough cases, the pore geometry may play an important role in the formation and size distribution of water clusters after breakthrough.

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MS13 / 510

Pore networks meet computational chemistry: a hybrid approach for studying the flow of fluid mixtures under various thermodynamic conditions in nanoporous materials.

Authors: Aleksey Khlyupin¹; Irina Nesterova¹; Rustem Sirazov²; Kirill Gerke³

¹ *Moscow Institute of Physics and Technology*

² *Shmidt Institute of Physics of the Earth (UIPE RAS)*

³ *RAS*

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An unconventional reservoir is a multiscale system in which pores with the size of several nanometers can reach 80% of the total pore volume. 1. Traditional methods of production processes modeling based on the Navier-Stokes equation, which describes the behavior of a continuous medium, are not suitable for this case, since they do not consider the molecular interactions of fluid and rock. In nanopores the interaction of fluid molecules with solid surface significantly affects the component composition, thermodynamic, phase and transport properties [2 - 4]. The development of technologies for effective production and design of enhanced oil recovery methods requires new approaches to modeling and understanding of the processes occurring at the molecular level. A wide range of

phenomena occurring at the nanoscale can be investigated using Molecular Dynamic (MD) modeling. However, since MD requires the numerical solution of the equations of motion for a system of interacting particles, the method is computationally expensive, and the calculations could take from several hours to several days [5]. To accelerate the calculation of the equilibrium state of the fluid in a multiscale pore system, a new hybrid approach is proposed. To study the behavior of hydrocarbon and carbon dioxide mixtures in nanoporous media a new method that combines modern Density Functional Theory (DFT) and MD with flow simulations in Pore Network models was developed in the current work.

At the first stage of the proposed method, the distribution of the component composition in micro- and nanopores and the equilibrium thermodynamic parameters is determined using DFT. Then, in the second step, a MD calculation of the system is conducted with the previously determined distribution of component composition between micro and nanopores. MD is used to calculate the fluid flow in the pore space and effective transport properties, considering the distribution of fluid components. Since the equilibrium distribution of the components in nanopores is calculated at the first stage, the time for calculating the transport properties will be significantly less than the time for direct MD simulation. Further, the transport and filtration properties of the entire porous medium are described and modeled based on the pore-network approach, taking into account the thermodynamic effects in nanopores.

As a result, we developed a multiscale technique for modeling and studying the properties of fluid mixtures in porous medium, depending on the thermodynamic conditions and the component composition of the fluid. The proposed method was applied to calculate the properties of various mixtures of hydrocarbons and carbon dioxide in nanoporous materials, so case studies are discussed in detail.

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References:

1. Yu W. et al. Compositional simulation of CO₂ huff'n'puff in Eagle Ford tight oil reservoirs with CO₂ molecular diffusion, nanopore confinement, and complex natural fractures //SPE Reservoir Evaluation & Engineering. –2019. –T. 22. –№. 02. –C. 492-508.
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Participation:

Unsure

MS14 / 511

Improving the efficiency of reservoir simulations with the Multi-scale Perturbation Method for Two-Phase Flows

Authors: Franciane Rocha¹; Het Mankad²; Fabricio Sousa¹; Felipe Pereira³

¹ *University of Sao Paulo*

² *Carnegie Mellon University*

³ *Mathematical Sciences Department, The University of Texas at Dallas, Richardson, TX, USA*

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The Multiscale Perturbation Method for Two-Phase Flows (MPM-2P, 1) is a procedure based on the Multiscale Perturbation Method (MPM, [2]) that uses classical perturbation theory to efficiently approximate velocity fields in the numerical solution of two-phase flow problems. We consider an operator splitting strategy, where a scalar conservation law for the saturation of one of the phases and the velocity field are updated sequentially. The velocity field is approximated by multiscale mixed methods, which allow for the global solution to be computed on a coarse mesh, while detailed basis functions are defined locally in a fine grid. The formulation of the MPM-2P introduces a modification on the operator splitting method to replace full updates of local solutions by reusing multiscale basis functions computed at an earlier time of the simulation. The new procedure provides a significant reduction of the computational cost in the approximation of challenging flow problems, while the accuracy is controlled by a tolerance criterion. Our numerical experiments demonstrate an exceptional speed-up of almost 90% of reduction in the computational cost of two-phase flow simulations with the MPM-2P.

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References:

1 F. F. Rocha, H. Mankad, F. S. Sousa, F. Pereira. The multiscale perturbation method for two-phase reservoir flow problems, *Applied Mathematics and Computation*, (2021): 126908.

[2] A. Ali, H. Mankad, F. Pereira, F. S. Sousa. The multiscale perturbation method for second order elliptic equations, *Applied Mathematics and Computation*, 387 (2020): 125023.

Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS08 / 512

Inertia and 3D Flow Effects on Mixing and Reaction at Channel Intersections

Authors: Peter Kang¹; Sang Lee^{None}; Woonghee Lee²; Jingxuan Deng¹; Etienne Bresciani³; Marco Dentz⁴

¹ *University of Minnesota*

² *UNIVERSITY OF MINNESOTA*

³ *CEAZA*

⁴ *IDAEA-CSIC*

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Mixing and reaction at channel intersections often control various processes and applications involving porous and fractured media. Fluid inertia effects can be important in such systems, but many previous studies are limited to Stokes flow. Lee and Kang 2020 [Physical Review Letters, 124(14)] namely observed that inertia effects can induce 3D recirculating flows at channel intersections and showed that the recirculating flows initiate local reaction hot spots, that is, locations where reaction rates are locally maximum. Nevertheless, we still lack comprehensive understanding of inertia and 3D flow effects on mixing and reaction at channel intersections.

In this study, we combine laboratory microfluidic experiments, pore-scale numerical simulations, and flow topology analysis to elucidate inertia and 3D flow effects on mixing and reaction at channel intersections. We show that mixing and reaction hot spots are strongly linked with flow topological properties that form the backbone of underlying flow fields. In particular, stagnation points constitute critical topological features that imply flow separation associated with strong stretching and folding, which has a major influence on overall mixing and reaction dynamics. We systematically vary both the injection rate and channel geometry to elucidate how various flow topologies emerge at channel intersections as a function of the Reynolds number and channel geometry. We then establish a quantitative link between flow topology, mixing, and reaction rates. Finally, we estimate mixing and dispersion measures at intersections and discuss the implications of inertia effects on mixing and reactive transport at larger scale.

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References:

Lee, S.H. and Kang, P.K., 2020. Three-dimensional vortex-induced reaction hot spots at flow intersections. *Physical review letters*, 124(14), p.144501.

Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Unsure

MS17 / 513

Micro-scale Laser-induced Fluorescence Thermometry for Multi-phase Flow in Porous Media

Authors: Samuel Simmons¹; Christian Pedrigal¹; Farzan Kazemifar¹

¹ *San Jose State University*

Corresponding Authors: farzan.kazemifar@sjsu.edu, christian.pedrigal@sjsu.edu, samuel.simmons@sjsu.edu

Multiphase flow in porous media is encountered in many important natural and industrial systems relevant to petroleum, water resources, and environmental engineering. In applications such as thermal recovery and thermal remediation of contaminated soil, heat transfer plays a central role. However, pore scale investigation of heat transfer is hindered by challenges such as complex geometry and lack of optical access. Optically accessible microfabricated 2D porous models, known as micromodels, enable the use of optical diagnostic techniques and have been extensively used for flow in porous media research. In this work, a laser-induced-fluorescence-based thermometry technique is introduced for simultaneous measurement of temperature in two immiscible liquid phases in micromodels. The temperature sensitivity of the fluorescence signal for various dyes are quantified using spectrofluorometric as well as in situ measurements in microchannels. Dye combinations with highest sensitivity are tested in multiphase flow configuration to demonstrate the characteristics of the measurement technique in terms of accuracy, temperature range, as well as spatial and temporal resolution.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS06-A / 514

Diffusion of methane and carbon dioxide within flexible kerogen from molecular dynamics simulations

Authors: Kristina Ariskina¹; Guillaume Galliero¹; Amael Obliger²

¹ Laboratoire des Fluides Complexes et leurs Réservoirs, UMR 5150, E2S UPPA

² Institut des Sciences Moléculaires, UMR 5255, Université de Bordeaux/CNRS

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The growing interest in shales stems from the presence of significant hydrocarbon reserves and the possibility of storing carbon dioxide in source rock's organic matter (kerogen). However, the impact of kerogen's microporosity on fluid dynamics is not fully understood yet. Phenomena such as strong adsorption effects have to be taken into account on fluid transport investigations due to the high surface to volume ratio in kerogen. Most of the previous molecular scale studies on the fluid dynamics in kerogen have been performed in the rigid solid approximation [1,2], which is a rather crude assumption in most cases. Thus, in this study, molecular dynamics and free volume theory have been applied to shed light on diffusion of methane (CH₄) and carbon dioxide (CO₂) in a flexible kerogen microporous structure. The molecular kerogen model described in the paper [3] has been reused to extend the methane diffusion study to the carbon dioxide transport properties and collective effects in fluid diffusion. Despite an anisotropy of the transport properties induced

by the size of our immature kerogen model ($\sim 6 \times 6 \times 6$ nm³), analysis of the diffusivity trends has shown that the anisotropic factor is approximately constant and remains small. This allows us to average over the three directions to obtain effective transport properties. In addition, we prove that fluid (CH₄/CO₂) transport in flexible kerogen microstructures is purely diffusive, as the dynamics of the host matrix does not promote collective effects through solid-fluid couplings. Thus, the self-diffusion coefficient is a sufficient measure of the transport properties of fluids confined in both rigid and flexible kerogen microporosity. Moreover, the diffusivity of a fluid in deformable kerogen increases with fluid loading due to adsorption-induced swelling, as opposed to the rigid solid case. Interestingly, this increasing trend is well captured by the Fujita-Kishimoto free volume model. In contrast to fluid adsorption, the replacement of CH₄ with CO₂ led to kerogen matrix shrinkage and decreased CO₂ diffusivity compared to that of CH₄ at certain conditions due to the stronger intermolecular forces of attraction in CO₂ reinforcing fluid-solid couplings. These results raise new issues of the impact of chemical and mechanical diversity of kerogen on fluid diffusion.

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References:

- 1 K. Falk, et al., Nature communications, 6: 6949, 2015.
- [2] J. Collell et al., The Journal of Physical Chemistry C, 119(39): 22587–22595, 2015.
- [3] A. Obliger et al., Journal of Physical Chemistry B, 123(26):5635–5640, 2019.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS06-B / 515

Characterisation of hydrocarbon bio-degradation in porous media

Authors: Anne Edith Larue¹; Yohan Davit¹; Michel Quintard¹; Manuel MARCOUX²

¹ Institut de Mécanique des Fluides de Toulouse

² Institut de Mécanique des Fluides de Toulouse

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In the context of bio-remediation of residual hydrocarbons in soils, we seek to understand the kinematics of mass exchange amongst the different phases of a polluted soil system namely the aqueous, oil or Non-Aqueous Phase Liquid (NAPL) and biofilm phases. In this work, we ran biodegradation experiments in 2D water-saturated porous media within which a residual NAPL phase has been established. As porous medium, we used a micro-fabricated epoxy photoresist (SUEx) network consisting of a disordered array of 160 μm diameter cylinders. This material was chosen as it allows experiments with organic compounds as well as being bio-compatible and transparent. After establishment of an irreducible decane (C₁₀) saturation, the micro-model is inoculated with an indigenous *P. fluorescens* strain isolated from a French polluted site. Experiments are run for 2 - 4 weeks under continuous flow of air-saturated, minimal mineral medium as we follow the temporal evolution of the three phases by bright and dark-field microscopy. We observe how the biofilm colonises the

pore space in accordance with preferential flow paths, how it develops around the NAPL phase being the sole carbon source and how bio-clogging induces redistribution of a partially degraded NAPL phase. After sophisticated image processing, several metrics distribution concerning the NAPL and biofilm phases are acquired such as volumes, contact angles and dimensions of NAPL ganglia along with biomass, biofilm type (agglomerate or streamer) and available surface area for mass exchange amongst the different phases. Analysis of the temporal evolution of these specific parameters' distributions unlocks multiple insights for the understanding of transport phenomena in such complex multi-phase systems.

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References:**Time Block Preference:**

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 516

Molecular dynamics of a fluid confined in kerogen from memory kernels

Authors: Kristina Ariskina¹; Guillaume Galliero¹; Amael Obliger²

¹ *Laboratoire des Fluides Complexes et leurs Réservoirs, UMR 5150, E2S UPPA*

² *Institut des Sciences Moléculaires, UMR 5255, Université de Bordeaux/CNRS*

Corresponding Authors: guillaume.galliero@univ-pau.fr, amael.obliger@u-bordeaux.fr, kristina.ariskina@univ-pau.fr

The depletion of conventional oil/gas reserves has led to the extensive exploitation of hydrocarbon-rich organic source rocks. However, recovery of hydrocarbons from kerogen, the main organic component of shales, has proved to be complicated due to the strong impact of kerogen microporosity on fluid transport. In order to understand the nature of solid-fluid couplings and its impact on fluid production/storage, a multiscale approach including advanced numerical and statistical methods should be applied. As a step towards this goal, we investigated the fluid dynamics which was affected by the solid dynamics through the application of molecular dynamics (MD) simulations and coarse-graining procedures based on the generalized Langevin equation. In this framework, the influence of the solid (kerogen) on the fluid flow is incorporated in the so-called noise, of which the autocorrelation function (ACF) is the memory kernel. To compute memory kernel, the post-treatment of trajectories from molecular simulations of fluids confined in rigid and flexible kerogen have been performed using two coarse-graining techniques, one based on the inversion of the Volterra equation of the second kind 1 and the other one based on the reconstruction of the backward orthogonal dynamics [2]. The latter method also gives access to the noise on top of the memory kernel while being computationally expensive. These approaches have allowed us to extract the feedback of the solid dynamics on the fluid one. It has been proven recently by a study on the memory kernel that, in the case of a bulk fluid, hydrodynamic modes govern the fluid dynamics even for colloids of molecular size [2]. In contrast, hydrodynamics is inadequate to describe the transport of a fluid trapped in rigid

pores of a kerogen molecular model [3,4]. Interestingly, the kerogen flexibility does not contribute to the cross-correlations between fluid molecules at long times leading to purely diffusive behavior. Nevertheless, our study has shown that the velocity ACF (VACF) scales exactly the way predicted by the hydrodynamic theory for both rigid and flexible solid cases despite negligible collective effects in fluid diffusion. The similar decay of the VACF has been determined by Lesnicki et al. for a tagged particle in a fluid [2]. All of that lead to the assumption that this scaling of the VACF ($\sim t^{-3/2}$) at long times is not restricted to hydrodynamics. Moreover, our analysis of memory kernel has shown that its decay does not follow the long-term trend prescribed by the hydrodynamics. Combining MD simulations with the memory kernels investigation will contribute to a more profound understanding of the impact of the environment (polymers, water, etc.) on confined fluid dynamics.

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References:

- 1 G. Jung et al., Journal of Chemical Theory and Computation, 13(6): 2481–2488, 2017.
 [2] D. Lesnicki et al., Physical Review Letters, 116(4): 1-5, 2016.
 [3] K. Falk, et al., Nature communications, 6: 6949, 2015.
 [4] J. Collell et al., The Journal of Physical Chemistry C, 119(39): 22587–22595, 2015.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

MS07 / 517

Positive DDFV scheme for degenerate parabolic equations arising from infiltration problem

Author: Mazen Saad¹

Co-authors: El Houssaine Quenjel²; Ben Mansour DIA³

¹ Ecole Centrale de Nantes

² CentraleSupélec

³ CIPR-CPG

Corresponding Authors: el-houssaine.quenjel@centralesupelec.fr, mazen.saad@ec-nantes.fr

Nonlinear degenerate parabolic equations are the main core to study some complex problems arising from petroleum engineering and hydrology. In our study, the problem describes the infiltration of a single fluid through a porous medium with no gravity effects.

We carry out the convergence analysis of a positive DDFV (Dual Discrete Finite Volume) method for approximating solutions of degenerate parabolic equations. The basic idea rests upon different approximations of the fluxes on the same interface of the control volume. Precisely, the approximated flux is split into two terms corresponding to the primal and dual normal components. Then the first term is discretized using a centered scheme whereas the second one is approximated in a non-evident way by an upstream scheme. The novelty of our approach is twofold: on the one hand,

we prove that the resulting scheme preserves the positivity and on the other hand we establish energy estimates. Some numerical tests are presented and they show that the scheme in question turns out to be robust and efficient with an accuracy of second-order on quadrilateral grids.

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References:**Time Block Preference:**

Time Block A (09:00-12:00 CET)

Participation:

In person

MS11 / 519

Nanoparticle-based suspensions and emulsions for enhanced oil recovery

Authors: Anastasia Strekla¹; Christina Ntente²; Maria Theodoropoulou³; Christos Tsakiroglou⁴

¹ Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences & University of Patras, Department of Physics

² Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences & University of Patras, Department of Chemistry

³ Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences

⁴ Foundation for Research and Technology Hellas - Institute of Chemical Engineering Sciences (FORTH/ICE-HT)

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The aqueous extracts obtained when boiling the leaves of plants (e.g. tea, parsley, coriander, etc) contain a mixture of polyphenols, which are natural polymers, and if mixed with a metal salt, they may act both as reductants and capping agents of the so-produced nanoparticles. Aqueous solutions of polyphenols extracted from the leaves of parsley were mixed with aqueous solutions of ferric chloride hexahydrate to produce suspensions of iron oxide nanoparticles. The total concentration of polyphenols was measured in terms of equivalent concentration of Gallic acid by using the Folin-Ciocalteu method. The creation of iron oxide nanoparticles was confirmed with X-ray diffraction (XRD) analysis, and scanning-electron microscope (SEM) images of solid material isolated with centrifuging. The suspended nanoparticle size distribution was determined with dynamic light scattering (DLS), while the stability of the nano-colloids was confirmed by measuring the ζ -potential as a function of the concentration of mono-valent (NaCl) and di-valent (CaCl₂) salts, and ionic strength. The static and dynamic surface/interfacial tension of aqueous phase/air and aqueous phase/oil were measured by using a tensiometer with DuNouy Ring, and combining the pendant drop method with the OpenDrop software of inverse modeling of Young-Laplace equation [2], respectively. These properties along with wettability, as quantified by the contact angle, enabled us to assess the capacity of nano-colloids to generate stable foams and emulsions. With the aid of an ultrasound probe, the nano-colloids were mixed with oil (n-decane) to prepare Pickering emulsions. The rheological properties (shear viscosity, loss and storage moduli) of emulsions were measured on a stress rheometer,

and their stability was inspected by observing the phase separation (macro-scale) and measuring the drop size distribution (micro-scale).

To assess the performance of the nano-colloid suspensions and emulsions as agents of enhanced oil recovery (EOR), tests of secondary and tertiary oil recovery were conducted in two types of porous media models: (i) transparent glass-etched pore networks [3]; (ii) sandpicks. In each test, the transient response of the oil displacement efficiency and pressure drop across the porous medium were recorded, and used as criteria to classify the performance of fluids as EOR agents, and select the most efficient ones for further studies in reservoir rocks.

Acknowledgements

The research project was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) under the “1st Call for H.F.R.I. Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment”(Project Number: HFRI-FM17-361, acronym: EOR-PNP).

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3. Theodoropoulou, M.A., V. Sygouni, V. Karoutsos, and C.D. Tsakiroglou, “Relative permeability and capillary pressure functions of porous media as related to the displacement growth pattern”, *Int. J. Multiphase Flow*, 31, 1155-1180 (2005).

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Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS06-A / 520

Ion composition effect on spontaneous imbibition in limestone cores.

Authors: Raymond Mushabe¹; Gbadebo Adejumo¹; Azizov Ilgar ²; Carl Fredrik Berg¹; Antje van der Net¹

¹ *Norwegian University of Science and Technology*

² *Norwegian University of Science and Technology*

Corresponding Authors: mushaberaymond@gmail.com, carl.f.berg@ntnu.no, antje.van.der.net@ntnu.no, adejumo-gbadebo94@gmail.com, ilgar.azizov@ntnu.no

Studies on low salinity oil recovery on mostly outcrop rock cores have accelerated in recent years. Detailed focus has been put on understanding competing underlying mechanisms behind observed

improved oil recovery. The main aim of this work was to understand how the ionic composition of imbibing brine dictates the wettability change in limestone outcrop cores basing on spontaneous imbibition (SI) experiments. The cores used in the study had a substantial difference in the degree of heterogeneity, and can therefore be representative of different actual reservoirs. It was observed through improved oil recovery that complete dilution of synthetic seawater had almost no impact on improved oil recovery on limestone cores, with the brine used in the tertiary mode. However, selective dilution of synthetic seawater with respect to the NaCl content resulted in high improved oil recovery. In line with this observation, two other brines depleted in NaCl and enriched in the magnesium (Mg^{2+}) and sulfate (SO_4^{2-}) ions were used to test the impact of minimal NaCl on the magnesium ion on the wettability alteration process.

Both brines (SSW-2S4Mg and SSW-2S8Mg) resulted in improved oil recovery in the tertiary mode. Contact angle measurements after placing polished rock chips, cut and shaped from the same rock material, in brines at 96 degrees Centigrade, were in line with the observed improved oil recoveries. What was striking was that all contact angle measurements in synthetic seawater depleted in NaCl content were in the water wetting window, based on the *Anderson et al.* criterion. Zeta potential measurements at both 25 degrees Centigrade and 70 degrees Centigrade, also supported both SI and contact angle measurements.

In this work, also a new and better experimental procedure and set up ideal for conducting high-temperature spontaneous imbibition (SI) experiments have been proposed. The set-up mainly focuses on minimizing interrupting the SI process during the experimental period. We have also been able to test its flaws and ultimately updated it. All the SI experiments in this work were done using this proposed setup.

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References:

- Anderson, W. G., et al. Wettability literature survey-part 1: rock/oil/brine interactions and the effects of core handling on wettability. *Journal of petroleum technology* 1986,38, 1-125.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS09 / 521

A new Pore Network stochastic generation approach utilising bulk pore characterisation data with application to mudrocks

Authors: Georgy Borisochev¹; Andreas Busch¹; Jingsheng Ma¹; Lin Ma²

¹ Heriot-Watt University

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With climate change mitigation actions in place, Carbon Capture and Storage (CCS) is by far the most industrially efficient technology to reach net-zero carbon emissions (HM Government, 2018), with current annual capture capacity exceeding 40 million tonnes of CO₂ world-wide (BP, 2020). While supercritical CO₂ is stored in conventional reservoirs or saline aquifers, overlying mudrock formations create a structural trap, preventing CO₂ leakage. Opalinus Clay, generally researched as a repository for radioactive waste, is a perfect candidate for CCS research, with a large dataset of mineralogical and petrophysical properties collected from existing publications (Bossart and Milnes, 2017) and experimental work allowing for good understanding of pore space geometry and underlying flow processes. It is necessary to estimate flow properties, such as permeability and capillary entry pressures, for mudrocks by numerical modelling, as the properties are difficult to obtain from laboratory tests on sample plugs.

Pore Network Modelling (PNM) is a method used for simulating pore-scale physiochemical processes on representative pore networks of sample pore space and estimating the flow properties, and is significantly more computationally efficient than most other methods. Techniques have been developed to extract networks from pore-grain resolved 3D images (Raeni et al., 2017, ThermoFisherScientific, 2020) and to integrate networks for specific sub-volumes of a sample (Ma et al., 2017, Jiang et al., 2013). However, submicron pores in mudrock are abundant and known to form critical flow pathways, but often distributed in a close association with large pores across the whole sample, other than scattered in isolation. This poses practical challenges to apply multiscale tomographic imaging for resolving pores at all scales. Stochastic pore network generation algorithms have been reported (Idowu and Blunt, 2009, Gostick et al., 2009, Jiang et al., 2012), and could be used to create networks where no images are available, but other specific pore characterisation data is present.

This work attempts to create an algorithm, which generates a representative pore network model with pore sizes ranging from sub-nanometre to over a micron, while using direct data input from bulk pore space measurements. An array of nodes was generated randomly based on low pressure adsorption and small angle neutron scattering data, with bonds defined based on nearest neighbours and coordination number. Pore-to-throat aspect ratio and element shape factors were adjusted using mercury intrusion measurements and specific surface area values. Model geometry was calibrated to match total porosity values measured by helium pycnometry.

Hydraulic conductivity was modelled following the method used in (Song et al., 2018), which accounts for real gas flow and diffusion effects across a full range of Knudson number. Gas adsorption effects were implemented by changing node and bond effective radii, using methane and carbon dioxide high pressure adsorption isotherms.

The nonlinear system of equations is solved iteratively to achieve effective permeability convergence, using the Pardiso sparse solver interface (Intel, 2021) for improved performance at large model sizes. Calculated results were verified against unsteady state single-phase gas permeability measurements, performed on Opalinus Clay plugs, at a range of confining conditions and absolute pressures.

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References:

- BOSSART, P. & MILNES, A. G. 2017. Mont Terri Rock Laboratory, 20 Years: Two Decades of Research and Experimentation on Claystones for Geological Disposal of Radioactive Waste, *Swiss Journal of Geosciences*.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS09 / 524

Lagrangian modeling and upscaling of pore-scale transport in random media

Authors: Giovanni Porta¹; Matteo Radice¹; Gael Guedon¹

¹ *Politecnico di Milano*

Corresponding Authors: matteo3.radice@mail.polimi.it, gael.guedon@polimi.it, giovanni.porta@polimi.it

We consider simulation and upscaling of advective-diffusive transport processes based on a Lagrangian modelling approach. Our study leverages simulated Lagrangian particle trajectories in periodic three-dimensional pore-spaces. These trajectories are then exploited through an upscaling method that relies on a spatial Markov model, ultimately yielding prediction of the particle travel times and locations at large distances and times. The key feature of the approach is that it can retain subscale features, as these are tied to the recorded trajectory paths. We demonstrate the application of this approach to modelling of transport in media characterized by a single or dual diffusivity. In the former case, transport is assumed possible only in the pore space via advection and diffusion, while in the latter we assume that transport may take place also in the solid grains via pure diffusion. The dual diffusivity case thus requires to deal with a spatially discontinuous diffusion coefficient, i.e. assumes different diffusion coefficients between liquid and solid phases. Our approach allows characterizing these transport scenarios with high computational efficiency. We discuss the validation of the method and the capabilities of the approach towards characterization of coupled processes. The results enable us to assess the impact of the sample porosity on the physical characterization of transport and on the performance of the method.

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Participation:

Online

MS06-B / 525

A quadrature-based scheme for numerical solutions to linearized unsaturated flow equation

Authors: Marco Berardi¹; Fabio Vito Difonzo²

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In this work we propose a numerical method for computing solutions to unsaturated flow equation within Gardner's framework. In order to do so, we resort to Kirchhoff transformation of Richards' equation in mixed form, obtaining a linear second order partial differential equation. Then, leveraging the mass balance condition, we integrate both sides of the equation over a generic grid cell and discretize integrals using trapezoidal rule. We prove that this method is l^2 -stable and convergent to the exact solution under suitably conditions on step-sizes, retaining the order of convergence from the underlying quadrature formula.

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Participation:

Online

MS14 / 526

INVERSE AND FORWARD UNCERTAINTY QUANTIFICATION OF RELATIVE PERMEABILITY AND FOAM MODEL PARAMETERS FOR EOR PROCESSES

Authors: RODRIGO Weber dos SANTOS¹; Gabriel Brandão de Miranda²; Luisa Silva Ribeiro²; Bernardo Rocha²; Grigori Chapiro²

¹ *Federal University of Juiz de Fora*

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In enhanced oil recovery (EOR) processes, foam can be injected into the porous media to reduce gas mobility and increase the recovery factor. Mathematical models of foam injection involve many parameters controlling the complex physics of this process. The quantification of uncertainties in a model is essential for developing robust simulators. However, neglecting some parameters during this analysis can hide important influences and interactions between them and their impact on propagated uncertainties. This work studies a more comprehensive approach for uncertainty quantification of two-phase flow models for foam flow using the same model implemented in STARS/CMG. We present a framework for the inverse and forward uncertainty quantification of Corey's relative permeability model and the apparent viscosity model from STARS with the dry-out component. The study is carried out for each submodel separately and then to the complete model using the Markov Chain Monte Carlo (MCMC) method for inverse uncertainty quantification. Preliminary results show that uncertainties propagated by apparent viscosity are more significant than those propagated by relative permeability models.

Acknowledgements: The current work was conducted in association with the R&D project ANP n° 20715-9, "Modelagem matemática e computacional de injeção de espuma usada em recuperação avançada de petróleo" (UFJF/Shell Brazil/ANP). Shell Brazil funds it in accordance with ANP's R&D regulations under the Research, Development, and Innovation Investment Commitment. This project is carried out in partnership with Petrobras.

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Poster / 527

Wetting/drying mechanisms associated with nanoconfined salt solutions: an optical reflectance study on vapour phase imbibition and adsorption

Author: Sujeet Dutta¹

Co-authors: Alexandre Littiere ; Hugo Bellezza ¹; Patrick Huber ²; Olivier Vincent ¹

¹ *Institut Lumière Matière, CNRS*

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The wetting and drying cycles of salt solutions confined in conductive nanoporous electrodes are conceived to generate energy from low-grade waste heat by coupling the pore drying/wetting process with the charging/discharging cycles of the electrodes. The key factor being the surface area of the electrode in contact with the adsorbing/desorbing liquid films. This objective could be realised by achieving the right set of physical conditions that allow a systematic control and manipulation of the electrically charged layers that develop inside the porous host matrices. The first step initiated in this direction is studying the percolation of water from the vapour phase in to the nanopores through a single exposed edge of the nanoporous host matrix (Vycor®). The porous host is maintained under controlled temperature and vapour pressure (humidity), and is illuminated by a diffuse white light source. The change in the grey-scale intensity with respect to the empty state is monitored to follow the pore-filling process as a function of time. Through systematic measurements at increasing relative humidity steps, the transition from diffusive percolation to imbibition is established. Likewise, the pore-emptying phenomenon is monitored by “degassing” the system in defined pressure steps, and the imbibition/drying mechanisms are rationalised with appropriate thermodynamic and kinetic models. The focus of the next phase of such investigations shall be on the wetting/drying mechanisms of nanopores carrying salt crystals, with complementary small/wide angle x-ray scattering experiments with the objective of obtaining information on the potential thin liquid films that may form in capillary bridges in the porous host matrices upon drying, and the re-distribution of ionic clusters as a consequence of such wetting/drying cycles, both of which could lead to spurious capacitances being exhibited by the porous electrodes. The thickness and electrical conductivity of such films have been investigated on flat macroscopic surfaces with similar surface chemistry as the pore walls of the nanoporous host with the objective of predicting the influence of such post-cursor films (left behind in the drying pores) on the electrode capacitance with respect to their dry state. In a separate set of experiments, vapour phase adsorption/desorption isotherms are obtained via optical reflectance with the objective of unravelling the influence of salt concentration on the vapour sorption characteristics, in particular playing with the contact angle of the meniscus of the adsorbed liquid film by appropriate pore- surface hydrophobization. The thermodynamic information revealed by such experiments, coupled with the imbibition characteristics will play an important role in fine tuning the pore filling and emptying kinetics in order to achieve electrodes with desirable energy storage capabilities.

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References:

- 1) Jain, Piyush, Olivier Vincent, and Abraham D. Stroock. “Adsorption, desorption, and crystallization of aqueous solutions in nanopores.” *Langmuir* 35, no. 11 (2019): 3949-3962.
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 528**Simplified simulation of two-phase flow in karst conduits in carbonate rocks**

Authors: Uebert Gonçalves Moreira¹; Franciane Fracalossi Rocha²; Alfredo Jaramillo¹; Fabricio Simeoni de Sousa¹; Roberto Federico Ausas¹; Gustavo Carlos Buscaglia¹; Felipe Pereira³

¹ *University of São Paulo*

² *Universidade de São Paulo*

³ *The University of Texas at Dallas*

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Oil reservoirs are composed of several combinations of matrices, fractures and cavity systems, which result in various properties of porosity, permeability and fluid transport behavior [1]. Thus, the problem of flow through a reservoir in the presence of karsts is complex and the predictive capabilities related to the flow and transport processes remain severely limited.

In this work, we perform computer simulations of the five spot problem in a domain $\Omega \subset \mathbb{R}^2$ to numerically describe an incompressible two-phase flow in a karstified carbonate rock. The methodology is based on the geometric treatment and simulation data proposed in [2], and on the application of the Karst Index (KI) concept presented by [3]. The use of the KI follows a similar approach to the application of the Well Index presented in [4]. Given the lack of knowledge of the precise geometry of karst network shape, we consider a particular arrangement of the branchwork type in the sense of the shape defined in [5] and idealized by [2]. The mathematical model used basically consists of a system of equations that includes Darcy's Law, a mass conservation equation for each component and a transport equation. The domain is discretized by a uniform mesh, where the karst is embedded, with different configurations of homogeneous and high-contrast heterogeneous media. The equations are discretized by standard finite volume schemes.

As a way of validating the results, we verified that the masses are conserved in all elements. In addition, the behavior of the pressure, velocity and saturation fields are consistent with the expected physical behavior. The results were compared with simulations in domains without the presence of karsts and substantial differences were noted between them. Our results emphasize the need to include karst regions in reservoir simulations and have potential to be used in more complete treatments that make use of Multiscale Methods and parallel simulations.

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References:

[1] C. Braester. Influence of block size on the transition curve for a drawdown test in a naturally fractured reservoir. SPE 10543-PA, 24(5), 1984.

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS07 / 529

A numerical approach to incorporating shear thinning effects of polymer in polymer flooding.

Author: Prabir Daripa¹

¹ *Texas A&M University*

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In mathematical modeling of chemical enhanced oil recovery by polymer flooding, it is desirable that non-Newtonian effects of polymer are properly accounted for. The two distinct effects that polymers exhibit are shear-thinning (stiff polymer) and visco-elasticity (flexible polymer). The shear thinning effect is important as the polymers used in chemical oil recovery are usually stiff polymers. We propose a data driven approach to incorporate this shear thinning effect. We describe the way we integrate this data driven approach with the hybrid numerical method for reservoir simulation, previously developed by Daripa and Dutta. The numerical method solves a system of coupled elliptic and transport equations modeling the polymer flooding process through heterogeneous porous media using a discontinuous finite element method and modified method characteristics. The simulations show (i) competing effects of shear thinning and mobility ratio; (ii) injection conditions such as injection rate and injected polymer concentration influence the choice of polymers to optimize cumulative oil recovery. (iii) permeability field also affects the choice of polymer as polymers show varying movement for different shear rates that are caused by heterogeneity; and (iv) shear thinning leads to complex fingering patterns with narrower fingers affecting the flow and displacement efficiency.

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Poster / 530

CO₂ storage site characterization using variational autoencoders

Authors: Bao Jichao¹; Hongkyu Yoon²; Jonghyun Lee³

¹ *University of Hawaii*

² *Sandia National Laboratories*

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Characterization of geologic heterogeneity is crucial for reliable and cost-effective subsurface management operations, especially in problems that involve complex physics such as field-scale carbon storage and unconventional oil and gas operations. With recent advances in computational power and sensor technology, large-scale aquifer characterization using various types of measurements has been a promising approach to achieve high-resolution subsurface images. However, traditional large-scale inversion approaches require high, often prohibitive, computational costs associated with large-scale coupled numerical simulation runs and large dense matrix multiplications. As a result, traditional inversion techniques have limited utility for problems that require fine discretization of large domains and a large number of hydrogeophysical measurements to capture small-scale heterogeneity. In this presentation, we apply a deep-generative model-based Bayesian inversion method for large-scale carbon storage site characterization and forecast. To be specific, novel variational autoencoders are used to learn the approximate distribution from multipoint geostatistics-derived training images as a prior and accelerated stochastic inversion is performed on the low-dimensional latent space in a Bayesian framework. Numerical examples with synthetic 2D permeability fields with fluvial channels confirm that our proposed method provides promising subsurface site characterization with reliable uncertainty quantification.

SNL is managed and operated by NTESS under DOE NNSA contract DE-NA0003525.

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MS03 / 531

Proppant Transport and Coverage in Rock Fractures –A Computational Modeling Approach

Authors: Farid Roustaf^{None}; Amir Mofakham¹; Dustin Crandall²; Goodarz Ahmadi¹

¹ *Clarkson University*

² *US Department of Energy - National Energy Technology Laboratory*

Corresponding Authors: dustin.crandall@netl.doe.gov, gahmadi@clarkson.edu, roustaf@clarkson.edu, abdolla@clarkson.edu

A pressurized liquid with proppants is injected into wellbores during hydraulic fracturing to create fractures in rock formations. After removing the high pressure, proppant (typically sands) are trapped throughout the passage keeping the fracture open. The extraction productivity from reservoirs is significantly affected by the distribution of proppants in the fracture. The goal is to have roughly uniform and high proppant coverage in the passage. Since the experimental investigations to examine the process are challenging and costly, in this study, computational modeling tools are used to provide significant insights into the process. Accordingly, a 4-way coupled Computational Fluid Dynamic and Discrete Element Method (CFD-DEM) using the Star CC+ and Rocky-Ansys-Fluent codes were used to simulate proppant transport into a numerically generated realistic rock fracture configuration.

A series of simulations with different proppant sizes and various fluid flow rates were performed. The corresponding fracture coverages for different proppant sizes and fracture apertures were evaluated and compared. It was also shown that the ratio of proppant diameter to the mean aperture size significantly affects the fracture coverage. The corresponding optimum proppant sizes for different fracture apertures were evaluated.

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MS06-A / 532

Thermodynamics of continuum scale immiscible and incompressible two-phase flow in porous media: A statistical mechanics approach using the Color Lattice-Boltzmann model

Authors: Håkon Pedersen¹; Santanu Sinha¹; Alex Hansen¹

¹ *PoreLab, NTNU*

Corresponding Authors: alex.hansen@ntnu.no, santanu.sinha@ntnu.no, hakon.pedersen@ntnu.no

Continuum scale steady-state two-phase flow in porous media can exhibit non-linear dependence on the pressure gradient, a phenomenon which is incompatible with relative permeability theory [1]. If the flow is immiscible and incompressible, it can be described in terms of a thermodynamic framework by considering averaged quantities through surfaces perpendicular to the overall direction of flow. With the assumption of Euler homogeneity on the flow, the seepage velocities can be replaced by a total flow velocity and a co-moving velocity, which consists of the difference between the two flow velocities and an additional term that depends on the saturation gradient of the total flow [2]. This function turns out to be linear in the correct choice of variables, resulting in a simple relation with only two parameters. A connection between this thermodynamic framework and statistical mechanics can be made by formulating a differential area distribution function associated with the local velocities in the slice from which the velocity distributions of the phases can be obtained. We demonstrate that only the total velocity distribution of a slice and the location and pore areas of the phases is needed to obtain the co-moving velocity, which eliminates the need to measure the individual velocities of both fluids. This simplifies the process of obtaining macroscopic flow properties, since knowledge of the co-moving velocity and one of the saturations can be used to determine the individual flow velocities [3]. This description, as opposed to relative permeability theory, is compatible with non-linearities in the flow [4], as these can be accounted for in the co-moving velocity without issue. We investigate the co-moving velocity via the differential pore-area distributions using Lattice-Boltzmann simulations on three dimensional CT-scans of real porous materials, and show that the results are compatible with the proposed thermodynamic description.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 533

Modeling contrast perfusion and adsorption in the 3D heart

Authors: RODRIGO Weber dos SANTOS¹; Evandro Dias Gaio²; Bernardo Rocha²

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This work presents a mathematical model to describe the dynamics of perfusion in cardiac tissue. The new model extends a previous one ¹ and is able to reproduce clinical exams of contrast-enhanced cardiac magnetic resonance imaging (MRI) of the whole heart (3D) obtained from patients with cardiovascular diseases, such as myocardial infarct.

The new model treats the extravascular and intravascular domains as distinct porous media, where Darcy's law is adopted.

We propose reaction-diffusion-advection equations to capture the dynamics of contrast agents that are typically used in MRI perfusion exams. The identification of myocardial infarct is modeled via adsorption of the contrast on the extracellular matrix.

Different scenarios were simulated and compared to clinical images: normal perfusion; endocardial ischemia due to stenosis; and myocardial infarct. Altogether, the results obtained suggest that the models can support the process of non-invasive cardiac perfusion quantification.

¹ Simulation of the Perfusion of Contrast Agent Used in Cardiac Magnetic Resonance: A Step Toward Non-invasive Cardiac Perfusion Quantification. JR Alves, RAB de Queiroz, M Bär, RW dos Santos. *Frontiers in Physiology* 10. 2019

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS14 / 535

Multiscale mixed domain decomposition methods for the simulation of heterogeneous black-oil flows

Authors: Fabricio S. Sousa¹; Vitor A. Pires¹; Rafael T. Guiraldello^{None}; Roberto F. Ausas²; Gustavo C. Buscaglia²; Felipe Pereira³

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² *University of São Paulo*

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Multiscale domain decomposition methods have proven to be a reliable way for solving single and two-phase flows in porous media. Among the advantages, the possibility to speed up the parallel simulation of huge domains with nearly ideal performance, is perhaps the most useful for applications in uncertainty quantification. However, in applications such as petroleum reservoir simulation, a more complex black-oil model is often required, which allows the simulation of three different components (water, oil and gas) that form at most three different phases (aqua, liquid and vapor), with possible mass transfer between phases. Among the multiscale domain decomposition methods employed in the solution of such models, are the MMMFEM 1 and MSFV [2].

In this work, we extend the Multiscale Robin Coupled Method (MRCM), a multiscale domain decomposition method recently introduced by the authors [3], for the solution of compressible heterogeneous black-oil model. The MRCM generalizes known mixed methods through the suitable choice of Robin-type boundary condition parameters and the finite element spaces used to span the interface unknowns, introducing flexibility and the possibility of adaptive schemes that greatly increase accuracy when compared to standard techniques. The hyperbolic conservation laws are handled by high order conservative finite volume schemes, while the parabolic pressure equation is discretized by implicit schemes, allowing the application of the domain decomposition method in each time step of the simulation.

We employ a number of test cases to evaluate the application of the MRCM for black-oil simulations, in homogeneous and heterogeneous media. The results show that the MRCM, combined with suitable downscaling techniques, can be successfully employed for the solution of black-oil flows, with good accuracy as compared to the solution of undecomposed cases.

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References:

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<https://doi.org/10.1016/j.jcp.2017.11.002>

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

Poster / 536

Chemotaxis promoted bacterial transport toward residual NAPL in a dual-permeability microfluidic device

Author: Beibei Gao^{None}

Co-authors: Roseanne Ford ; Xiaopu Wang¹

¹ *China University of Petroleum*

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Nonaqueous phase liquid (NAPL) contaminants which persist in subsurface environments due to low solubility and flow heterogeneity may be more accessible to chemotactic bacteria in bioremediation contexts. Chemotactic bacteria bias their swimming motion upon sensing chemical gradients, such as performing longer runs toward sources of chemoattractants (e.g., naphthalene), which increases the contact of microbes and NAPLs. This work aimed to investigate the transport of chemotactic bacteria in a dual-permeability microfluidic device with chemoattractant-containing NAPL under flow conditions, mimicking NAPL contaminated aquifers. Microscopic imaging of bacteria in the pore space revealed accumulation of chemotactic bacteria near NAPL surfaces at the junction of high and low permeability areas; however, no chemotaxis was observed near NAPL in flow through pathways. Weak convection and steeper chemoattractant gradients in the junction regions strongly regulated the transport of chemotactic bacteria, according to our simulations, which fully captured the pore geometry. We also applied continuum-level models of bacterial transport where dispersion was included in diffusion term to account for the effect of flow heterogeneity. Chemotactic bacterial transport in porous media often requires adjustments of chemotactic velocity to a certain extent to match experimental data. However, our simulation required no modification in chemotaxis convection term, rather a 50% increase in the dispersion of chemotactic bacteria, which is consistent with conclusions in de Anna et al. (2020) that chemotaxis can modulate bacterial dispersion in porous media. The experiment and simulations provide insight into the interplay between chemotactic bacteria and pore-scale chemical gradients, and its impact on macroscale transport in subsurface environments.

Studies in liquid media showed chemotaxis toward NAPL was undermined at higher flow velocities. However, in porous media, chemotactic bacteria can benefit from stronger convection by being brought to closer contact with residual NAPL in the junction regions. In our experiments of bacterial transport under varying pore velocities, maximum accumulations of chemotactic bacteria at the junction were achieved at fluid velocities much higher than those in Wang et al. (2012). To understand the effect of pore confinement on bacterial transport, we proposed two time scales related to convection and chemotaxis, respectively, and applied machine learning techniques to investigate the correlation between bacterial accumulation and physical conditions such as pore velocity, chemical distribution, and pore dimension.

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References:

- 1 T. Long and R. M. Ford, "Enhanced transverse migration of bacteria by chemotaxis in a porous T-sensor," *Environ. Sci. Technol.*, vol. 43, no. 5, pp. 1546–1552, 2009.
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS12 / 537

A macro-scale elasto-thermo-viscoplastic constitutive model for saturated frozen soils

Authors: Dana Amini¹; Maghoul Pooneh²; Hollaender Hartmut³

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Slow-rate time-dependent behavior (i.e., creep) of frozen soils is experimentally observed in the literature. From a poromechanical point of view, frozen soil is a medium composed of a deformable solid skeleton and a porous space filled with unfrozen water and ice. In addition to pore ice, ice-rich permafrost can also contain thin ice lenses. The rheological properties of saturated frozen soils due to the coexistence of ice and viscous unfrozen water cause slow rate deformation and loss of shear strength of the soil. Temperature, applied stress conditions, ice content, soil type, and density are key factors controlling the viscoplastic reorganization of the inter-particle microstructure and, subsequently, the creep rate of frozen soils. In this study, an Elasto-Thermo-ViscoPlastic (ETVP) constitutive model for frozen soils is formulated within the framework of two-stress state variables in which the cryogenic suction and the net solid phase stress are defined as state variables. In the proposed model, the impacts of the aforementioned factors and their interdependencies, as well as the current state of the frozen soil structure on the creep deformation of frozen soils, are properly considered based on a phenomenological (macro-analytical) point of view.

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MS16 / 538

A One-Dimensional Numerical model of Carbon Corrosion in Catalyst Layers of Proton Exchange Membrane Fuel Cells

Authors: Dong Enci¹; Zhang Ruiyuan¹; Chen Li¹

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The short lifetime of membrane electrode assemblies (MEAs) is one of the main obstacles for large-scale commercialization of proton exchange membrane fuel cells (PEMFCs). Carbon corrosion under certain transient operations such as start-up/shutdown and local hydrogen starvation can induce significant degradation of the catalyst layer, which will destroy the connectivity of carbon skeleton, cause collapse of the solid structures, change the wetting characteristics, increase the catalyst particle size, and reduce the cell performance. In order to accurately predict the lifetime of MEAs, a one-dimensional numerical model of carbon corrosion in catalyst layer (CL) is established in this study. It is found that carbon weight loss is about 4% after 2000 square wave potential cycles, and the numerical results are in good agreement with the experimental data. Besides, this study develops the quantitative relationship between carbon corrosion ratio and catalyst layer structural parameters such as carbon particle size, catalyst layer porosity and catalyst layer thickness. It is found that carbon corrosion has a significant effect on the structure of catalyst layer and will further increase the mass transport resistance of oxygen. It is demonstrated that an in-depth understanding of the carbon corrosion mechanism and the according structure evolution of the catalyst layer are of far-reaching significance to further improve the lifetime of the PEMFCs.

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MS07 / 539

Influence of Pore Morphology on Mechanical Properties of Second Gradient Materials

Authors: Pania Newell¹; Bozo Vazic¹

¹ *The University of Utah*

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Porous materials with heterogeneous porous structures possess a wide range of mechanical, thermal, or electrical properties. Therefore, they are widely used in different engineering fields, such as energy-storage technology, geothermal engineering, and bio engineering. Considering the strong influence of pore morphology on material properties and their diverse application, over the years variety of homogenization techniques based on averaging different fields, such as stress, strain, and deformation energy density, have been developed to efficiently transfer material properties from micro to macro scale. For porous materials with complex pore morphology, most homogenization techniques fail to capture the absolute size and distribution of the pores as they are based on classical continuum theory. To account for the pore shapes and variability in the pore distribution besides the

porosity, in this study, we adopt a higher-order asymptotic homogenization method. The advantage of higher-order homogenization becomes apparent when developing complex multiscale structures is best described by incorporating higher-gradient effects. This can be especially observed in biological materials that are highly heterogeneous (e.g. bone tissue) and have hierarchical structures that demand higher-gradient effects to be included in modeling their mechanical responses as well as in their multi-physics simulations. The higher-order scheme is an extension of the first-order computational homogenization framework where the use of a generalized continuum enables us to introduce the length scale into the material constitutive law and capture the absolute size of the pores and pore distribution. By employing this model, we studied a set of numerical problems with different combinations of porosity, pore shapes, and distributions. The results show a strong influence of pore shape on the effective material properties, with some shapes having a more noticeable impact than others (e.g., circle and square pores have an almost identical effect). However, analysis of pore distribution demonstrates little to no effect on effective material properties. Moreover, we observed that even for isotropic matrix material, different pore shapes will produce different material behavior, such as elliptic pores producing orthotropic material behavior while circular and square pores lead to cubic material behavior. Furthermore, the results for higher-order parameters show a strong influence of the pore shape/distribution and the size of the representative volume element.

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MS01 / 541

Monitoring of Brine Leakage form Carbon Storage in Deep Saline Formations: Method Validation Using Intermediate-Scale Testing

Author: Tissa Illangasekare^{None}

Co-author: Ahmad Askar¹

¹ *Intera*

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Injecting CO₂ for storage into deep saline formations is a promising technology for minimizing the amount of released greenhouse gas released into the atmosphere, contributing to global warming. The pressure build-up in the storage formation during an injection can affect the caprock integrity, leading to pressure-driven leakage of native brine or CO₂, posing a contamination risk in shallow aquifers. Hence, developing strategies for monitoring such leakage events and possible remediation action should be a part of selecting and implementing carbon capture and storage (CCS) operations. Regulatory constraints are in place to protect the aquifer water used for drinking. The complexities associated with deep geological settings and flow and transport in multiple heterogeneous layers

of the storage, intermediate and shallow aquifers preclude the direct adaptation of the monitoring methods and approaches that have been developed and validated for traditional problems in shallow aquifers. Hence to address problems associated with brine leakage, new approaches have to be developed and validated before field implementation of CCS. As field CCS systems are at pilot testing stages and no field data exists on leakage events, the only currently available option for validation is the use of numerically generated synthetic data. This approach has a significant shortcoming as the available models are not validated for their ability to capture complex processes. This paper presents a method where an intermediate scale test system was used to generate data to validate a model that is used to develop a monitoring approach. A framework for designing monitoring systems that optimally use relatively readily available shallow zone data and hard-to-make deep zone observations was developed and validated. Basic to this framework is calibrating a transport model using monitoring data to determine leakage source conditions and then predicting brine plume contaminating the shallow aquifer. As it is expected that cost considerations limit monitoring the deep zone, the framework is developed to minimize the deep zone observations (e.g., using sensors). The best placement locations selected from a predefined number of observation points to provide the most worthwhile monitoring data that reduces predictive uncertainty is determined by integrating linear uncertainty analysis with the Genetic Algorithm. The framework was tested in an intermediate-scale soil tank, where monitoring data on brine leakage plume development from the storage zone to the shallow aquifer was collected. Predictions using a transport model using the data were then compared with experimental observations to evaluate the informativity of the monitoring locations. The results demonstrated the ability of the framework to select the most informative deep monitoring locations. It was also found that the deep observations and shallow zone data are worthwhile to determining source conditions. The results showed the possibility of identifying the likely areas of impact of shallow aquifer using early-stage monitoring data.

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MS08 / 542

Laboratory-Scale Investigation of Secondary Sulfate Precipitation in Marcellus and Wolfcamp Shales

Author: Asli Gundogar¹

Co-authors: Adam Jew²; John R. Bargar³; Anthony Kavscek⁴

¹ *Postdoctoral Scholar*

² *SLAC*

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⁴ *Stanford University*

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Geochemical changes in fractured shales may influence long-term production efficiency. The complex composition and morphology of shale minerals and formation brine composition as well as stimulation fluid make the interpretation of shale-fluid interactions very challenging. Reaction-induced evolution of shale fabric, pore water, and the associated evolution of porosity and permeability alteration remain unclear. There is a need for further investigation to improve recovery and environmental sustainability. In this reactive flow-through study, multi-instrument (X-ray computed tomography (CT) and scanning electron microscopy (SEM)) imaging from nm's to cm's together with mineral surface (energy dispersive spectroscopy (EDS)), and time-resolved fluid analysis (inductively coupled plasma-mass spectrometry (ICP-MS)) were employed for a comprehensive evaluation of the shale-brine-fracture fluid interactions. The study cores were from Marcellus and Wolfcamp formations, that are major contributors to US gas and oil supply. According to quantitative X-ray diffraction and EDS analysis, both samples have a clay-rich mineralogy (over 30.8 wt%) and a small carbonate content (less than 5 wt%). Lab-generated brine and fracture fluid (pH 2) solutions were sequentially injected under confining stress (up to 500 psi) at reservoir temperature (80°C). This experimental study simulated deeper matrix zones with mostly microcracks away from the main fractures where the flow rate is much slower (below 0.02 mL/min) than the vicinity of the main flow channels. For the Marcellus sample, synthetic brine was used that mimics the basin-specific formation brine composition, while the reactive fluid was formulated based on field-based stimulation fluid with typical industrial additives. For the Wolfcamp sample, actual cleaned brine from the Permian Basin of Texas was used as the formation water and as the base fluid of the HCl-acidified fracture fluid without additives. After reactive flooding occurred, the permeability and fracture porosity values of both cores decreased significantly. Based on the SEM-EDS data, barite crystals were prominent throughout the reacted MSEEL inlet, outlet, and crack surfaces. Barite was attributed to the mixing of Ba-rich brine solution with fracture fluid, including persulfate-containing breakers. Time-resolved ICP curves revealed that barite formation occurred as soon as the fracture fluid mixed with the resident brine and continued until dissolved Ba was consumed. Similarly, secondary strontium sulfate precipitates were evident on the reacted Wolfcamp surfaces as well-formed euhedral crystals and concentrated adjacent to the microcracks and grew along the microcrack surfaces. This intense interaction of the shale surfaces with the injected fluids leads to large, impermeable precipitates that plug and seal fractures thereby reducing permeability, preventing reactive fluid from passing through the inner matrix layers, and inhibiting recovery from the deeper zones. These findings provide direct experimental confirmation under in situ conditions of sulfate scale formation, particularly near microcracks that are suspected to be critical in productivity of fractured shale wells. These observations provide data crucial to help producers develop scale mitigation methods by optimizing the stimulation fluid compositions and produced water treatment practices.

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MS06-B / 545

Factors influencing shale wettability from nano to macro-scale

Authors: Ahmed Reda Fathy¹; Muhammad Arif¹; Stefan Iglauer²

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² *Edith Cowan University*

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Shale rocks remain the least understood sedimentary rocks. In particular, shale rocks depict a complex wetting behavior which is arguably due to complex microstructure of shales. This work investigates wettability of shale/decane/brine systems as a function of pressure, temperature and brine salinity. Moreover, nano-fluid aged shale surfaces are also investigated to examine the potential nanoparticles for shale wettability alteration. To elucidate the wetting behavior, advancing and receding contact angles are measured for pressures ranging from 0.1 MPa to 20 MPa and temperatures ranging up to 323 K. Three shale samples (Mancos, Eagle Ford and Wolf Camp) are investigated. The results indicate that all shale surfaces demonstrate distinct wetting behavior at ambient and high pressure conditions. For instance, Mancos was water-wet while Eagle Ford and Wolf Camp depicted oil-wet state. Increase in pressure resulted in a slight increase in contact angle –which contradicts some previously published literature findings. Notably, the temperature effect was quite inconsistent i.e. for Mancos and Wolf camp increase in temperature led to more oil-wet surfaces while Eagle Ford turned more water-wet with increasing temperature. This discrepancy may be attributed to high quartz content of Eagle Ford samples. Moreover, with increasing concentration silica nanoparticle, shale surfaces turned much more water wet. This can have implications for the use of silica as an additive in hydraulic fracturing and potential chemical EOR options. The optimum concentration for maximal wetting alteration were 1 wt. % for Eagle Ford, and 5 wt. % for Wolf Camp and 2 wt. % for Mancos.

A high degree of heterogeneity was also evident from the obtained SEM images of all samples and nanoparticle adsorption was also observed in some of the samples at micro-scale. More interestingly, surface roughness of all shale samples were investigated via AFM (Atomic Force Microscopy) before and after exposure to nano-fluids and the results indicated an increase in nanoscale surface roughness after nano-fluid treatment. Lastly, Fourier Transfer Infrared Spectroscopy measurements were also conducted on all shale samples and an abundance of oxygen containing functional groups was observed for Mancos sample which explained its water-wet behavior.

The results of this study thus provide new insights into the factors affecting shale rock wettability from nano to macro-scale. The results have implications for understanding fluid flow in shale rocks.

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Reactive Transport Modeling of Dissolution/Precipitation in Fractured Porous Media

Author: Hossein Fazeli¹

Co-author: Florian Doster

¹ *The Heriot Watt University*

Corresponding Authors: f.doster@hw.ac.uk, hf2014@hw.ac.uk

During CO₂ injection into geological reservoirs, CO₂ may flow through faults and fractures present in the seals. CO₂ dissolution can acidify the formation water and drive a range of mineral reactions; For instance, the CO₂-acidified water can cause silicate mineral dissolution, which releases ions to solution. These ions can later react and form secondary minerals such as carbonates. These reactions may either increase the porosity (mineral dissolution) or decrease it (mineral precipitation). The reactions creating porosity may increase the permeability of the fracture networks in the seals and also reduce the capillary entry pressure, which can lead to the CO₂ leakage. On the other hand, formation of new minerals may decrease the permeability of the fracture systems and increase the caprock integrity. To predict how the dissolution and precipitation reactions affect the permeability of the fracture network in the fractured caprocks, we develop a model that can simulate the reactive transport processes in fractured networks. The reactive transport model is based on the Discrete fracture and matrix (DFM) model and is implemented in the MATLAB Reservoir Simulation Toolbox (MRST). Since in the fractured media the fluid transport rates are usually high, most of the mineral reactions considered in the model are treated as kinetic reactions. The developed model is then used to simulate the reactions between CO₂-acidified brine and minerals in different fracture networks (including a fracture network from Svalbard).

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MS09 / 547

Predictive multi-scale network models with micro-porosity

Authors: Sajjad Foroughi¹; Branko Bijeljic²; Martin Blunt³

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In pore-scale imaging, it is often not possible to visualize pores of all scales present in one experiment due to the resolution/sample size trade-off. This sub-resolution pore space for some rocks such as Estailades or the reservoir sample is a significant fraction of the total porosity. We consider this sub-resolution pore space as the micro-porosity. Differential imaging makes it possible to identify micro-porosity in a micro-CT experiment and to quantify its porosity. Including micro-porosity in the pore network model leads to correct saturation and pore volume. Also, it is essential to improve our prediction of connectivity and permeability. Furthermore, it has a significant effect on the accessibility to network elements. In this study microporosity is modeled using a multiscale pore network model. Sensitivity analysis on the effect of micro-porosity in pore network modeling demonstrates the importance of microporosity in pore network modeling for both single-phase flow and multiphase flow.

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MS07 / 548

Linear lignin as a potential consolidant for archaeological wood treatment: a hybrid Monte Carlo and molecular dynamics study

Author: Ali Shomali¹

Co-authors: chi zhang ²; Wenqiang Liu ³; Benoit Coasne ⁴; Eleanor J. Schofield ⁵; Dominique Derome ⁶; Jan Carmeliet ⁷

¹ *ETH Zurich*

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Lignin is one of the abundant polymers found in wood cell wall composite acting as the cohesive matrix that surrounds the wood holocellulose and provides increased hydrophobicity and chemical

stability to the composite. Due to its less susceptibility to biological attack and high compatibility with holocellulose, synthesized lignin-like oligomers have been considered as potential consolidation material for archaeological wood [1]. In addition, cellulose mixtures have attracted increased attention for the production of novel material, biofuels and, chemicals. Due to the highly heterogeneous structure of lignin and complications of its extraction in experimental approaches, relatively little evidence exists on lignin and cellulose interaction and its response to water adsorption on molecular level. In the present study, atomistic modeling is employed to investigate hygromechanical properties of lignocellulose mixtures and to inform the role of lignin as a consolidation agent in wood composite. Mixtures of amorphous cellulose with uncondensed coniferyl and sinapyl lignin are prepared by employing an iterative hybrid all-atom molecular dynamics and grand canonical Monte-Carlo (GCMC) simulation [2] as a model representing wood holocellulose and lignin matrix, hydrated in a range relative humidity from fully dry to saturation pressure. The hybrid GCMC/MD technique provides an excellent tool to capture the highly coupled nature of sorption-induced swelling in the lignocellulose mixture by enabling us to capture the sorption by applying relative humidity in GCMC and allowing the resultant swelling during relaxation in the MD stage of the simulation. The presented model, methodology and the choice of simulation parameters such as system size are validated through comparison with available simulation and experimental data. By applying the mechanical tests to hydrated samples role of lignin in adsorption-induced mechanical softening in wood polymer is also studied. The sorption isotherms, swelling curves and mechanical data reveal reduced moisture adsorption and swelling together with mechanical softening as the lignin content increase signifying the effect of the polymer interaction, which is further characterized by measuring porosity pore size distribution, hydrogen bonding network and cohesive energy calculation. Rule of mixture is introduced as an analysis tool to reveal the role of polymer interphase [3]. The underlying molecular mechanism describing the lignocellulose Hygromechanical response is compared to what we learned in our recent studies regarding molecular phenomena involved in polyethylene glycol consolidation of wood in order to unravel molecular characteristics of an inspired wood cell wall consolidant.

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MS02 / 549

Effects of Fluid Saturation on Unsaturated Soil Hydraulic and Solute Transport Parameters

Authors: Luwen Zhuang¹; Rien van Genuchten²

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² Utrecht University, Netherlands

Corresponding Authors: rvangenuchten@hotmail.com, luwen.zhuang@outlook.com

Through this Interpore 2022 presentation we like to acknowledge the exceptional scientific and professional contributions by Sjoerd van der Zee during his nearly 40-year career at Wageningen University. His contributions covered multiple topics in soil hydrology, geochemistry, contaminant transport, ecohydrology, water reuse, soil salinity, and stochastic modeling at a range of spatial and temporal scales. We present several examples consistent with his long-time work. One set of examples concerns the formulation and testing of alternative descriptions of the unsaturated soil hydraulic properties in attempts to cover the water retention (Pc-S) and unsaturated hydraulic conductivity (relative permeability) relationships over the entire pressure head range. A second example deals with the water content dependency of the solute dispersivity in both classical equilibrium and nonequilibrium contaminant transport models. Detailed laboratory tracer experiments showed a clear non-monotonic relationship between the dispersivity and soil water saturation, with the extent of non-monotonicity depending upon soil texture.

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MS07 / 550

Numerical investigation of the flow and phase transitions of CO₂ near its triple-point during a blowout from a plugged well

Authors: Pramod Bhuvankar¹; Abdullah Cihan¹; Jens Birkholzer¹

¹ *Lawrence Berkeley National Laboratory*

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The dry-ice formation of CO₂ near its triple-point can occur during a blowout event in plugged wells, and this process can impact the mass flux of the leaking CO₂. From a risk assessment standpoint relating to geologic carbon sequestration, we wish to understand which scenarios will lead to the dry-ice formation, and how this process affects the CO₂ flux. In the current work we present a numerical method that can solve for the flow and the supercritical-liquid-gas-solid phase transitions of CO₂ over a wide range of pressures.

The first part of the presentation explains the numerical method. Our in-house code solves the compressible 1D Navier Stokes and energy transport equations along with a hybrid equations of state module. To capture any shocks that may occur during the blowout, we use a Godunov-type Riemann-solver based scheme explained in the work of Toro et al. (1994). Our hybrid equations of state comprise of two modules, the first of which covers the gas-liquid-supercritical phase transitions above the triple-point pressure. The second module covers gas-ice and triple-point phase transitions occurring below the triple-point pressure. The former module is an open-source code made available by Fang et al. (2019), and the latter module consists of a Span-Wagner based lookup table that we created by following the work of Hammer et al. (2013). It is important to mention that all phase transitions in the present work are assumed to obey the Homogeneous Equilibrium Model. This

model assumes all phases of CO₂ at a fixed point in space and time to have the same temperature, pressure, and velocity. In the case of ruptured flow, the outlet pressure is assumed to be atmospheric pressure, unless we observe choked outflow, wherein the speed of CO₂ exceeds its speed of sound. In the case of choked outflow, we iteratively determine the outlet pressure such that the resulting outflow has a Mach number of 1. We demonstrate the effectiveness of the numerical method by presenting two benchmark simulations of the shock-tube problem and a simulation of the CO₂ leak experiment of Brown et al. (2014).

The second part of this work presents simulations of the blowout from a 1500m deep plugged well that is linked to an infinite reservoir of CO₂. The cement plug at the top end of the well ruptures at $t = 0$, causing a blowout of the CO₂. We simulate different reservoir pressures and their impact on the CO₂ flux. We also examine the mass fraction of dry-ice at the rupture location and its impact on the leakage flux of CO₂. We conclude the presentation by laying out our future work in this project on CO₂-hydrate modeling and the related challenges.

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References:

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS22 / 551

Gold Nanocomposite Contact Lenses for Ocular Health Management

Authors: Haider Butt¹; Ahmed E. Salih¹; Mohamed Elsherif^{None}; Fahad Alam^{None}

¹ *Khalifa University*

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Color vision deficiency (CVD) or color blindness is an inherited genetic ocular disorder affecting millions of people around the globe. CVD is a common ocular disorder affecting, for example, an estimated 8% of males and 0.5% of women of Northern European descent. It limits distinguishing between specific colors depending on the CVD type and severity of the disorder. CVD patients may

experience problems in work and everyday life when matching or discriminating between fine colors. Since there is no cure for color blindness so, the sufferers use wearables to enhance the color perception. The most commonly used wearables include tinted glasses, which act as optical filters and filter out the optical bands (540-580 nm) for the red-green CVD patients. In contrast there are a few studies, which have presented the fabrication of tinted contact lenses for color blindness, and several issues related to their mechanical properties and toxicity were reported. In this study, gold nanoparticles were integrated into the soft hydrogel material based contact lenses, thus forming nanocomposite contact lenses targeted for red-green CVD application. The integration of nanomaterials into hydrogels is a prominent research challenge for a myriad of healthcare applications, such as bio-sensing, cancer therapy, and bone tissue engineering. In particular, practical contact lenses, functionalized with metallic nanoparticles are of interest for therapeutics and targeted therapy. Several types of nanoparticles were synthesized, characterized and incorporated within the pHEMA hydrogel material based contact lenses, and their resulting optical, mechanical, hydration and material properties were assessed. The optical transmission properties of the developed nanocomposite lenses were found to be analogous to those of the commercial CVD glasses, and their water content and wettability properties were better in comparison to some of the commercially available contact lenses used for cosmetic/vision correction purposes. Hence, this work demonstrates the potential usage of gold nanocomposite contact lenses in ocular health management and, more generally, color filtering applications.

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A.E. Salih, M. Elsherif, F. Alam, A.K. Yetisen, H. Butt*, Gold Nanocomposite Contact Lenses for Color Blindness Management, ACS Nano, 10.1021/acsnano.0c09657 (2021) IF: 14.59

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS02 / 552

A Novel Mass Transport Model for Direct Contact Membrane Distillation Flux Prediction

Authors: Isam Janajreh¹; Khadije Elkadi¹

¹ *Khalifa University*

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Owed to its promising permeate flux production, direct contact membrane distillation (DCMD) has been promoted as competitive substitute for conventional water purification and desalination technologies. In DCMD, a porous hydrophobic membrane is placed in partition between a hot feed and fresh cold permeate channels. Water vapor transports through the porous membrane from the feed side to the permeate side due to pressure gradient. This mass transport phenomenon is typically explained by the Kinetic Theory of Gases which suggests Knudsen diffusion, molecular diffusion or Poiseuille flow 1. The non-uniformity of fabricated membrane pores can lead to the occurrence of

more than one transport phenomenon, and thus, a combination of the previously mentioned models is also possible. Deciding which one of these options is appropriate to describe vapor flow in the porous membrane is challenging. Deep understanding of membrane morphology and operational conditions is crucial for accurate description of mass transport. So far, several attempts of mass transport combination models were spotted in literature to predict the actual DCMD membrane permeability. Nevertheless, a wide discrepancy is still present between the available models when tested for the same experimental setup and operating condition [2]. This is due to the marginalized impact of DCMD operating conditions, e.g., inlet feed and permeate velocities. In this work, a unique combination model is proposed to predict permeate flux of DCMD taking into account different inlet conditions. Assessments are performed utilizing a validated steady non-isothermal computational fluid dynamics (CFD) model. Eventually, the proposed model is compared with existing models to assure a reliable estimation of the permeate flux under a wide range of operating conditions.

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- 1 M. Khayet, M. Godino, J. Mengual, Modelling transport mechanism through a porous partition, *J. Non-Equilib. Thermodyn.*, 26 (2001) 1–14.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS01 / 553

Direct pore-level multiphysical model for solar thermochemical fuel production reactor based on structured porous media

Authors: Da Xu¹; Meng Lin²

¹ *Department of Mechanical and Energy Engineering, Southern University of Science and Technology*

² *Southern University of Science and Technology*

Corresponding Authors: 12049050@mail.sustech.edu.cn, linm@sustech.edu.cn

Solar-driven thermochemical fuel production cycle is one of important route for effective conversion and storing dilute and fluctuation solar energy into value-added fuels. The performance of a thermochemical reactor is largely dependent on the porous media design. The reacting porous media should simultaneously facilitate heat and mass transfer, provide reaction sites, as well as maintain large mass loading. Optimization of porous media structures are essential for further reactor optimization to achieve high solar-to-fuel efficiency. In this study, we developed a fully coupled multiphysical model in 3D based on the actual morphology of porous media under direct solar irradiation. This model couples solar absorbing in volumetric photo-absorber, fluid flow of inert sweeping gas, multi-mode heat transfer, as well as detailed bulk and surface chemical reactions. The coupled 3D model offers a high fidelity to access the solar-to-fuel performance of various structured porous media. Owing to its 3D nature, the model allows for accurate calculation for the gradient structure

design (e.g., artificially introduced anisotropy) to balance mass loading (thermodynamics) and reaction kinetics can be identified. Particularly, a detailed reaction kinetics model including chemical diffusion as well as chemical surface exchange is considered to identify the kinetic limiting regimes for various structure designs. Further, the impact surface roughness factor on the surface kinetics is studied in order to figure out potential of introducing surface modifications in the case of surface limited reaction kinetics.

This study offers a high-fidelity modeling framework for the optimization of porous structures for solar thermochemical applications. The coupled multiphysical model enables to simultaneously coordinate various involved physics including heat and mass transfer, species transport, solar absorption, as well as bulk vs. surface kinetics.

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Time Block A (09:00-12:00 CET)

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Online

MS15 / 555

Machine Learning for Porosity and Absolute Permeability Prediction from Carbonate Rock Images

Authors: Ramanzani Kalule¹; Hamid Abderrahmane^{None}; Waleed Alameri¹; Mohamed Sassi^{None}

¹ *Khalifa University*

Corresponding Authors: mohamed.sassi@ku.ac.ae, kramanzani@gmail.com, waleed.alameri@ku.ac.ae, hamid.abderrahmane@ku.ac.ae

Abstract—Several empirical or theoretical models have been proposed in the literature to predict or correlate porosity and permeability and other reservoir-based properties, their generalizability is still quite prohibitive [2]. This is because several reservoir property relationships are highly complex and nonlinear. Properties such as permeability cannot accurately be estimated using simplified or linear relationships [3]. The nonlinear relationship can make the estimates of rock properties using linear relationships inaccurate. Numerous machine learning (ML) models and deep neural networks (DNN's) have been reported to accurately handle nonlinear relationships in various scientific studies [4]. Several successful studies on predicting porosity and absolute permeability using ML or DL have been reported in the literature.

This study presents the capabilities of various machine learning-based regression algorithms in predicting rock porosity and absolute permeability from carbonate rock images. We adopt an ensemble learning approach, stacking that integrates predictions from several machine and or deep learning-based models into a single model to accelerate predictions and generalizability. Stacking is presented in two different ways with one based on typical ML models and the other designed with multiple DNN models of various architectural designs. The ML models adopted are both linear and non-linear including multiple linear, ridge, lasso, random forest, and gradient boosting regression models. We also adopt the use of the randomized search algorithm for optimal hyperparameter search over a wider hyperparameter space for each of the models. Our dataset is a set of micro-CT images scanned

at different resolutions, from four different carbonate core samples. The selected rock samples exhibit different levels of heterogeneities and a wide range of absolute permeability. Averaged rock pore properties are extracted from each of these images using a watershed-scikit-image technique to represent the input features to the selected models. Results obtained from this study, show that both stacking approaches proposed can outperform the individual selected models. However, stacked ML models require more computational time, in contrast to stacked DNN's and the individual ML and DNN-based models. Concerning the individual models, we note that linear models are not able to generalize the dataset while nonlinear models require higher computational time than linear and DNN models. The trained individual models and the proposed ensembled stacked models predict the rock porosity and absolute permeability accurately in a few seconds. The study provides a valuable approach for predicting rock sample porosity and absolute permeability from several rock image samples within seconds.

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References:

- 1 S. M. R. Niya and A. P. S. Selvadurai, "A Statistical Correlation Between Permeability, Porosity, Tortuosity and Conductance," *Transp. Porous Media*, vol. 121, no. 3, pp. 741–752, 2018.
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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 556

Pore-scale imaging of asphaltene deposition with permeability reduction and wettability alteration

Authors: Yihuai Zhang^{None}; Qingyang Lin¹; Ali Qaseminejad Raeni²; Yutaka Onaka^{None}; Hiroki Iwama³; Katsumo Takabayashi³; Martin Blunt⁴; Branko Bijeljic⁵

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To better understand asphaltene deposition mechanisms and their influence on rock permeability and wettability, we have developed an in situ micro-CT imaging capability to observe asphaltene precipitation during multiphase flow at high resolution in three dimensions. Pure heptane and crude oil were simultaneously injected to induce asphaltene precipitation in the pore space of a sandstone rock sample. The heptane permeability across the sample was nine times lower after the first asphaltene precipitation, while it was reduced by a factor of ninety due to asphaltene migration and growth after subsequent brine injection. Furthermore, through quantifying the curvatures and contact angles on the images before and after asphaltene precipitation, we observed that the wettability of the porous medium changed from water-wet to mixed-wet. Overall, we demonstrate a micro-CT imaging and analysis workflow to quantify asphaltene deposition, permeability reduction and wettability change which can be used for reservoir characterisation and remediation.

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MS01 / 557

A Novel Technique to Investigate Effects of Thermal Shocks on Cement for CCS Well Integrity

Authors: Kai Li¹; Anne Pluymakers¹

¹ *Delft University of Technology*

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Carbon capture and storage (CCS) gains much attention as it contributes to mitigating climate change. However, during CCS, the periodic injection of pressurized CO₂ leads to strong thermal cycling and shocks in the subsurface, due to the endothermic expansion of pressurized CO₂ upon injection. Under these temperature variations, the wellbore and subsurface formations cyclically contract and expand. As a result, leakage pathways such as micro-annuli between wellbore casing and cement, and cracks in the cement can develop. They impair well integrity, and thus impede safe geological storage of CO₂. Therefore it is of significance to understand how the sealing ability of the cement sheath of CCS wells is affected by thermal cycling or shocks.

In this paper, we report a novel technique to investigate cracking in cement by thermal shocks under in-situ temperature and pressure. To this end, we use a triaxial deformation apparatus capable of mounting a cement sample in a vessel at a confining pressure of up to 70 MPa, with an axial stress up to 26 MPa. An internal furnace is used to achieve an elevated temperature in the vessel. Pore fluid lines are fitted in upper and lower axial pistons to allow water injection. In this study, we use a solid neat cement sample (Ø30×70 mm, water-to-cement ratio: 0.3) cured at 20°C and ambient pressure for 28 days. During the experiments, the triaxial vessel is filled with heat-resistant oil which provides the confining pressure. The cement sample is isolated from the oil using a thin Teflon jacket. We load the sample at different in-situ states of hydrostatic stress and heat the sample assembly to

various elevated temperatures (60 - 120°C). We then inject cold water (20°C) through the sample using two high-pressure syringe pumps at a designated flow rate for a given time. In the vessel, three linear variable differential transducers (LVDT) mounted parallel to, and span around the sample are used to calculate axial and radial strain, respectively. Two thermocouples, one mounted on the middle of the sample (outside the jacket), and another inside the upper pore fluid line, are used to measure temperature. To study the extent of cracking, how and where cracks initiate and grow in the cement under thermal shocks, we measure permeability of the sample with a differential pressure transducer measuring the difference between the up- and down-stream pore fluid line, and we use a micro-computed tomography (μ -CT) scanner to characterize the microstructure of the cement sample before and after the experiments. This technique provides valuable expedience to investigate the thermal effects on the integrity of cement under different in-situ conditions for CCS wells.

The pistons of the setup can also be readily adjusted to study how de-bonding between casing and cement, and cracks in the cement develop for composite cement samples (with analogous casing) under thermal cycling. Our overall goal by using these techniques is to develop and test novel cement designs for enhanced CCS well integrity.

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MS20 / 559

Multiscale Finite element models with Poromechanics for Myocardial Blood Perfusion

Authors: Sumesh Sasidharan¹; Jacques Huyghe¹; Peter Bovendeerd²

¹ *University of Limerick*

² *Eindhoven University of Technology*

Corresponding Authors: p.h.m.bovendeerd@tue.nl, sumesh4sai@gmail.com, jacques.huyghe@ul.ie

Computational cardiac models are promising tools to enhance the design of clinical trials and aid cardiovascular surgeons in decision making during interventional therapies. Multiscale haemodynamic models are gaining popularity to evaluate perfusion in a virtual environment both in healthy and diseased patients. Failure of a heart is usually induced by a mismatch between blood perfusion and metabolic needs of the cardiomyocytes. Because heart failure is associated with blood perfusion and present day computational models do not address this failure mechanism, there is an urgent need for a computational strategy for blood perfusion in deforming myocardial tissue. The computational models on myocardial blood perfusion rely on the finite element method specifically to estimate how perfusion is altered in patients before during, and after various treatment modalities.

Upscaling of the vessel trees to a continuum opens the way to computation of coronary blood flow in a multi compartment poro-mechanical model of the beating heart. The porous mechanics models of myocardial perfusion approximate blood pressure and perfusion distributions reliably even on

a coarse grid with first order elements. On the other hand, higher order elements are essential to mitigate errors in volumetric blood flow rate estimation. The aim of the study is to compare the multi scale finite element models used in computational analysis of myocardial perfusion with parameter optimization sensitivity analyses. The findings show how selection of appropriate models and their couplings can improve its applicability in the treatment development for cardiovascular conditions.

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MS02 / 560

Optimizing laterite soil bed filters via predictive modelling and simulations

Author: Zahra Lakdawala^{None}

Corresponding Author: zahra.lakdawala@lums.edu.pk

The presence of arsenic in drinking water can have significant effects leading to cancer, including skin, lung and bladder carcinoma, on both chronic and acute exposure. The increased use of pesticide and fertilizer to meet agricultural needs (especially in places like Pakistan, India, Nepal and Bangladesh) has led to the release of arsenic from rocks contaminating groundwater. The quality of our drinking water and its treatment depends critically on filtration solutions. Recent studies have reported the success of laterite soil bed filter to filter arsenic. Depending on the operating conditions and the material properties, a comprehensive understanding of the dependence of filter life is investigated in a virtual environment using 3D predictive modeling and simulation framework. We employ the mathematical model from R.Mondal et. al (2019), and extend the flow model to a coupled Navier–Stokes–Brinkman system of equations. The flow model is coupled to the convective, diffusive, advective transport equation for the arsenic. The adsorption is incorporated as a functional change of porosity/permeability over time, which is essential towards predicting the efficiency and lifetime of the filter. We use different CAD filter designs for domestic use to predict the lifetime of these filters under real operating conditions in a virtual environment.

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MS15 / 561

Deep Learning Accelerated History Matching and Forecasting for Geologic CO₂ Sequestration

Authors: Bailian Chen¹; Bicheng Yan²; Qinjun Kang¹; Rajesh Pawar³¹ *Los Alamos National Laboratory*² *King Abdullah University of Science and Technology*³ *Los Alamos National Laboratory***Corresponding Authors:** rajesh@lanl.gov, qkang@lanl.gov, bicheng.yan@kaust.edu.sa, bailianchen@lanl.gov

Traditional physics-simulation based approaches for inverse modeling and forecasting in large-scale subsurface flow and transport problems, e.g., geologic CO₂ sequestration, is a very time consuming process. In this work, we developed a deep learning assisted workflow to speed up this process. First, we developed a deep learning model to predict the pressure/saturation evolution in large-scale storage reservoir. A feature coarsening technique was applied to extract the most representative information and perform the training and prediction at the coarse scale, and further recover the resolution at the fine scale by 2D piecewise cubic interpolation. Thereafter, the feature coarsening based deep learning model was utilized as forward model in the inverse modeling process where a classical data assimilation approach, ES-MDA-GEO, was applied. The efficiency and effectiveness of the proposed deep learning assisted workflow for large-scale inverse modeling and forecasting was demonstrated with a reservoir model (~1.34 million grid cells) built upon Clastic Shelf storage site.

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MS07 / 562

Tightly Coupled Hyperbolic Treatment of Buoyant Two-Phase Flow and Transport in Porous Media

Authors: Patrick Jenny¹; Rasim Hasanzade²; Hamdi Tchelepi³

¹ *Swiss Federal Institute of Technology, Switzerland*

² *Stanford University, USA*

³ *Stanford University, USA*

Corresponding Authors: rasim@stanford.edu, jenny@ifd.mavt.ethz.ch, tchelepi@stanford.edu

Buoyant incompressible multiphase flow and transport in porous media typically is simulated by coupling an elliptic flow equation with a hyperbolic transport description. The tight coupling between flow and transport either requires a fully implicit solution algorithm or very small time steps, if solved sequentially. In any case, however, a large linear system has to be solved each time step.

Here a new solution approach is devised, which relies on solving a coupled hyperbolic system of conservation laws with an explicit finite volume method. Consequently, only local operations have to be performed, which is a great advantage in case of massive parallel simulations and if GPUs are employed.

The devised method is based on the isothermal Euler equations with momentum source terms accounting for resistance due to the porous medium and buoyancy. In this system the pressure is proportional to the density and in case of very small Mach numbers and relative density changes, the computed velocity field is divergence free and converges towards the total volumetric flow in the porous domain. To account for saturation transport, the system was augmented by an additional hyperbolic equation. In order to obtain the numerical fluxes, a characteristic based approximative Riemann solver was developed and 2nd order accuracy in space and time is achieved by piecewise linear reconstruction.

Two-phase flow test cases with buoyant plumes and a lock exchange problem demonstrate that the devised hyperbolic approach recovers the correct incompressible solutions. Numerical experiments also demonstrate that the method is accurate and efficient.

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MS13 / 563

Molecular Transport in Nanoporous Gold Thin Films for Drug Delivery Applications

Author: Erkin Seker¹

¹ *University of California, Davis*

Corresponding Author: eseker@ucdavis.edu

Nanoporous materials have been commonly utilized in drug delivery platforms due to their large specific surface area for higher loading capacity and tunable morphology for controlling drug release profile. In these platforms with large surface area, the interfacial phenomena (surface-molecule interactions) play a significant role in dictating loading capacity and release kinetics. In a collection of works, we use nanoporous gold (np-Au), produced by a nanoscale self-arrangement process, to study the influence of pore morphology, surface chemistry, halide content of the microenvironment, and surface charge on release kinetics and loading capacity for fluorescein (small-molecule drug surrogate). We demonstrate np-Au thin films' utility in releasing biologically-relevant small-molecules to control cell proliferation on np-Au surfaces. We conclude by showing in-plane transport of fluorescein from a distal reservoir to the site of delivery enabling continuous replenishment and release of small molecules. We expect that our investigation of the revealed physical mechanisms will provide a better understanding of the operation of various platforms (e.g., tunable drug delivery, electrochemical biosensors).

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References:

Palanisamy, B., Goshi, N., Seker, E., "Chemically-Gated and Sustained Molecular Transport through Nanoporous Gold Thin Films in Biofouling Conditions," *Nanomaterials* 11:498 (2021)

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

MS07 / 564

Coupled Thermo-Hydro-Mechanical-Chemical Analysis of CO₂ Injection in a North Sea Chalk Reservoir

Authors: Seyedbehzad Hosseinzadeh¹; Frédéric Amour²; Mohammad Reza Hajiabadi^{None}; Hamid M. Nick³

¹ *Technical University of Denmark*

² *The Danish Hydrocarbon Research and Technology Centre*

³ *DTU*

Corresponding Authors: hamid@dtu.dk, amour@dtu.dk, mreza@dtu.dk, behzadh@dtu.dk

Growing global demand for renewable energy and reducing CO₂ emissions drive researchers to materialize Carbon Capture and Storage (CCS) to achieve a net-zero emission by 2050. With several depleted offshore hydrocarbon fields, Denmark is taking this opportunity to reduce the CO₂ levels during the energy transition from fossil fuels to renewable energy. However, most reservoirs in the Danish part of the North Sea are chalk, and contrary to sandstone formations, chalk formations show reactive behavior in the presence of CO₂. Moreover, calcite dissolution in the presence of carbonated water in chalk reservoirs may also induce compaction around the injection well and within the reservoir. Other than that, low matrix permeability and high porosity chalk reservoirs have been subjected to geomechanical alteration due to the cold seawater injection that has been started at the early field lifetime. This geomechanical alteration consists of the softening of rock mechanics properties such as yield stress and bulk modulus, referred to as the water weakening effect, which occurs due to i) the adsorption of specific ions from seawater to the calcite rock surface and ii) calcite and quartz dissolution at high temperature, and Ca-Mg substitution at the grain surface [2]. Therefore, CO₂ injection may expedite the weakening mechanical properties of chalk even further by inducing chemical interactions with the surface of chalk [3].

Considering the impact of the coupled interactions on the non-isothermal transport of multi-phase fluids and reservoir deformation, this study aims at illustrating the dynamic behavior of a mature North Sea chalk reservoir for the CO₂ injection after injecting cold seawater. A wrapper in Matlab is developed that integrates Eclipse reservoir simulator and Visage geomechanics simulator to update the mechanical properties at each time-step based on Eclipse's output and developed yield stress correlations at various temperatures, ions concentrations, and CO₂ saturation.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

The yield surface of reservoir chalk from the North Sea: influence of age, mineralogy and water saturation.

Authors: Frédéric Amour^{None}; Mohammad Reza Hajiabadi^{None}; Hamid M. Nick¹

¹ DTU

Corresponding Authors: hamid@dtu.dk, amour@dtu.dk, mreza@dtu.dk

The exploitation of chalk reservoirs in the context of hydrocarbon production and CO₂ and thermal storage causes in situ changes in stress and saturating fluid, which in turn entail rock compaction, seafloor subsidence, wellbore instability and fault reactivation that can ultimately jeopardise the economic viability of a field [1,2]. The efficiency of new technology such as radial jet drilling and time-lapse seismic interpretation in stimulating and monitoring production are also impeded by subsurface deformation [3,4]. Reliable prediction of chalk deformation is therefore of primary importance so that suitable field development plan can be implemented in a safe manner. To this purpose, experimental studies were conducted to quantify the geomechanical properties of outcrop chalks considered as analogues for reservoir rocks [5,6]. However, there is a lack of systematic assessments comparing quantitatively the properties of outcrop and reservoir rocks to ensure that experimental data can be transferable. In this context, our study assesses and compares the shear and plastic behaviour of Maastrichtian and Danian reservoir chalk from the North Sea by using an extensive experimental database (>80 triaxial tests). The impacts of water saturation (Sw) and mineralogy on rock geomechanics are considered by analysing tests carried out on oil- and water-saturated specimens with various mineralogical composition. Overall, the porosity of the core samples ranges between 30% to 45% porosity, thereby allowing to cover a wide spectrum of reservoir rock types that are likely to deform in a field.

The results indicate that the impact of Sw on rock strength differs between the outcrop and reservoir chalk. Contrary to observations reported on outcrop specimens, the water weakening effect is porosity dependent for subsurface chalk. This mechanical contrast may be due to a change in mineralogy. Besides, the analysis of the core samples shows that clean Danian lithology (<3% quartz content) is stronger than the clean Maastrichtian counterpart, especially towards low porosity values. For instance, at 34% porosity, the specimens from the Tor Fm. start deforming plastically at 34 MPa hydrostatic stress, which is 8 MPa lower than the estimated pore collapse stress of clean chalk from the Ekofisk Fm. Calcite cementation is thought to be the main controlling factor, although further investigation is needed to confirm this hypothesis. Impure Danian chalk (>4% quartz content) appears as the strongest lithology likely due to the presence of quartz cement in pore space that strengthens the rock fabric. Finally, the yield surfaces (shear failure line and end cap) of intact, Danian and Maastrichtian chalk from the North Sea are reconstructed and compared in a mean-deviatoric stress plot with porosity as a third axis. The outcomes of this work can be integrated in constitutive models and assist engineers and geologists in developing geomechanical simulators that capture the specific mechanical behaviour of the Ekofisk and Tor Fms in the context of hydrocarbon exploitation as well as CO₂ and energy storage.

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References:

- 1 Schutjens PMTM, Kokker P, Rai UBB, Kandpal J, Cid Alfaro MV, Hummel ND, et al. Compaction- and shear-induced well deformation in Tyra: Geomechanics for impact on production. 52nd US Rock Mech. / Geomech. Symp., Seattle: ARMA; 2018.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

MS14 / 566

Quantifying the uncertainty associated with reservoir compaction forecasting: Role of the experimental estimation of the hydrostatic yield stress.

Authors: Frédéric Amour^{None}; Mohammad Reza Hajiabadi^{None}; Hamid M. Nick¹

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Geomechanical simulators aim at predicting the irreversible deformation taking place in hydrocarbon and CO₂ reservoirs to optimise profits and reduce risks associated to the exploitation of chalk fields. In the context of compaction studies, accurate forecasting of the plastic strain relies on well-calibrated constitutive equations to capture the mechanical response of rocks according to, amongst others, the porosity, water saturation, age of the rock, and stress and temperature conditions [1,2]. The constitutive equations correlating lithological, petrophysical and geomechanical properties under various in situ conditions are based on experimental database that show a non-negligible data scattering [3]. Although raising questions about the reliability of the predicted strain, the uncertainty on the representativeness of these correlation functions to capture the plastic behaviour of chalk is not yet addressed in the literature.

The present study assesses how the change in the hydrostatic yield stress (σ_{hy}) estimated from laboratory studies impacts the amount and distribution of plastic strain modelled in four depleted reservoirs from the Danish North Sea (Dan, Halfdan, Gorm, and Kraka fields). The selection of the parameter σ_{hy} is motivated by the difficulty that scientists face to assign a stress value to a specimen tested in the laboratory. The transition from the elastic to plastic regime is not abrupt i.e., occurring at one specific stress value. On the contrary, the elastic-to-plastic transition is progressive taking place over a stress interval delimited by the initial ($\sigma_{(hy,in)}$), and final yield stresses ($\sigma_{(hy,fin)}$). Besides, the method used to determine the representative yield stress ($\sigma_{(hy,rep)}$) of chalk varies between studies [4–6].

Two 1-D simulation scenarios are carried out per study areas by considering in the constitutive equations the $\sigma_{(hy,in)}$ and $\sigma_{(hy,fin)}$ value of Danian and Maastrichtian chalk. The first scenario is considered as a conservative approach and the latter is an optimistic approach that results in a smaller deformation. The geomechanical simulator is a strain-rate dependent constitutive model using a modified Mohr-Coulomb yield function to capture the change in mechanical properties as irreversible strain accumulates in the rock [7]. The stress paths are reconstructed from repeated formation tests and the reservoir properties are extracted from well log data. Note that the simulation outcomes are quality-checked by subsidence data.

The results indicate that the creep deformation does not contribute to the contrasts in compaction prediction between the conservative and optimistic model. Secondly, changing σ_{hy} of chalk from its initial to final value obviously shifts the onset of plastic deformation towards high stress conditions. This shifting in σ_{hy} reduces by a factor of 26% to 73% the amount of strain simulated. The contrast in the simulation outcomes between the conservative and optimistic model is dependent on a subtle interplay between rock porosity, virgin stress, and stress path. Thus, the uncertainty related

to the determination of the σ_{hy} of subsurface chalk can potentially modify crucial decisions taken during a field development such as, platform height design and the drilling trajectory.

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References:

- [1] Angus DA, Dutko M, Kristiansen TG, Fisher QJ, Kendall JM, Baird AF, et al. Integrated hydro-mechanical and seismic modelling of the Valhall reservoir: A case study of predicting subsidence, AVOA and micro-seismicity. *Geomech Energy Environ* 2015;2:32–44.
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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 567

Pore-scale displacement and trapping mechanisms for underground hydrogen storage

Author: Maksim Lysyy¹

Co-authors: Per-Hilmar Knut van der Hart¹; Geir Ersland²; Martin Ferno¹

¹ *University of Bergen*

² *University of Bergen (UiB)*

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Hydrogen will have a major role in low-carbon energy transitions, and it is vital to develop hydrogen storage facilities to accommodate widespread implementation. Underground hydrogen storage (UHS) offers a widely available large-scale and long-term storage option, but this storage technology lacks experimental efforts of multiphase hydrogen flow. We use microfluidics to experimentally

describe pore-scale hydrogen-water flow behavior in porous media, previously unaddressed by scientific community. Under imbibition experiments we report the effect of capillary number on displacement and trapping mechanisms and quantify dissolution kinetics. We observe that hydrogen displacement is mainly controlled by I1 imbibition mechanism, whereas hydrogen residual trapping is triggered by I2 imbibition mechanism. Dissolution trapping initiates after residual trapping and is governed by one- and two-end dissolution processes. Hydrogen bubble dissolution kinetics show dependency on injection rate and bubble size. Dissolved global hydrogen concentration corresponds to 7-56 % of literature hydrogen solubility, indicating pore-scale non-equilibrium dissolution. Our results provide key UHS experimental data to enhance understanding of hydrogen flow behavior in porous media.

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Participation:

In person

MS14 / 570

Optimal control analysis of leakage risk in geological CO₂ sequestration under uncertainties

Authors: Ben Mansour Dia¹; Mazen Saad²; Manal Alotibi³

¹ CPG, KFUPM

² Ecole Centrale de Nantes

³ CCM, KFUPM

Corresponding Authors: manal.alotibi@kfupm.edu.sa, diabenmansour@gmail.com, mazen.saad@ec-nantes.fr

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References:

Dia, B.M. (2021), "Bayesian experimental design for CO₂ sequestration with leakage risk assessment", *Engineering Computations*, Vol. 38 No. 3, pp. 1385-1401. <https://doi.org/10.1108/EC-03-2020-0143>

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 571

Design and Fabrication of 4D Fresnel Lenses for Optical and Thermal Sensing Applications

Author: Murad Ali¹

Co-author: Haider Butt²

¹ *Khalifa University of Science and technology*

² *Khalifa University*

Corresponding Author: murad.ali@ku.ac.ae

The demand for additive manufacturing is on the rise in the optical industry. Notably, 3D printing provides solutions to most limitations inevitable for conventional processes. 3D printing offers novel design and fabrication of complex geometries rapidly and cost-effectively. Here, we demonstrate the fabrication of functionalized optical device (4D Fresnel lens) for the first time using a computer-aided design for 3D printing based on the digital light process (DLP) technique. The fourth dimension is introduced by adding the thermochromic pigment powders (blue, green, and red) to a transparent resin that utilizes spectral color response to variation in temperature as an external stimulus. The thermally active powder added two functionalities: selective color filtering at room temperature and thermal sensing (25° C to 32° C) to Fresnel lenses. The printed lenses were assessed for light focusing performance and thermal sensing using homemade experimental setups. Contact angle measurements revealed the hydrophilic nature of lens material, while XRD confirmed no other phase formation during photopolymerization. The surface topography of lenses was investigated using scanning electron microscopy (SEM) and atomic force microscopy (AFM) characterizations that confirmed the surface integrity of our printing process (often used for lenses ($\lambda/4$ to $\lambda/10$)). As a potential alternative to traditional Fresnel lenses, 3D printing offers custom-built optical devices with optimized materials for optical sensing applications.

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Time Block B (14:00-17:00 CET)

Participation:

Online

Invited & Plenary Speaker / 572

Life in a Tight Spot: How Bacteria Swim, Disperse, and Grow in Porous Media

Author: Sujit Datta¹

¹ *Princeton University, USA*

Corresponding Author: ssdatta@princeton.edu

Bacterial motility and growth play central roles in agriculture, the environment, and medicine. While bacterial behavior is typically studied in bulk liquid or on flat surfaces, many bacterial habitats—e.g., soils, sediments, and biological gels/tissues—are complex porous media. Here, using studies of *E. coli* in transparent 3D porous media, we demonstrate how confinement in a porous medium fundamentally alters bacterial behavior. In particular, we show how the paradigm of run-and-tumble motility is dramatically altered by pore-scale confinement, both for cells performing undirected motion and those performing chemotaxis, directed motion in response to a chemical stimulus. Our porous media also enable precisely structured multi-cellular communities to be 3D printed. Using this capability, we show how spatial variations in the ability of cells to perform chemotaxis enable populations to autonomously stabilize large-scale perturbations in their overall morphology. Finally, we show how when the pores are small enough to prevent cells from swimming through the pore space, expansion of a community via cellular growth and division gives rise to distinct, highly-complex, large-scale community morphologies. Together, our work thus reveals new principles to predict and control the behavior of bacteria, and active matter in general, in complex environments such as porous media.

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Time Block A (09:00-12:00 CET)

Participation:

In person

Invited & Plenary Speaker / 573

Modelling & Simulation of Multiphase Flow in Highly Heterogeneous Geologic Porous Media

Author: Stephan Matthai¹

¹ *The University of Melbourne*

Corresponding Author: stephan.matthai@unimelb.edu.au

Geologic heterogeneity presents itself in the form of nested accumulations of granular porous media, ranging from poorly indurated soils to brittle rocks. The depositional environment determines the association of sediment types, and the environmental processes shape, structure, and juxtapose different deposits. Desert dunes, for example, are hundred-metre-tall stacks of mm-thin sand sheets varying in grain size and composition. This layering is disrupted by slides, slumps, and other discontinuities. It is amplified by chemical interactions with infiltrating fluids, bonding grains together while selectively dissolving and-or precipitating mineral phases.

This presentation explores complex emergent behaviour that arises from the interplay of geoheterogeneity with multiphase flow. Sophisticated digital outcrop models resolving geologic features across multiple length scales are used to constrain digital twins of the real world, offering the unique opportunity to investigate system behaviour in response to engineering interventions and reveal side effects. Of particular interest are the performance analysis and optimisation of multiphase flow systems such as CO₂ geo-sequestration complexes, geothermal reservoirs, and gas storage sites. These simulations can also constrain uncertainty aggravated by the sporadic nature of measurements and the limitations of the geophysical imaging of the subsurface.

The rich behavioural dynamics of geologic porous media saturated with brine and CO₂ will be illustrated with results of hybrid FEM-FVM computations expressing jump discontinuities during simulation.

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Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS01 / 574

Impact of Relative Humidity on the Adsorption of Volatile Organic Compounds by Industrial Porous Materials

Author: Meishan Guo¹

Co-authors: Majid Naderi¹; Manaswini Acharya¹; Damiano Cattaneo¹; Daryl Williams¹

¹ *Surface Measurement Systems*

Corresponding Authors: dwilliams@surfacemeasurementsystems.com, macharya@surfacemeasurementsystems.com, mnaderi@surfacemeasurementsystems.com, mguo@surfacemeasurementsystems.com, dcattaneo@surfacemeasurementsystems.com

The presence of pollutants in the air is becoming an area of significant interest and there has been an increasing concern about air quality and its impact on health due to the presence of volatile organic compounds (VOC) in the air. VOC molecules include toluene, formaldehyde, methylene chloride, tetrachloroethylene, xylene, acetone and benzene which may appear in different forms as in solvents, paints or packaging materials. It is important to find a solution for the removal of volatile organic pollutants from the air. Porous materials are considered as a cost effective route to capture VOC pollutants and the reason for their success is the high fraction of pore volume and adsorption sites for trapping volatile species. Zeolites and activated carbons are widely used due to their low cost and ease of availability.

VOC concentrations can vary in different environments but are significantly lower than the moisture concentration. Therefore, water molecules would be competing for the same adsorption sites as VOCs and it would be important to assess the impact of humidity on the choice of porous material for removing certain VOC molecules. This study will look at the impact of humidity on a series of common industrial porous materials which are potentially usable for capturing VOCs.

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References:

- 1 Elwin Hunter Sellars, J J Tee, Ivan P Parkin, Daryl R Williams, *Microporous Mesoporous Mater* 298 2020 110090
- [2] Elwin Hunter Sellars, Paola A Saenz Cavazos, Anthony R Houghton, Sean R McIntyre, Ivan P Parkin, Daryl R Williams, *Adv Funct Mater* 2020 2008357
- [3] N Chanut, S Bourrelly B Kuchta C Serre, J S Chang, P A Wright, P L Llewellyn, *ChemSusChem* 10 2017 1543 1553

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

Invited & Plenary Speaker / 575

Experimental Investigation of Conditions Favoring Enhanced Gas Storage in Shales

Author: Zuleima Karpyn¹

Co-authors: Xuanqing Lou²; Nirjhor Chakraborty³

¹ Penn State U.

² Pennsylvania State U.

³ BP

Corresponding Authors: nirjhor.chakraborty@bp.com, xxl234@psu.edu, zkarpyn@psu.edu

Shale gas reservoirs are currently viewed as an emergent opportunity to sustain growing energy needs while reducing the carbon intensity of energy systems relative to other fossil fuels. However, these reservoirs are geologically complex in their chemical composition and dominance of nano-scale porosity, resulting in limited predictability of their effective storage capacity. To predict gas storage and estimate volumetric gas-in-place, in-situ gas properties need to be defined. However, only a few direct experimental measurements on in-situ gas properties are available in the literature, and the interactions between gas and the surrounding surface area of the medium remain poorly understood. In this study, gas invasion experiments were conducted in conjunction with X-ray microCT imaging on three different shales, i.e., Bakken, Haynesville and Marcellus. Results show evidence of enhanced storage capacity in all cases, with different degrees of gas densification across the three shale specimens. The average of measured in-situ xenon density within the Bakken, Haynesville and Marcellus shale samples were found to be 171.53kg/m³, 326.05kg/m³ and 947kg/m³, respectively. These measured densities are higher than their corresponding theoretical free gas density, though lower than the xenon density at boiling point, indicating that current practices of estimating adsorbed gas and gas in place, using boiling point liquid density, may be overestimated. The xenon densification factor in the Marcellus sample was found to be 7.4, indicating the most significant degree of localized densification. This densification factor drops to 2.6, and to 1.4, in the Haynesville and the Bakken sample, respectively. Characterization of shale composition and pore structure are discussed, in order to assess the shale properties favoring enhanced gas storage. Statistical results indicate that compositional properties are weakly correlated with gas densification, while pore structure is a strong indicator of gas densification levels in shales. The findings in this work lay a foundation to evaluate enhanced storage capacity for various gases in ranging tight formations.

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Time Block C (18:00-21:00 CET)

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Online

Poster / 578

Surrogate models for aquifer management

Authors: VANESSA A. GODOY¹; Janire Uribe-Asarta¹; Gian F. Napa-García²; J. Jaime Gómez-Hernández³

¹ *Universitat Politècnica de Valencia*

² *Research*

³ *Universitat Politècnica de València*

Corresponding Authors: jgomez@upv.es, j.uribeasarta@gmail.com, godoyalmeida@gmail.com, giannagar@gmail.com

Different artificial intelligence methods are evaluated for the construction of surrogate models of the flow of the Requena-Utiel and Cabrillas-Malacara aquifers, in Valencia, Spain. The objective is to provide a quick, open, and minimally accurate tool that allows managers to assess the impact

of possible changes in the flows extracted from existing wells and the impact of rainfall on the decrease/rise of piezometric levels. The different surrogate models resulted in very similar and precise approximations in the ranges of inputs and outputs for which training data were generated. In addition, the speed and ease of use were also verified.

Research financed by the InTheMED project, which is part of the PRIMA Programme supported by the European Union's Horizon 2020 Research and Innovation Programme under Grant Agreement No 1923.

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Time Block A (09:00-12:00 CET)

Participation:

In person

MS11 / 579

Measurement of capillary pressure and relativity permeability relations for two-phase air-water cross flow in thin sintered metal wicks

Author: Bhaskarjyoti Sarma¹

Co-authors: Srivathsan Sudhakar¹; Dominik Tomasz Nasilowski¹; Justin A. Weibel¹

¹ School of Mechanical Engineering, Purdue University

Corresponding Authors: sarma5@purdue.edu, jaweibel@purdue.edu, dnasilow@purdue.edu, ssudhak@purdue.edu

Thin capillary wicks provide an integral function serving as evaporators in vapor chamber thermal management devices [1]. The application of high heat fluxes at the evaporator causes boiling to occur in the wick; the resulting two-phase flow dynamics dictates the thermal performance and critical dryout limits. These wicks are commonly composed of high thermal conductivity copper powders sintered into thin layers. While the physiochemical properties and single-phase flow characteristics in such wicks are widely known, the two-phase flow properties, namely, capillary pressure and relative permeability as a function of the liquid saturation, have been scarcely explored. We propose a novel experimental technique for characterizing the air-water capillary pressure and relative permeability curves of sintered copper wicks using two complementary facilities that together yield both properties. For measuring the capillary pressure as a function of liquid water saturation during both drainage and imbibition, a facility inspired by a previous microfluidic method of Fairweather et al. [2], is developed. The sintered sample is sandwiched between a hydrophilic membrane and a hydrophobic membrane prior to performing sequential liquid and gas (air) intrusion experiments in opposite directions based on the membrane configurations. The capillary pressure difference across the sample is measured as a function of the liquid saturation based on active weighing of the liquid in the sample. Next, the liquid relative permeability is measured from a core flooding experiment [3], a modified version of the earlier stationary liquid method proposed by Leas and co-workers [4]. In this method, the porous sample is continuously flooded with water at a constant flow rate from

a reservoir at high pressure, which flows through the length of the sample. Subsequently the non-wetting phase (air) is injected at different flow rates through the sample thickness in a cross-flow manner using a syringe pump. The injection flow rates of air are varied in a wide range (2-15 ml/min) to alter the local two-phase flow saturation and subsequently, relative permeability as a function of saturation, using sintered samples of three different particle sizes (45 –53 μm , 90 –106 μm and 180 –212 μm). The sintered porous samples are treated with a controlled oxidation process so that they are stably wetting with water throughout the experiments. We first validate the proposed two-step measurement technique by characterizing the properties of carbon paper and comparing to the results reported by Koido et al. [5]. Post-validation, the single-phase liquid permeability, capillary pressure, two-phase pressure drop, and water saturation are sequentially collected for each different sintered copper sample. Using the appropriate data reduction techniques and Darcy's equation for two-phase flow, we obtain capillary pressure and relative permeability as a function of saturation. The experimental results highlight the sensitivity of these properties to the two-phase flow orientation and nature of the porous media configuration. The developed method can be used as a tool for characterizing the two-phase flow behavior of a variety of salient porous media types including sintered mesh wicks or sintered fiber wicks.

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References:

- 1 Sudhakar, S., Weibel, J. A., & Garimella, S. V. (2018). Design of an area-scalable two-layer evaporator wick for high-heat-flux vapor chambers. *IEEE Transactions on Components, Packaging and Manufacturing Technology*, 9(3), 458-472.
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- [4] Leas, W. J., Jenks, J. H., & Russell, C. D. (1950). Relative permeability to gas. *Journal of Petroleum Technology*, 2(03), 65-72.
- [5] Koido, T., Furusawa, T., & Moriyama, K. (2008). An approach to modeling two-phase transport in the gas diffusion layer of a proton exchange membrane fuel cell. *Journal of Power Sources*, 175(1), 127-136.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Unsure

Poster / 580

Application of Lattice Boltzmann Method in Pore-scale Characterisation of Flow Dynamics in Three-Dimensional Porous Medium

Author: Mehrdad Vasheghani Farahani¹

Co-author: Mohaddeseh Mousavi Nezhad²

¹ *Institute of GeoEnergy Engineering, Heriot-Watt University*

² *Associate Professor*

Corresponding Authors: m.mousavi-nezhad@warwick.ac.uk, mv47@hw.ac.uk

A profound understanding of the fluid flow characteristics in porous media is essential in various industrial and engineering applications such as enhanced oil recovery, geological CO₂ and H₂ storage, geothermal energy storage, groundwater remediation, and pharmaceutical engineering. In this study, lattice Boltzmann method (LBM) is utilised for 3D simulation of fluid flow through two porous media, consisting of grains with the same diameter: (i) a homogeneous porous domain, in which the grains are placed with a simple cubic packing configuration, and (ii) a real randomly packed porous domain reconstructed by X-ray micro-CT images. Constant velocity and pressure boundary conditions are imposed for the inlet and outlet boundaries, respectively, and the curved solid boundaries are adequately mapped with Bouzidi boundary condition. The simulations are carried out in a wide range of Reynolds to investigate the effect of both laminar and turbulent regimes on the flow dynamics. While a Single-Relaxation-Time (SRT) LBM is applied for Reynolds lower than 1000, a Smagorinsky turbulent BGK model is adopted for higher Reynolds to ensure the stability of the simulation.

Upon convergence, the velocity magnitudes and components (along and transverse to the imposed flow direction) are extracted and analysed in order to investigate the dynamics of the flow. The analysis is conducted over a broad range of length scales, from the scale of individual pores to the scale of the entire medium, providing insights regarding the underlying pore-scale correlations in the flow. The simulation results show that even though the pore space available for the flow becomes more complex when the heterogeneity of the medium increases, its dynamics would not be completely random and could be correlated with the geometry of the medium. The fundamental insights from this study can be used to shed light on the effect of the pore geometry and grain heterogeneity on pore-scale phenomena associated with fluid flow in porous media such as solute transport and mixing, fluid-solid interaction, and sorption phenomena.

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Time Block B (14:00-17:00 CET)

Participation:

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Invited & Plenary Speaker / 581

Phase-field modeling and simulation of desiccation-induced cracking

Authors: Chenyi Luo^{None}; Lorenzo Sanavia¹; Laura De Lorenzis²

¹ *University of Padova*

² *ETH Zürich*

Corresponding Authors: ldlorenzis@ethz.ch, cheluo@ethz.ch, lorenzo.sanavia@unipd.it

We developed a phase-field approach to model desiccation-induced fracture in porous media. The model describes the coupling of deformation, fluid flow and fracture in partially saturated materials. Different coupling options are discussed and compared, and physically motivated improvements with respect to previous models are introduced. The discretization setting hinges upon a stabilized low-order finite element to maximize efficiency within a three-dimensional implementation. We also discuss the comparison of numerical results to predictions of semi-analytical approaches and to experimental results.

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Time Block A (09:00-12:00 CET)

Participation:

In person

Poster / 582

Adsorption and Transport Behaviors of Shale Oil in Kerogen Slit by Molecular Dynamics Simulation

Author: Liu Jie¹

Co-authors: Sun Shuyu¹; Yang Yongfei²; Yao Jun²; Kou Jianlong³

¹ *KAUST*

² *China University of Petroleum(East China)*

³ *Zhejiang Normal University*

Corresponding Authors: kjl@zjnu.cm, yaojunhdpu@126.com, shuyu.sun@kaust.edu.sa, jie.liu.1@kaust.edu.sa, yangyongfei@upc.edu.cn

In the last decades, shale oil, mainly distributed in organic nanopores of shale, has been considered as the representative of unconventional energy to alleviate the energy crisis. Kerogen plays a complex and key role for adsorption and transport behaviors of shale oil, and the ideal pore models greatly overestimate the flowing capability of shale oil, thus it is crucial to identify the associated mechanisms. In this paper, molecular dynamic simulation had been performed to quantify the adsorption and transport behaviors of shale oil in kerogen slits. Both the distribution of shale oil properties and potential of the mean force (PMF) were used to identify the interaction mechanisms between the light and heavy components respectively represented by methane and asphaltene. To get more accurate and reasonable flow behavior, the multicomponent shale oil in the realistic kerogen channel is studied. Both density and velocity distributions that along and perpendicular to the flow direction are studied in kerogen channel, where the influence of branch chain of kerogen is also took into consideration. We also examined the effects of different temperatures and apertures on the

adsorption behavior. Owing to the extremely strong adsorption capacity between the asphaltene and kerogen, the adsorbed asphaltene layers reduce the slit width, preventing the light components from adsorbing on the kerogen slits due to the energy barrier formed by heavy components. It is found that, with an increase in temperature, the distribution of hydrocarbons performs more homogeneously. In addition, the adsorption quantity of medium components displays a reduction in kerogen slit, while the heavy component shows a rising as its greater competitive, suggesting that the medium components are the most potential fraction in thermal exploitation, and the light components keep a steady quantity with the combined action of medium and heavy components. The small slit (aperture < 2 nm) can be blocked by asphaltene molecules, and the adsorption density of hydrocarbons reaches the maximum at 2 nm aperture. On the flow direction, the velocity profile preforms the peristaltic behavior due to the effect of branch chain of kerogen, and the toluene and asphaltene components contribute it mostly. According to the heterogeneous characteristics of shale oil flow, we define the fictitious slip boundary, which corresponds to the boundary between bulk phase and adsorbed phase, to describe shale oil flow precisely. The potential energy distribution and the interaction force contour verified the peristaltic flow behavior and the validity of fictitious slip boundary.

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References:

Liu J, Yang Y, Sun S, et al. Flow Behaviors of Shale Oil in Kerogen Slit by Molecular Dynamics Simulation[J]. Chemical Engineering Journal, 2022: 134682.

Yang Y, Liu J, Yao J, et al. Adsorption behaviors of shale oil in kerogen slit by molecular simulation[J]. Chemical Engineering Journal, 2020, 387: 124054.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS02 / 583

Development of Carbon membranes and carbon/CNT membranes for wastewater treatment

Author: ilyes JEDIDI¹

Co-authors: Marc Cretin ²; Mohamed Saif Al Saidi ¹; Sulaiman Al Isae ³; Mohamed Mihoub ¹; Mohamed Salah ³; Baskaran Krishnan ³; Makki Abdelmouleh ⁴

¹ University of Technology and Applied Science - SOHAR

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Carbon membranes are well-known for their excellent performance in gas separation, as well as liquid separation, particularly for water-oil emulsions and the purification of industrial corrosive solutions. Carbon membranes are mostly prepared by carbonizing at a temperature varying from 600°C to 900°C under an inert atmosphere a shaped green body made of an organic precursor. As a result, a porous carbon membrane with vitreous carbon is formed.

A process for preparing carbon membranes was developed previously, and it consisted of a new and simple approach to preparing carbon MF and UF membranes. These membranes were prepared by extruding a green body or a paste made of a mixture of mineral coal or graphite powder, porogen compounds, and a solution of phenolic resin/ethanol. To obtain the final porous structure, carbonization at 700°C in an inert atmosphere is required. These membranes performed very well when applied to the treatment of different industrial wastewaters such as the Textile industry wastewater and the soft drinks industry wastewater.

Adding a carbon nanotubes growth catalyzing agent to the steps of preparation of these carbon membranes allowed us to grow CNT's and iron nanoparticles inside the porosity of the material. The CNTs grew on the material's external surface as well, resulting in MF and UF layers with vertically grown CNTs on top. Such a structure is thought to be very effective at fouling reduction during filtration.

When both materials, the Porous carbon, and the porous carbon/CNTs, were used as adsorbents in synthetic aqueous humic acid solutions, we saw clearly that CNTs played an important role in enhancing the material's adsorption capacity.

Using a diluted solution of Phenolic resin/Ethanol, we were able to deposit, by slip casting, a thin nanofiltration layer and tailor its average pore size within 1 to 2 nm by varying the thermal treatment conditions. The layer had a thickness of less than 1 nanometer and the carbon structure of the layer was graphene-like according to the TEM analysis.

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References:

1 I. Jedidi, M. Cretin, S. Cerneaux, M. Saif AL Saidi, S. Al-Isaee and al., Detailed manufacturing process of a tubular carbon microfiltration membrane for industrial wastewater treatment, *Journal of Porous Materials*, 29, 2022, pp.291–306.

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

In person

Invited & Plenary Speaker / 584

Transport and Multiphase Flow in Porous Media for Electrochemical Technologies

Author: Adam Weber¹

¹ *Lawrence Berkeley National Laboratory*

Corresponding Author: azweber@lbl.gov

As low-temperature electrochemical technologies become increasingly important in our energy paradigm, there is a need to examine them holistically. For commercialization and optimization, one requires a detailed understanding of the underlying physics and phenomena, which is directly coupled to their structure that is composed of various porous media including porous electrodes and porous backing layers. Furthermore, for such technologies to become practical, they need to operate at high current densities, which drives the need for efficient transport of reactants and removal of products from the reaction site. Finally, such interactions most often involve multiphase flow, whether it is hydrogen fuel cells, water electrolyzers, CO₂ reduction devices, etc. In this talk, we will explore the commonalities and approaches towards understanding multiphase flow in these systems with a focus on the importance that such phenomena play on the overall transport phenomena and cell performance.

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MS19 / 585

Ex-situ visualization of wetting dynamics in a microporous layer of polymer electrolyte fuel cells by X-ray computed tomography under water vapor supply

Authors: Satoru Kato¹; Satoshi Yamaguchi¹; Yoriko Matsuoka¹; Akihiko Kato¹; Yasutaka Nagai¹; Takahisa Suzuki¹

¹ TOYOTA Central R&D Labs., Inc.

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The cell potential of polymer electrolyte fuel cells (PEFCs) is reduced by accumulation of liquid water in the cathode gas diffusion layers (GDLs). The GDL is usually composed of a substrate (i.e., carbon paper) and a microporous layer (MPL). The MPLs are usually made of carbon nanoparticles and fluoropolymers. It is well known that MPLs suppress water accumulation in the GDL. Water accumulation in the MPL is conventionally observed by operando (during the measurement of the performance) X-ray radiography. The obtained results are the one-dimensional average saturation in the X-ray incidence direction. For example, if the water distribution in the MPL is heterogeneous, this cannot be observed by Operando X-ray radiography. Therefore, three-dimensional information of water distribution can help understand water behavior in the MPL. Operando X-ray computed tomography (CT) is a powerful tool to visualize 3D water distribution in the substrate. The method is, however, difficult to visualize 3D water distribution in the MPL because the CT image of the MPL near the catalyst layer (CL) is blurred by strong X-ray absorption by Pt loaded in the CL.

We developed an ex-situ method for visualizing the 3D distribution of the wet domain in the MPL1. The sample was a punched GDL without a CL to circumvent the problem in the Operando X-ray CT mentioned above. A GDL with an MPL was cooled down in a wet atmosphere so that water vapor could condense in the pores of the MPL. X-ray CT scanned the wet domain in the MPL. The visualization results revealed that the wet and dry domains coexisted in the MPL. In addition, the liquid water distribution in the through-plane direction indicated that liquid water formed in the MPL drained to the substrate side and the outer surface side. The dynamic behavior of liquid water, however, could not be analyzed because it took 6 minutes to conduct a CT scan.

Here, we report the dynamic behavior of the wet domain in the MPL. Wet domain in the MPL was produced similarly to the previously reported method. A series of CT images were scanned with a time resolution of 4 seconds. With supplying water vapor, the average volume of the wet domain increased, and the number of wet domains decreased. This means that wet domains expanded by absorbing water vapor and combined. The wet domains finally reached the outer surface of the MPL and covered 20% of the area. This two-dimensional wet area may hinder oxygen transport at the MPL –CL interface.

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References:

1 Satoru Kato, Satoshi Yamaguchi, Wataru Yoshimune, Yoriko Matsuoka, Akihiko Kato, Yasutaka Nagai, Takahisa Suzuki, "Ex-situ visualization of the wet domain in the microporous layer in a polymer electrolyte fuel cell by X-ray computed tomography under water vapor supply", *Electrochemistry Communications*, 111 (2020) 106644.

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Unsure

MS10 / 586

Hysteresis in Multiphase Flow and Application to Hydrogen Storage

Author: Sepideh Goodarzi¹

Co-authors: Abdulla Alhosani²; Martin Blunt²; Branko Bijeljic³

¹ *PhD student*

² *Imperial College London*

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Energy storage has been an area of interest for many decades. Underground storage is a way to store a huge amount of energy, but it has many challenges along with safety and economic impacts. Hydrogen storage in the subsurface can be considered as a long-term energy storage solution. Green hydrogen can be produced from the excess electricity during peak production, it can be injected into

the surface reservoir and withdrawn for the time of high demand. The focus of this project is to understand the hysteresis phenomenon and study the behaviour of fluids in porous media, which can be applied to underground hydrogen storage processes. Two experiments were performed at an unsteady state to investigate the pore-scale observation during the cycle of drainage and imbibition steps. This work studied hydrogen and nitrogen injections at representative subsurface pressures and a wider range of hysteresis cycles, coupled with measurements of capillary pressure from interfacial curvature and relative permeability. This research utilises the advantages of using computed tomography on a micro-scale to image the dynamic behaviour of the flow through the sample. This technique helps to have a better understanding of multi-phase flow characterisation in porous media by providing three-dimensional images. The purpose of the work is to provide pore-scale insights into hydrogen storage and withdrawal while providing multiphase flow properties for input into the reservoir-scale simulation.

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Time Block A (09:00-12:00 CET)

Participation:

In person

Poster / 588

Polymeric Membranes' Morphology and Water Flow Simulation

Author: Meixia Shi¹

¹ *Ningbo Polytechnic*

Corresponding Author: 732103628@qq.com

The membrane morphology significantly influences membrane performance. For osmotically driven membrane processes, the morphology strongly affects the internal concentration polarization. In this work, different membrane morphologies were generated by simulation and their influence on membrane performance was studied. The simulation results were experimentally validated for two classical phase-inversion membrane morphologies: sponge- and finger-like structures. Membrane porosity and scanning electron microscopy image information were used as model input. The permeance results from the simulation fit well those experimentally measured. Water permeances were predicted for different kinds of finger-like cavity membranes with different finger-like cavity lengths and various finger-like cavity sets, as well as for membranes with cylindrical cavities using 3-D simulation. The results provide a much more realistic representation of the system, than just considering a simple porosity estimation. The method was confirmed as a validated tool to predict how different morphologies would affect the accurate water permeance and is being now explored to facilitate further modeling solute transfer as a valuable help to estimate the performance in osmotically driven membrane processes.

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References:

Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Invited & Plenary Speaker / 589

Discrete models, continuum models and scale transitions for the drying of porous media

Author: Evangelos Tsotsas^{None}

Corresponding Author: evangelos.tsotsas@ovgu.de

Continuum models similar to those used for diffusion, heat conduction or viscous flow are since long available for drying processes, so one might think that tabulating respective transport coefficients for various materials should be the main research task left to be fulfilled. However, the opposite is true, because expansion and, especially, deepening of the research on the drying of porous media in the last years has unveiled, how severely restricted common continuum models for drying in reality are. This has mainly been achieved by using pore network simulations as in silico experiments of much superior resolution and accuracy than real experiments can provide to derive continuum model parameters. Tremendous variability, missing uniqueness of such parameters at local scale, and the necessity of corrections by so-called non-local-equilibrium functions are some of the deficiencies diagnosed. They can explain the notorious hardship in identifying the transport parameters of drying porous media, but can also result in serious misunderstanding of the physics behind the drying process. On the other hand, discrete, pore-resolving models are not just the starting point of coarsening, but they can also be used on their own to better understand, which structural features of porous media correlate with their drying behaviour, how, and why. Pointing in the direction reverse engineering towards materials with superior properties, such aspects indicate how ample the potential of research on drying porous media still is.

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Time Block A (09:00-12:00 CET)

Participation:

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Poster / 593**Modeling Microbial Enhanced Oil Recovery (MEOR) Optimization Augmented with Formation Damage Mitigation Within Sandstone Core Under Adverse Subsurface Oil-Field Conditions****Author:** Susmit Chakraborty¹**Co-authors:** Suresh Kumar Govindarajan¹; Sathyanarayana N. Gummadi¹¹ Indian Institute of Technology Madras, Chennai 36, India**Corresponding Authors:** gummadi@iitm.ac.in, bt16d301@smail.iitm.ac.in, gskumar@iitm.ac.in

For an efficient field implementation of MEOR process, crucial microbial, formation rock and physicochemical properties, and operational parameters must be characterized and optimized. The present study numerically investigates the impacts of nutrient competition, toxicity, pulse injection time (t_{pulse}), media heterogeneity, and microbial reversible attachment and detachment rates on tertiary *in-Situ* MEOR mediated with biosurfactant and biofilm production within a sandstone core system under extreme field-like conditions of varying temperature, salinity and brine pH.

Herein, the developed highly coupled multi-species reactive-transport black oil model simulates heat transport; cation and anion transport with multi-component ion exchange (MIE); pH variation with temperature and salinity; injected *Pseudomonas putida* metabolism, and carbon and nitrogen substrate utilization, with maximum specific growth rate being a combined function of temperature, salinity and pH; biosurfactant and biofilm induced oil/water interfacial tension (IFT) and rock wettability alteration (WA), respectively; and capillary desaturation, relative permeability and fractional flow curve variations. Finite difference technique with iterations and error tolerance limit of 10^{-7} is used to solve the nonlinear governing equations. MIE-transport is solved by operator splitting and bisection methods.

Verification and validation results determine the present model to be numerically stable and reliable enough. The injected microbe possessing highest specific affinity towards both carbon and nitrogen limiting substrates is clearly found to possess maximum competitive advantage over other microbial populations within sandstone core, thus causing maximal growth and biosurfactant production under extreme conditions. Whereas, the microbes are found to be highly susceptible towards toxic effects of water-soluble organics and indigenous chemicals, reducing growth and biosurfactant production by 70% and 64%, respectively. This loss can be further attenuated by increasing t_{pulse} for all species just by 1.5 times (38.4 to 57.6 h), thus enhancing biomass and biosurfactant production by 38% and 74%, respectively. Although biofilm formation is important for rock WA towards water-wet condition, in order to prevent formation damage induced by excessive bio-clogging of pore-throats, sandstone core with intermediate heterogeneity is preferred. Formation damage near core inlet can be further prevented by injecting microbes possessing lower reversible attachment-to-detachment ratio, thus attenuating porosity and permeability reduction, and enhancing biomass and biosurfactant production by 10%, 60%, 97% and 35%, respectively. Furthermore, temperature (40 to 55 degree Celsius) and salinity (0.32 to 3.15 mol/l) variations had maximal debilitating effect on microbial reactive transport, whereas pH change from 8.0 to 8.9 had marginal impact. The combined effects of IFT reduction (from 25 to 0.001 mN/m) and rock surface WA (from weakly oil-wet towards intermediate wet state) prompted >5 times residual oil saturation reduction (from 60% to <10%), consequently with significant increase in oil relative permeability, fractional flow and recovery for a wide range of oil API gravities (29, 35 and 40 degree API).

Thus, the developed MEOR mathematical model and numerical solution technique at core-scale with lower run time and computational cost proposes an innovative, more realistic and environmentally sustainable strategy for quickly but efficiently selecting suitable microbial and sandstone oil-field candidates for sustainable and profitable MEOR application while simultaneously mitigating bio-clogging induced formation damage.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Invited & Plenary Speaker / 597

The Pulse of Plants

Author: Abraham Stroock¹

¹ *Cornell University*

Corresponding Author: abe.stroock@cornell.edu

Plants give life to our planet by pulling critical reagents out of the soil from below (water and micronutrients) and out of the atmosphere from above (light and carbon dioxide). To achieve this feat, they master a wide range of fluid mechanical contexts, from flows in unsaturated porous media around their roots, through nanoconfined flows in their tissues, to turbulent air flows around their leaves. They regulate these steps in the transpiration process passively through their internal and external structure and actively through valves (stomates) that control the coupling to the atmosphere. Through each day, the flux and stress within a plant pulse due to physical and biological responses to fluctuations in sunlight, wind, temperature, and humidity in the microenvironment. This pulse of plants defines their productivity and efficiency in both natural and agricultural contexts. In this talk, I will describe our work measuring these dynamics with a microfluidic sensor that itself borrows design principles from the vascular structure of plants. I will use our efforts to model the observed dynamics to illustrate the coupling of the various flows mentioned above with the physiology of plants. I will also point toward implications for improved understanding of the biology and increased efficiency in the management of water in agriculture.

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Time Block C (18:00-21:00 CET)

Participation:

Online

Invited & Plenary Speaker / 598

Lessons from flows through porous media for solving nonlinear hyperbolic problems

Author: Eduardo Abreu¹

¹ *University of Campinas, Sao Paulo, Brazil*

Corresponding Author: eabreu@ime.unicamp.br

Hyperbolic problems and balance laws are relevant on the foundations of mathematical modeling and numerical simulation to the study of fluid dynamics in porous media. Such nonlinear models appear naturally in basic and applied sciences related to energy, climate, water, agriculture and they are also current events for a green world. We will discuss how fresh insights from flows through porous media on conservation properties, dimensional analysis and relaxation are key ingredients for construction of new effective schemes for solving hyperbolic transport models and a new desingularization analysis tool for construction of computationally stable numerical flux in locally conservative form. In fact, the approach is more general. We will also present advances in the mathematical

modeling and design of a new class of positive Lagrangian-Eulerian schemes with rigorous numerical analysis for solving multidimensional hyperbolic-transport problems and related applications in geosciences.

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References:

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

Online

Poster / 600

Numerical study of single droplet drying in an acoustic levitator

Authors: Martin Doß¹; Eberhard Bänsch¹; Nadja Ray²

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² *Friedrich-Alexander Universität Erlangen-Nürnberg*

Corresponding Authors: ray@math.fau.de, baensch@math.fau.de, martin.md.doss@fau.de

To examine the drying kinetics inside a spray dryer, it is essential to understand the heat-induced transformation of a single colloidal droplet into a solid dry particle. During the last decades, numerous researchers applied acoustic levitation to perform single droplet drying experiments using a standing ultrasound wave to immobilize the droplet in one of its pressure nodes. Even if this approach requires no physical contact, secondary acoustic effects (namely the acoustic radiation pressure and the acoustic streaming) still have a significant impact on the heat and mass transfer within the area of levitation. Our aim is to investigate the drying and particle formation of a single colloidal droplet in an acoustic levitator by means of mathematical modeling and numerical simulations [DB22]. More precisely, we apply the finite element method to simulate the phase transitions during the drying process and to quantify the impact of the aforementioned secondary acoustic effects. Once a critical amount of solvent has evaporated from the droplet, its liquid suspension turns into a porous medium consisting of a wet core and a dry crust. The evaporation front is modeled as a sharp interface and the drying rate is derived locally from the thermodynamic non-equilibrium between the saturated and the actual vapor pressure. Finally, empirical data from the literature and our collaboration partners are taken into account to confirm the validity of our numerical results.

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[DB22] Martin Doß, Eberhard Bänsch, Numerical study of single droplet drying in an acoustic levitator before the critical point of time, *Chemical Engineering Science*, Volume 248, Part A, 2022, 117149, <https://doi.org/10.1016/j.ces.2021.117149>.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

MS02 / 603

Fenton Reaction in Porous Media

Author: Ambika Selvaraj¹

¹ Assistant Professor, Department of Civil Engineering; Adjunct Faculty, Department of Climate Change

Corresponding Author: ambika@ce.iith.ac.in

The Fenton reaction is studied and applied for a long-time by global researchers worldwide. However, the investigation of Fenton reaction in porous media to remove pollutants is the least attempted due to the associated complexity. This study attempted applying the Fenton reaction in detoxifying the contaminated-groundwater. The hypothesis behind this study is utilizing the advanced oxidation viz a viz the greatest benefit of the Fenton reaction for the complete and quicker degradation of groundwater organic pollutants. The coarse, meso and nano-sized iron particles were arranged in a column such a way that the generated radicals break the bonds of the complex-structured organic molecules to undergo the degradation. The representative pollutant chosen was phenol due to its wide-application in industries and domestic cleansing agents. Columns with different configurations

varying in ZVI distribution and location of H₂O₂ were investigated for factors influencing sustainable phenol removal. Distribution of mZVI contributed 61-84% more interaction between Fe²⁺ ions and H₂O₂, promoted good radical generation and continuous corrosion, invigorated effective Fe²⁺-Fe³⁺ cycling, retained active iron surface area and circumvented precipitation and secondary sludge production which extended the active corrosion stage by 5 to 8 times and resulted in 3 to 7 times increment in mg phenol removed/mg mZVI along with 80% to 99.8% utilization of mZVI.

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

In person

MS02 / 604

A novel technology to remove co-occurring arsenic and atrazine in the groundwater used for drinking

Authors: Siva Rama Satyam Bandaru^{None}; Arkadeep Kumar¹; Mohit Nahata²; Dana Hernandez³; Ashok Gadgil²

¹ Lawrence Berkeley National Laboratory

² University of California Berkeley

³ University of California

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Water supplies of many communities are contaminated with both naturally occurring arsenic and anthropogenic toxic chemicals. Globally, 200 million people are exposed to toxic levels of naturally occurring arsenic in the groundwater used for drinking (Podgorski and Berg 2020). Chronic exposure to arsenic causes various types of internal cancers, cardiovascular diseases and low I.Q in children (Smith et al. 2002). Further, unsafe levels of persistent organic contaminants (e.g., insecticides, nematicides, and antibiotics, from farming activities) are observed in the arsenic contaminated

groundwaters (Dutttagupta et al. 2020). Low-income resource-poor communities are disproportionately impacted by groundwater contamination because of the lack of affordable remediation technologies that can be operated over long periods (Amrose, Burt, and Ray 2015).

Recently, we reported Air Cathode Assisted Iron Electrocoagulation (ACAIE) as a promising low-cost technology to remove arsenic in the groundwater used for drinking. In ACAIE, low-voltage direct current is applied between a steel plate (anode) and an air diffusion cathode (herein called “air cathode”) to promote anodic dissolution of Fe(II) from the anode and cathodic reduction of O₂(g) from air, to form H₂O₂ in the solution at the air cathode. In bulk solution, Fe(II) and H₂O₂ react rapidly to form insoluble Fe(III) (oxyhydr)oxides which have high affinity for As(V) adsorption. Reactive intermediates (OH, O₂⁻, Fe(IV)), generated during the oxidation of Fe(II) by H₂O₂, oxidize dissolved As(III) to As(V) that can be easily adsorbed (Hug and Leupin 2003), and can also breakdown toxic organic contaminants (Bocos et al. 2016) to non-toxic byproducts.

Although ACAIE is a promising technology to treat contaminated groundwater for drinking, long-term performance of ACAIE—especially the longevity of the air cathode—is poorly understood. In ACAIE, the Fe(III) (oxyhydr)oxides precipitates formed in the bulk solution can deposit on the air cathode causing a decrease in H₂O₂ generation. Poorly conducting iron oxides, can increase the charge transfer resistance and can also catalyze the decomposition of H₂O₂ at the surface, which leads to decreased H₂O₂ concentrations in the bulk solution (Pham et al. 2009; Rusevova Crincoli and Huling 2020). Adequate production of H₂O₂ is critical for efficient contaminant removal in ACAIE.

In this work, we demonstrate the effectiveness of ACAIE in removing co-occurring realistic concentrations of arsenic and atrazine to safe levels in a realistic water matrix. Further, we will discuss the influence of operating time and electrolyte composition on the longevity of the air cathode with respect to the Faradaic efficiency of H₂O₂ generation. Various analytical characterization tools (e.g., SEM, XPS, Raman, LSV) are used to understand the mechanisms responsible for the decrease in H₂O₂ Faradaic efficiency. Finally, we will present effective strategies for the regeneration of fouled air cathodes to recover their H₂O₂ Faradaic efficiency to near the original value.

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MDPI Energies Student Poster Award:

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References:

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Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

In person

Invited & Plenary Speaker / 605**Fractal Theory of Porous Media**

Author: Peng Xu¹

¹ *China Jiliang University*

Corresponding Author: xupeng@cjlu.edu.cn

Over the past four decades, fractal geometry has sparked considerable interest in many disciplines to characterize irregular and disorder objects that traditional Euclidean geometry fails to analyze. Since Katz and Thompson presented experimental evidence indicating that pore spaces of sandstone are self-similar in 1985, fractal geometry has been successfully applied into variety of porous media such as soil, rock, coal, shale, fiber, wood, ceramic, concrete, tissue, etc. In this talk, I will firstly review the background and applications of fractal geometry in porous media. And the fractal theory and methods to characterize and reconstruct the complex structures of porous media are illustrated. I will also introduce the fractal models for the transport properties of porous media.

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References:**Time Block Preference:**

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 606**Print Quality and Particles: pore-scale simulations of particles/liquid interaction with printing substrate**

Authors: Hamed Aslannejad¹; Amir Raouf¹

¹ *Utrecht University*

Corresponding Authors: h.aslannejad@gmail.com, a.raouf@uu.nl

Application of inkjet printing as a versatile technique has gain a great attention during last decade. Not only in paper printing industry but also in pharmaceuticals, electronics, sensors, etc. In order to deliver the highest print quality possible, the droplet landing, distribution and penetration into the media needs to be well controlled. In this paper, we studied the ink, containing liquid phase but also the Latex particles, and the coated media interaction during printing process. Pore-scale two-phase flow simulation was conducted to evaluate the liquid-phase of ink infiltration into the media. While DEM was used to simulate particle-particle and particle-media interactions. The results of model provide a unique overview about pore-scale detailed phenomena happening during ink droplet landing on the coated media.

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Participation:

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Poster / 608

Simulation of turbulent mixing in channels with reactive boundary conditions

Authors: Alisdair Soppitt¹; Mohaddeseh Mousavi Nezhad²; Alberto Guadagnini³; Thomas Hudson¹

¹ *University of Warwick*

² *Associate Professor*

³ *Politecnico di Milano*

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Reactive boundary conditions are employed to model an increasingly wide range of transport scenarios (e.g., [4];1;[5]). While the capability of a variety of computational schemes for reliable description of such reaction-diffusion processes at the boundary of a given domain has been assessed in the literature [2], the effects of hydrodynamic processes on the rates of reactions taking place at the boundary are still largely unexplored. We present a computational algorithm based on a probability density function approach to model turbulent mixing and transport of scalars through a channel in the presence of reactive boundary conditions. The Parametrised Scalar Profile theory (PSP) originally proposed by Meyer and Jenny [3] is used to model turbulent mixing. A Lagrangian stochastic particle technique is used to model scalar transport. We consider a system with a partially adsorbing boundary condition. The latter is formulated in upon considering that, upon interacting with the boundary only some particles are adsorbed, while other particles are reflected. The formulation rests on a Gaussian updating rule which is derived with the assumption that particle reactions are families of weakly dependent events. This allows such reactions to be incorporated in the modelling system, while maintaining the ability to use the full probability density function (PDF) of the scalar

concentration across time and space. We apply our computational framework to a scenario comprising of turbulent flow in a narrow channel with a single reactive wall. We observe that increasing the turbulence frequency leads to a reduction in the peak concentration variance along the channel, corresponding to an increase in mixing rate. Additionally, an analysis on the effects of a key model parameter driving the reaction enable us to provide a method for reducing the initially observed multi-modal behaviour of concentration distribution in the channel.

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References:

- 1 Steven S Andrews and Dennis Bray. Stochastic simulation of chemical reactions with spatial resolution and single molecule detail. *Physical Biology*, 1(3):137–151, aug 2004. doi: 10.1088/1478-3967/1/3/001. URL <https://doi.org/10.1088/1478-3967/1/3/001>.
- 2 Radek Erban and S Jonathan Chapman. Reactive boundary conditions for stochastic simulations of reaction–diffusion processes. *Physical Biology*, 4(1):16–28, feb 2007. doi: 10.1088/1478-3975/4/1/003. URL <https://doi.org/10.1088/1478-3975/4/1/003>.

Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 609

Numerical modelling of CO₂ sequestration in coal-seams based on a parallel hybrid discrete fracture –dual porosity model

Author: Shakil Masum¹

Co-authors: Min Chen ¹; Hywel Thomas ²

¹ *Cardiff University*

² *Cardiff Unviersity*

Corresponding Authors: masumsa1@cf.ac.uk, thomashr@cf.ac.uk, chenm24@cf.ac.uk

Coal-seams or coal deposits are not only critical to global energy supply but also recognized as a potential reservoir/ target formation for geologic carbon dioxide CO₂ storage. Detailed understanding of coal-CO₂ interaction and assessment of reservoir performance are fundamental for successful design and operation of coalbed CO₂ storage strategies. Coalbeds are complex porous media consisting of multi-scale fracture networks and multi-pore matrices. Coal matrix blocks are generally separated by well-defined, small-scale fractures or cleat network inherent to the material, whereas large-scale fractures are associated with hydraulic fractures or geological fault lines. Numerical modelling of subsurface fluid flow, reaction, and mechanical deformation in coal deposits, in such discrete but inter-connected system of domains, especially for large spatio-temporal problems, are challenging and computationally expensive. Therefore, implementation of robust numerical techniques is essential for efficient and accurate solutions.

By focusing on fluid conductivity regimes or separate flow regions, an advanced hybrid discrete fracture –dual porosity (HDF-DP) model is developed on a coupled thermo-hydraulic-chemical-mechanical (THCM) modelling framework. In the model, large hydraulic conduits are simulated as discrete fractures while the cleats and matrices are simulated, combinedly, under a dual-porosity system. In the numerical procedure, large fractures are idealized as lower-dimensional geometric objects and discretized by lower-dimensional interface elements, such as, lines (1D) in 2D planar domains or 2D planes in 3D volumes, however share the same nodes at the interface elements between two continua. In the model, Galerkin finite element method is used for spatial discretization and a fully implicit mid-interval backward difference time-stepping algorithm is used for temporal discretization. Furthermore, the model is parallelized using a hybrid message passing interface/open multi-processing (MPI & OpenMP) scheme to reduce computational time. The model is applied to investigate carbon dioxide storage in coal-seams accounting realistic subsurface conditions. For large-scale simulations, significant reduction of simulation runtime was achieved using the parallel HDF-DP model. To demonstrate accuracy of the model, predicted results were compared against an in-situ field dataset on coalbed methane production obtained from literatures. The model predicted results agreed well with the field-data highlighting its utility to studying complex subsurface processes regarding carbon storage and/ coalbed methane recovery.

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Time Block B (14:00-17:00 CET)

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MS22 / 610

Linking structure and catalytic properties of automotive and heterogeneous catalysts for industrial applications through X-ray nanotomography, scanning electron microscopy and cryogenic focused ion beam microscopy in three dimensions

Authors: Andy Holwell¹; Maadhav Kothari¹; Markus Boese²

¹ Carl Zeiss Microscopy Ltd

² Carl Zeiss Microscopy GmbH

Corresponding Authors: maadhav.kothari@zeiss.com, markus.boese@zeiss.com, andy.holwell@zeiss.com

Heterogeneous catalysts are a broad and versatile set of engineered porous materials, of high surface area and surface functionalization. Automotive catalysts have removed billions of tons of pollutants from entering the atmosphere since their deployment in the 1970s and must withstand long service lives. Their structure-property relationships are complex, determined by porosity, particle size, voids and adhesion between substrate, washcoat base layer and precious metal active components. Catalysts can therefore be challenging to image and characterize at high resolution and in three dimensions.

We demonstrate several novel 3D microscopy approaches to imaging the internal solid and pore structure of catalysts and using those 3D datasets to simulate the performance of gasoline particulate filters (GPF), polymer electrolyte fuel cells (PEFC) and metal organic frameworks (MOF). We describe the use of X ray microscopy for 3D imaging, pore analysis, and differentiation and quantification of washcoat and substrate layers on a honeycomb support.

As part of this work, deep learning was used for reconstruction, measurement and multiphase segmentation of 3D datasets of GPF. Reconstructed data was used for input into gas flow simulations to relate pressure drop to performance. Property simulations were able to predict pressure drop along channels and through channel walls, and reactivity, through experimentally derived structure-boundary conditions.

Further, X-ray nanotomography was used to study porous PEFC catalyst agglomerate structures and used to simulate gas diffusion through pore networks. Non-destructive 4D studies were enabled by time resolved in situ experiments.

Novel field emission scanning electron microscopy “sweet spot” techniques were then deployed for imaging and understanding platinum nanoparticle decoration on A-site deficient perovskite catalysts for automotive applications, revealing details of terracing and platinum exsolution not previously visible and quantifiable in the scanning electron microscope.

Finally, a novel cryogenic focused ion beam scanning electron microscopy technique was applied for 3D volumetric analysis and lamella preparation for nanoanalytics of MOF materials.

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Participation:

In person

Poster / 611

Novel techniques in X-ray nanotomography, scanning electron microscopy and cryogenic focused ion beam microscopy Linking structure and catalytic properties of heterogeneous and automotive catalysts in three dimensions

Authors: Andy Holwell¹; Maadhav Kothari²; Markus Boese³

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Corresponding Authors: markus.boese@zeiss.com, andy.holwell@zeiss.com, maadhav.kothari@zeiss.com

Heterogeneous catalysts are a broad and versatile set of engineered porous materials, of high surface area and surface functionalization. Automotive catalysts have removed billions of tons of pollutants from entering the atmosphere since their deployment in the 1970s and must withstand long service lives. Their structure-property relationships are complex, determined by porosity, particle size, voids and adhesion between substrate, washcoat base layer and precious metal active components. Catalysts can therefore be challenging to image and characterize at high resolution and in three dimensions.

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Chris Morgan, Johnson Matthey Technol. Rev., 2014, 58, (4), 217
doi:10.1595/205651314x684726

Time Block Preference:

Time Block C (18:00-21:00 CET)

Participation:

In person

Poster / 613

Experimental Research and Application of Fracture Stress Sensitivity

Author: Junjie Liu¹

Co-authors: jian xiong ; jingpeng wang ; xiangjun liu

¹ 13008119162

Corresponding Authors: 767559931@qq.com, 361184163@qq.com, 2577138004@qq.com, wangjinpeng2018@petrochina.com.cn

Abstract: Stress sensitivity is a typical reservoir damage. Before large-scale development of tight gas reservoir, a correct understanding of reservoir stress sensitivity is very important for the protection and efficient development of tight sandstone gas reservoir. Therefore, taking the tight sandstone cores of the lower accumulation assemblage in the southern margin of the Junggar Basin as the research object, the stress sensitivity experiment and electron microscope scanning experiment were carried out, and the gas well productivity model considering the stress sensitivity coefficient was deduced. The results show that: The micro pores and micro fractures of the original tight sandstone matrix are not developed, the permeability and porosity are low, and have high stress sensitivity coefficient; The stress sensitivity coefficient of fractured rock sample increases with the increase of fracture angle; In the process of the gradual increase of the production differential pressure, the productivity of the gas well also increases, but the rate of productivity increase gradually slows down; Under the same production differential pressure, the productivity of gas well decreases gradually with the increase of the fracture angle.

Key words: Tight sandstone; Fracture; Stress sensitivity test; Gas well productivity model

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Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 614

Dependence of hydraulic conductivity on effective confining pressure in rocks and concretes

Author: Kotone Sakemoto¹

Co-authors: Masaji Kato ¹; Yusuke Ishii ²; Kiyofumi Kurumisawa ¹; Yoshitaka Nara ³

¹ Hokkaido University

² Taiheiyo Cement Corporation

³ Kyoto University

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The geological disposal of radioactive waste is designed to confine radioactive nuclides for a long period of time based on the concept of a multiple barrier system consisting of engineered and natural barriers. In this study, the hydraulic conductivity of mudstone and granite as natural barrier

materials and high strength and ultra low permeability concrete (HSULPC) as engineered barrier materials were measured using the transient pulse method. The results showed that both materials have low permeability, and the effective confining pressure dependency and hysteresis were also observed. Therefore, the coefficient of effective confining pressure dependency was introduced to discuss quantitatively. The results showed that there is a difference in the hysteresis between rock and concrete, and SEM observations were carried out on HSULPC to investigate whether there is a difference in the porosity affecting permeability. It was pointed out that the skeletal structure of HSULPC was not easily deformed and there were few flat cracks. It was also suggested that hydration reactions in the unhydrated part of HSULPC may have promoted the closure of voids and cracks during the permeability test. These results suggest that HSULPC exhibits significant hysteresis. Therefore, HSULPC is expected to stabilize at a low hydraulic conductivity after being buried in the ground and subjected ground pressure.

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Participation:

Online

Poster / 615

Capillary sealing efficiency of caprock: Implications for hydrogen and carbon-dioxide geo-storage

Authors: Amer Alanazi¹; Muhammad Ali¹; Hussein Hoteit¹

¹ King Abdullah University of Science and Technology

Corresponding Authors: hussein.hoteit@kaust.edu.sa, amer.alanazi@kaust.edu.sa, muhammad.ali.2@kaust.edu.sa

Geo-storage of hydrogen (H₂) and carbon dioxide (CO₂) is a promising solution for a low-carbon global economy (Ali, 2021; Ali et al., 2022a; Ali et al., 2021b; Bui et al., 2018; Pan et al., 2021b). The knowledge of the capillary entry pressure of caprock is critical, which provides a rapid assessment of the capillary sealing efficiency and sealing capacity, particularly in the presence of impurities (organic acids) and formation brine (Hosseini et al., 2022a; Pan et al., 2021a). However, the literature lacks such analysis on caprock under storage conditions, specifically for H₂. An efficient and safe structural storage requires a deep understanding of key parameters such as pore geometry, organic acid contents, pressure, temperature, and salinity on the wetting characteristics of the rock/gas/brine system for comprehending the capillary sealing efficiency (Al-Ansari et al., 2018; Al-Yaseri et al., 2022; Ali et al., 2020; Ali et al., 2021a; Arif et al., 2019; Hosseini et al., 2022b; Iglauer et al., 2021). Therefore, it is pertinent to determine the wetting characteristics of caprock and interfacial tension (IFT) between liquid and gas to mitigate any potential sealing problems.

The capillary sealing efficiency and entry pressure of the gas is determined using the interfacial tension (IFT) between liquid and gas, the contact angle of the rock surface in the presence of liquid and gas, and the typical pore throat radius of caprock, i.e., 5 nm and 10 nm (Hosseini et al., 2022a). The capillary sealing works against the buoyancy pressure exerted by the gas column height, therefore,

the maximum static column height of the gas is crucial in these calculations (Hosseini et al., 2022a; Iglauer et al., 2015). The geological formation contains organic molecules and their effect on wetting characteristics is widely reported (Akob et al., 2015; Ali et al., 2020; Ali et al., 2019a; Ali et al., 2019b; Ali et al., 2021a; Ali et al., 2021b; Ali et al., 2022b; Lundegard and Kharaka, 1994). Therefore, this work investigates the capillary-sealing efficiency using contact angle measurements of pure mica as a proxy of caprock compared to organic-aged mica, and the effect of alumina nanoparticles on organic-aged mica substrates under various geological conditions (i.e. up to 25 MPa and 343 K). The results indicate that the sealing efficiency and storage capacity for H₂ and CO₂ decreased with pressure and higher organic surface concentration but increased with temperature. The analysis demonstrates the theoretical inverse relationship between the capillary entry pressure and the pore throat radius. The smaller the pore size, the more suitable the conditions for sealing and storage capacity. The analysis of the alumina-nano-organic-aged mica/CO₂ systems showed improved wettability and better sealing efficiency. In a nutshell, this work provides a detailed theoretical workflow to assess the influence of organic molecules on the sealing efficiency and storage capacity of caprock for safe and secure geo-storage of H₂ and CO₂.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 616

Permeability estimation in the low-porous rock sample using the Navier-Stokes equation at slip and no-slip conditions

Authors: Paweł Madejski¹; Paulina Krakowska-Madejska¹

¹ AGH University of Science and Technology

Corresponding Authors: krakow@agh.edu.pl, madejski@agh.edu.pl

Porosity and permeability are particularly important parameters in the petroleum industry, where the possibilities of hydrocarbons exploitation depend on reservoir properties. The computational methods have become more popular in the analyzes of fluid flow and heat transfer in porous media. The flow of gas at the microscale differs with respect to flow at the conventional scales 1. The primary difference is that slipping of gas molecules may occur at the solid-gas interface [2]. The paper presents the results of CFD modeling in the form of mass flow rate changes and permeability changes for the examined pore space. The permeability was determined based on the results of CFD modeling and the modified Darcy equation [3]. Computational analysis of fluid flow through the pore space was performed with the use of the Finite Volume Method (FVM). To solve Navier-Stokes equations using the FVM method, a numerical mesh was generated by dividing the entire 3D geometric model into small Control Volumes (CV) and calculating the desired values in each mesh cell. The fluid flow simulation results are the local velocity, mass flow of the fluid, and pressure in each grid cell, depending on the pressure difference at the inlet and outlet of the analyzed sample (boundary conditions). The 3D geometrical model used in simulations can be obtained using various measurement techniques. The presented work uses the results of a computed X-ray tomography (CT) and a specialized study of pore space using a developed tool for image analysis - poROSE software [4]. In the case of low porous rocks, it is necessary to consider the phenomenon of slip to determine the permeability value correctly. The calculation results at slip conditions were carried out using the Maxwell model in the presented work. The effective permeability can be up to 1.68 times greater considering the slip phenomenon. The change in the mass flow rate of gas and the effective permeability of the rock sample showed a high impact of slip conditions on the achieved results. The proposed approach can be used to estimate TMAC values for different porous materials by comparing measured core samples and calculated permeability.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 617

A Potential Energy based Lattice Boltzmann Model for Two-Phase Flow in Fractured Porous Media

Authors: Zhongkun Niu¹; Zhengming Yang²; Yutian Luo^{None}; Yapu Zhang^{None}; Yilin Chang³; Xinliang Chen³; Xinli Zhao³

¹ *Institute of Porous Flow and Fluid Mechanics, Chinese Academy of Sciences*

² *PetroChina Research Institute of Petroleum Exploration & Development*

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The flow law of two-phase flow in complex porous media can be used to explain the variability of development efficiency during the displacement, imbibition, and huff-and-puff process with different construction parameters. Therefore, with the help of nuclear magnetic resonance, micro-CT (micro computed tomography), and tracer method, core samples and microfluidic chip experiment are commonly used as laboratory means to study the displacement and imbibition process in porous media. However, the flow field information obtained by laboratory methods is extremely limited. While, from the perspective of numerical simulation, more detailed flow field information of two-phase flow in complex porous media can be obtained through various computational fluid dynamics methods.

The computational fluid dynamics applied to the simulation of two-phase flow in porous media includes two types of calculation methods: the conventional Navier-Stokes solvers and the particle-based solvers. Specifically, the common numerical simulation methods for two-phase flow include direct numerical simulation, finite element method, volume of fluid-finite volume method, lattice Boltzmann method (LBM), and molecular dynamics method. Whereas, LBM is more suitable to simulate flows in complex porous media because of its simplification and advantageous boundary conditions processing. Thus, the numerous studies have carried out to analyze the flow field in porous media through the pore-scale LBM combined with digital core technology. While, pore-scale LBM depends on the specific interconnected pore network structures which have been the important influence in the flow field. It indicates that few mechanisms of two-phase flow between fractures and matrix would be deduced because of the lower modeling accuracy of simulated structures. For instance, the submicron structures would be omitted due to smaller size than the microfractures or dispersed dissolution pores contained in tight porous media.

In order to obtain more inherent mechanisms of the two-phase flow in fractured tight porous media.

This paper extends the application of the free-energy based LBM and adjusts the equilibrium distribution function and the potential energy model to make the two-phase flow algorithm more suitable for REV-scale porous media. The novel algorithm can be applied in trans-scale, where free-energy model is used in the fracture flow, and the two-phase seepage model is used in porous media simulation. Based on the slices of the real rock samples scanned by micro- and nano-CT, the two-phase flow in tight porous media with discrete fracture network is simulated by the novel algorithm. Compared with the original two-phase flow LBM algorithm, it can reveal not only the two-phase flow mechanism with the presence of discrete fracture network, but also the imbibition process between fracture and matrix. Therefore, it can provide a guidance of trans-scale flow simulations in tight porous media after hydraulic fracturing.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 618

The SOPHIE initiative –The first interlaboratory comparison of the wet end of the soil water retention curve

Author: Benjamin Guillaume¹**Co-author:** Aurore Degré¹¹ *Uliège***Corresponding Authors:** aurore.degre@uliege.be, benjamin.guillaume@uliege.be

Soil water retention curves (SWRCs) are key inputs to feed Richards's equation-based hydrological models. Knowing that these models play a role in a wide range of societal issues, they must be based on reliable data. SWRCs are usually obtained in laboratory on soil samples using one/some of the available methods. Although some studies show that different non-harmonized elements of the procedures for the determination of SWRCs in laboratories can significantly influence the measurement of retention properties, to date, these procedures are not harmonized. The impact of these non-harmonized procedures on the legacy SWRCs data and on the hydrological models they feed remains to be investigated.

The challenge was to carry out an interlaboratory comparison using an artificial constructed porous reference sample set with controlled retention properties that can be transferred safely between laboratories. The reference sample was composed by a mix of glass beads and cement. The inter-laboratory comparison involved 14 European laboratories with 3 successive rounds of measurements of four retention points (10, 50, 100 & 300 hPa) on 84 reference samples. The samples followed specific inter-laboratory exchange schemes designed to assess both the intra-/inter-laboratory variability and the effect of sample transfer. The random effect related to the laboratories, samples and transport between laboratories on the SWRCs were determined based on a Bayesian linear mixed model programmed in the "Stan" language.

A simple bulk density analysis showed that the reference samples were not uniform, with bulk densities ranging from 1.575 to 1.835 g/cm³. Nevertheless, the linear mixed model shows that the variance explained by the differences between laboratories is more important than the variance explained by the intrinsic differences between samples. This underlines the fact that differences in SWRC measurements, on a same sample, from one laboratory to another can be substantial. However, the dry mass of the samples increased significantly between the first and last series of measurements, despite the fact that some material losses were reported. Although not considerable, the transfer of samples between laboratories seems to significantly influence the retention curves. This indicates that the retention characteristic of the reference samples could change over time. In this case, the methodology used to analyze sources of variability can be biased and could lead to inaccuracies in the estimation of the variability attributed to the laboratories or samples.

These results shows us that the uncertainty associated with the determination of the retention curve in the laboratory can be substantial and should be a concern. However, a more appropriate porous reference sample is needed to refine the investigation and gain insight into the underlying causes of this uncertainty.

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Participation:

Online

Invited & Plenary Speaker / 619

Advances in pore-scale characterisation of multiphase flow and transport in porous materials

Author: Vahid Niasar¹

¹ *University of Manchester*

Corresponding Author: vahid.niasar@manchester.ac.uk

Understanding fundamentals of flow and transport in porous media has been significantly enhanced using pore-scale characterisation methods, such as pore-scale modelling and imaging. During the last five decades “pore-scale characterisation” has been established as a major field of porous media research, has imposed new questions and highlighted gaps in knowledge that has enhanced our understanding for practical implications.

In this presentation, I present some key pore-scale findings related to solute transport in saturated and unsaturated porous media. The experimental results have been obtained using three different complementary approaches : (a) optical imaging of quasi-3D micromodels, (b) 4D X-ray microCT imaging glass-bead and sand packing, (c) GPU-enhanced pore-network models.

Two main aspects of the results will be discussed in this presentation (i) the non-Fickian behaviour of transport in unsaturated porous media and the critical role of saturation morphology (ii) time scale of transport during loading and unloading of a solute and the potential role of non-linear transport.

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References:

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Time Block Preference:

Time Block B (14:00-17:00 CET)

Participation:

Online

Poster / 620

Predicting thermal potential of a shallow ground to support design of low-temperature district heating and cooling networks

Authors: Shakil Masum¹; Wu Gao¹; Hywel Thomas²

¹ *Cardiff University*

² *Cardiff University*

Corresponding Authors: thomashr@cardiff.ac.uk, gaow11@cardiff.ac.uk, masumsa1@cf.ac.uk

To limit the global temperature rise to 1.5°C, significant reduction of fossil fuel usage and promotion of zero-carbon, renewable energy solutions are essential. Energy sector is one of the largest emitters of greenhouse gases (GHG), dominated by space heating and cooling demand. The 5th generation district heating and cooling networks, that are designed to operate at near ground temperature, offer cost-effective, zero-carbon energy solution. For successful design and optimum performance of such network, detailed investigation of ground processes and accurate estimation thermal storage and recharge potential are of great importance. Thermal potential of shallow grounds is influenced by atmospheric conditions as well as subsurface soil types or profiles. Numerical studies which incorporated the complex boundary conditions and coupled soil heat and moisture processes in support of ground energy network design and assessment are limited.

Therefore, in this study, an advanced numerical model, based on a coupled Thermal-Hydraulic (TH) modelling framework, is developed to evaluate a shallow horizontal ground loop system. It calculates and predicts temperature and soil-moisture behaviour of a shallow ground under complex and coupled atmospheric, temperature and hydraulic boundary conditions. Atmospheric data e.g., solar radiation, rainfall, humidity, air temperature, wind velocity is incorporated in the model with soil-soil boundary and diverse layered soil profiles to investigate thermal and hydraulic responses of the ground, and performance of a DHC network. The model is applied to predict evolution of long-term ground temperature and saturation level of a potential site located at the Warwickshire County in the UK. The total and net heat content per unit area of the site per annum/ season/ month are simulated for a five-year period. The heat content varied between 2.0-55 MJ/m² depending on the subsurface soil layers. The simulations also revealed that a considerable amount of heating and cooling demand of the site could be met sustainably, solely from the shallow ground, implementing the proposed horizontal ground loop system. In addition, sensitivity of the model parameters investigating the effects of soil types and hydraulic drainage conditions on the ground heat supply potential revealed significant impact of underlying soil layers on spatio-temporal distributions of ground heat. The findings of this study highlight the influences of atmospheric conditions and coupled ground processes on accurate design of a 5th generation low-temperature heat network and estimation of ground thermal behaviour.

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Time Block B (14:00-17:00 CET)

Participation:

In person

Poster / 623

Digitizing and Exploring 16 Years of the Registry of Contaminated Sites in the state of São Paulo, Brazil

Author: Nouha Samlani¹**Co-authors:** Daphne Pino²; Carlo Bianco³; Nathaly Lopes Archilha⁴; Tannaz Pak¹¹ Teesside University² University of São Paulo³ Polytechnic University of Turin⁴ Brazilian Synchrotron Light Source**Corresponding Authors:** t.pak@tees.ac.uk, nathaly.archilha@lnls.br, carlo.bianco@polito.it, n.samlani@tees.ac.uk, daphne.pino@usp.br

Brazil is a water-rich country with nearly 90% of its freshwater lying on its subsurface¹. Brazilian groundwater plays a crucial role in the water supply as 16% of the population depends solely on it^[2]. However, rising anthropogenic contamination threatens this resource, especially in urban areas, industrial districts, and storage areas¹. The most prevalent contaminants –petroleum and chlorinated products–have low water solubility and constitute separate phases in the subsurface^[3], making remediation procedures in situ a challenge.

The state of São Paulo is the most densely populated in Brazil and is heavily industrialized. It is also one of the most dependent states on groundwater. Its environmental agency, CETESB –The Environmental Company of the State of São Paulo –was the first of its kind to be created in Brazil in 1968 ^[4] and has contributed to the leap of advances in contaminated sites (CSs) management that São Paulo has on the other Brazilian states. Indeed, it is one of three Brazilian states with a database^[5] and a publicly published registry of its CSs.

This registry promotes identifying CSs and yearly monitoring of remediation and controlling measures applied to each site. This study looks into 16 years of this registry and presents an overview of CSs management in São Paulo. The objective is to provide insights on the state of remediation and the efficiency of used techniques and thus lay the ground for future studies planning the use of innovative technologies within the Brazilian context.

To this aim, a computer vision program was developed to digitize the openly available survey forms. An optical character recognition (OCR) engine and edge detection techniques were deployed in a python script to transform the data from a portable document format into a tabular format for data analysis in Microsoft Excel.

This study shows that not only the number of identified contaminated sites has multiplied over the years, but also more sites have been rehabilitated. Indeed, nearly 30% of the 6434 sites of 2020 are classified as rehabilitated and 16% as reused sites, against a meager 1,5% of finished rehabilitation cases among the 1336 cases of 2004. Groundwater has been the most impacted media by the contaminated sites (59%, in 2020). The most-reported polluting activity is gas stations (70%, 2020), causing automotive fuels to be the most detected contaminant and the pump and treat as the most used remediation technique in the sites surveyed. This focus on the gas station's cases surveillance followed a licensing legislation and does not represent the real distribution of the CSs. In fact, industrial activities being responsible for only 20% of the CSs is proof of this bias.

Although the real number of CSs in the state of São Paulo is expected to be around 20 000 sites [5], significant progress has been made over the last 16 years and needs to be acknowledged. Furthermore, in preparation for a future big-data stage, automating data entry of publicly available forms and subsequent data analysis will become an indispensable step toward a more efficient and fact-based communication with stakeholders.

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References:

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Time Block Preference:

Time Block A (09:00-12:00 CET)

Participation:

Online

Poster / 624

Experimental study on porosity and permeability characteristics of unconventional reservoir under overburden pressure

Authors: Xinliang Chen^{None}; zhengming Yang¹; Xinli Zhao²; yapu Zhang^{None}; Zhongkun Niu³; Wen Li²; Yilin Chang²

¹ *PetroChina Research Institute of Petroleum Exploration & Development*

² *University of Chinese Academy of Sciences*

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The changes in the porosity and permeability characteristics of rocks under overburden pressure often have a series of effects on the development of oil reservoirs, especially for unconventional

reservoirs. In order to study the porosity and permeability characteristics of unconventional reservoir under overburden pressure, a large number of overburden porosity and permeability experiments on unconventional reservoir cores are carried out. Meanwhile, the microscopic pore structure characteristics of unconventional reservoir cores with different permeability are analyzed by using synchrotron radiation imaging technology. The results show that: ① The relative porosity ratio and relative permeability ratio of unconventional reservoirs have a good correlation with the effective overburden pressure. With the increase of overburden pressure, the relative porosity ratio and relative permeability ratio change greatly, which is different from the traditional view; ② Under reservoir conditions, the relative porosity ratio, relative permeability ratio, and irreversible permeability loss of unconventional reservoir cores all have a good semi-logarithmic relationship with permeability. The values of porosity and permeability under reservoir conditions are quite different from those on the ground, and their influence cannot be ignored; ③ The lower the permeability of unconventional reservoir cores, the stronger the microscopic heterogeneity and the worse the pore connectivity.

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References:**Time Block Preference:**

Time Block A (09:00-12:00 CET)

Participation:

Online

Invited & Plenary Speaker / 626

Supercritical CO₂ flow and heat/mass transfer in micro/nano-porous structures in CO₂ geological utilization and storage

Author: Ruina Xu¹

¹ *Tsinghua University*

Corresponding Author: ruinaxu@tsinghua.edu.cn

CO₂ geological storage and its use to enhance geothermal systems and shale oil/gas recovery are critical technologies for addressing climate change. CO₂ is in a supercritical condition among the above methods. One of the most important challenges in improving recovery efficiency and long-term storage safety is the migration and heat/mass transfer of supercritical fluids in reservoir porous structures. Under the subsurface conditions, micro/nano-scale confinement, interface effect, and rapid changes in supercritical-fluid physical properties all have a significant influence on transport behavior in the porous structure. This talk will be divided into three parts: (1) heat transfer characteristics of supercritical CO₂ in rocks; (2) CO₂/CH₄ adsorption in kerogen nano pores; (3) supercritical CO₂, water, and oil multiphase flow in micro-porous structures.

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Time Block A (09:00-12:00 CET)

Participation:

Online

Invited & Plenary Speaker / 627**Hysteresis of mass transport in porous media**

Author: Dominique Derome¹

¹ *Universite de Sherbrooke*

Corresponding Author: dominique.derome@usherbrooke.ca

A discussion on the occurrence of hysteresis in different aspects of mass transport in porous media, including contact angle of advancing and receding flow in capillaries, occurrence of capillary condensation hysteresis at mesopore scale and hysteretic swelling of hygroscopic polymers upon sorption. Relevance of considering hysteresis in computational modeling, namely lattice Boltzmann and atomistic modeling.

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