# Book of Abstracts

# 8th Interpore UK Chapter Conference on Porous Media

1-2 September 2025

Loughborough University,
Loughborough, UK

# Keynote & Invited Lectures

# Kimberly-Clarke Distinguished Lecture

## From the Brain to Water Uptake of Roots to Fuel Cells: - Porous Media are "Almost" Everywhere

Professor Rainer Helmig

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Porous media are almost everywhere. The understanding of flow, transport and deformation processes in porous media is important for the optimization of fuel cells, energy storage, the prediction of landslides due to heavy rainfall or the spread of tumors in human tissue.

In this lecture, we will first give a brief overview of the importance of porous media. Using selected examples, we will cover the range from environmental to technical and relevant bio-issues.

Then we would like to present selected modelling approaches and analyses using two concrete application examples:

First, we can use the knowledge of porous media to make better predictions when multiple sclerosis flares. What happens in the porous medium "brain" when the blood-brain barrier no longer functions properly? How can research in the field of porous media positively influence the treatment of multiple sclerosis?

Secondly, we would like to discuss whether it is possible to improve water management in fuel cells as a drive technology with our knowledge of porous media. What role does the understanding of porous media play in the context of alternative forms of mobility such as fuel cells? Are our "classical models" for water transportation helpful?

Regarding both of the above-mentioned topics, the use of simulations helps because they make the invisible processes in the brain and in the fuel cell visible (I hope).

# Invited Lecture

## It's the Stickiness: How Winnowing, Substrate Structure and Pore Space Dynamics Limit Estuarine and Coastal Morphodynamics

Professor Dan Parsons

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Estuarine environments are hotspots of ecological productivity and sedimentary complexity, yet our ability to predict their morphological evolution is hindered by a critical gap: the role of substrate cohesion and microstructure in mediating sediment transport. This talk explores new insights from a series of controlled flume experiments that systematically varied substrate clay and extracellular polymeric substance (EPS) content to replicate natural estuarine bed conditions. We show that biologically and physically cohesive sediments not only delay bedform development, but significantly alter winnowing processes with limitations of flow through pore spaces likely a key control. The "stickiness" introduced by even trace amounts of EPS profoundly stabilises substrates, reducing bed sediment mobility and preventing effective winnowing, which is a key trigger for bedform initiation. This leads to morphological hysteresis, with long lags in response to flow forcing and incomplete bedform equilibration over tidal timescales. Pore space dynamics and substrate structure further mediate how cohesion impacts erosion thresholds and sediment reworking. These findings challenge conventional assumptions in bedform phase diagrams and morphodynamic models toat seek to predict the evolution of estuaries and coasts, and point to the urgent need to integrate the impacts of cohesive microstructural dynamics into estuarine and coastal modelling frameworks. As climate-driven pressures reshape estuarine systems, understanding the microscopic controls on macroscopic change is essential for forecasting and managing future coastal landscapes.

# Invited Lecture

## Degradation of PFAS During Thermal Reactivation of Granular Activated Carbon for Water Treatment

Professor Jan Hofman

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Granular activated carbon (GAC) is used throughout the water industry to remove organic micropollutants such as pesticides, pharmaceuticals and other chemicals. GAC can also effectively remove PFAS compounds, although the adsorption capacity is much lower than for other target compounds. Therefore, GAC that is used for PFAS removal requires more frequent regeneration actions. GAC regeneration is done in a high temperature furnace (800-1000°C) in a non-oxidising atmosphere. Until now it was unclear what the fate of the PFAS was during regeneration: are they desorbed, and will by-products be formed? In this project we investigated the fate of PFAS molecules during thermal regeneration of GAC. We found that PFOS and PFOA were fully removed above 500°C. We could also detect the formation of by-products that were consistent with decomposition pathways.

# Invited Lecture

## Minimally Invasive Technologies for Transdermal Delivery and Diagnostics

Dr Conor O'Mahony

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At Tyndall National Institute, our research is focused on merging miniaturized sensors, actuators, power sources, communications and control electronics to form a new generation of wearable healthcare devices that we refer to as Micro Transdermal Interface Platforms (MicroTIPs). MicroTIPs will ultimately be capable of independently diagnosing physiological conditions, autonomously delivering appropriate therapeutic agents, and wirelessly interacting with clinical personnel and mHealth networks.

In many cases, these platforms utilize arrays of microneedles - microfabricated structures that penetrate the outermost layers of the skin but yet are too short to strike nerve endings or draw blood, and that are therefore perceived as painless by the user. Working in collaboration with a wide range of industrial and academic collaborators, we are assembling microneedle-based, closed-loop smart systems that in-crease patient adherence and lead to improved treatment outcomes.

This talk outlines examples of progress in key aspects of those platforms, such as smart systems and microneedle technologies for transdermal and subcutaneous drug delivery, interstitial fluid sampling, electrochemical diagnostics and embedded sensors for closed-loop theranostics.

# Invited Lecture

## Inkjet Printing of ZIF-67 based-polymer composite membranes

Professor Begum Tokay

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Inkjet printing (IJP) has been adopted to fabricate zeolitic imidazolate frameworks (ZIFs) on commercial membranes. ZIFs, the subclass of metal-organic frameworks (MOFs), are achieving significant progress in applications such as adsorption, gas sensors, gas separation, drug delivery, and more due to their tunable porosity and high surface area. Employing IJP allows the fabrication of ZIF/MOF layers of desired geometry and thickness on porous substrates to address the limitations of traditional manufacturing techniques related to processability and mechanical strength, including scale up. This talk will present in-situ inkjet printing of ZIF-67 on a commercial nylon membranes and their application to remove dyes from water.

# Oral and Flash Presentations

## Session 2

## Porous Media in Environmental and Water Engineering

# Transcending Diffusional Limits: Microchannel Structured Substrates for Intensified Catalysis and Separation

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Porous substrates serve as an indispensable interface, bridging nanoscale functional materials from laboratory settings to meter-scale industrial unit operations. Historically, the inherently stochastic nature of their pore architectures has dictated the limits of diffusional transport, consequently imposing a significant performance upper bound on micro-scale functional materials in macro-scale engineering applications. This fundamental limitation is pervasive across critical engineering processes, including catalysis and separation. Current suboptimal solutions often involve adjusting substrate dimensions or optimizing unit operation characteristics to merely mitigate the adverse effects of diffusional constraints. These compromises invariably lead to reduced process efficiency, increased energy consumption, and higher operational costs. Fundamentally, these trade-offs stem from the absence of a scalable substrate technology capable of transcending conventional random pore architectures.

Our recent breakthrough in this domain centres on the development of microchannel-structured beads. Utilizing a controlled phase inversion process, a technique widely employed in the preparation of organic, inorganic, and composite membranes, we have successfully engineered beads of approximately 3 mm in industrial-standard diameter. These beads are characterized by an abundance of radially oriented microchannels, explicitly designed to intensify diffusional mass transfer. Furthermore, we have established pilot-scale infrastructure to facilitate their scaled-up production. We are actively engaged in validating the profound advantages of this unique pore architecture in augmenting diffusional transport and substantially enhancing the efficiency and sustainability of catalytic and separation processes across diverse fields, including water treatment, chemical synthesis, and energy & environmental applications.

# Multiscale Modelling of Reverse Osmosis Membranes: Asymptotic Derivation and Numerical Validation

Matteo Icardi, John King, Nicodemo Di Pasquale, Omomayo Akele, Anna Kalogirou, Ye Ma

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We develop a multiscale model for reverse osmosis desalination that couples fluid flow, solute transport, and surface scaling. Starting from the Navier–Stokes and advection-diffusion equations, we derive a reduced 1D model via lubrication theory and matched asymptotics, capturing the impact of osmotic pressure and surface precipitation on membrane performance. Two permeability update models (porosity reduction and surface layer growth) are incorporated to describe clogging dynamics. The asymptotic results are validated against 2D simulations implemented in OpenFOAM, with custom membrane boundary conditions. This approach provides both analytical insight and a flexible numerical tool for membrane design and optimization.

# Urban mining at Loughborough - a summary of activities using biochar to extract metal ions from solution.

Mark Leaper, Diganta B. Das

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This presentation summarises projects over the last 5 years involving biochar adsorbing metal ions from solution at the Chemical Engineering Department at Loughborough University, within the university remit of the circular economy. Biochar is organic waste material that is heated in the absence of oxygen (a process known as pyrolization) to produce stable particles that are mostly carbon. The pyrolization time and temperature affect the properties of the biochar, including the functional groups such as hydroxyl and carbonyl, inorganic compounds such potassium and sodium oxide and porous structure, with temperatures varying between 300$^{O}$C and 800$^{O}$C. Treatment of the feedstock and biochar before and after pyrolization can also create bespoke properties. Metals of interest include copper, iron and neodymium as recovery examines distillery wastewater, coagulants in sewage treatment and the recycling of permanent magnets as areas of application.

# Oxygen Dynamics in Smouldering Combustion: Impacts on Reaction Zones and Biochar Production

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Smouldering combustion is a flameless process driven by the interplay between pyrolysis, oxidation reactions, and oxygen diffusion within porous media. In self-sustained smouldering, the energy released by oxidation reactions is sufficient to offset energy losses from endothermic processes and heat dissipation. Applied smouldering has been demonstrated as a cost-effective technology for soil remediation and waste treatment, and a few studies have also shown that it can be tuned to produce syngas, biooil, and biochar. However, the influence of oxygen dynamics on product formation through reaction zone transformations has not been fully explored. This study addresses this knowledge gap by examining oxygen ($O_2$) sensitivities in applied smouldering experiments, which resulted in self-sustained biochar production.

Experiments were conducted with inflow $O_2$ concentrations ($Y\_O_2$) of 21%, 10%, 5%, 4%, 3%, and 2% at a constant total Darcy air velocity of 5 cm/s. The fuel bed consisted of crushed walnut shells and sand mixed at 1:10 mass ratio. Results showed self-sustained smouldering at $Y\_O_2$>3%, while smouldering velocity increased from 0.24 to 0.81 cm/min at Y_O2= 3% to 21%. Oxygen-limited conditions ($Y\_O_2$<10%) favoured biochar production. This study provides valuable insights into how O2 dynamics control the reaction zone for smouldering applications, such as biochar production.

# Numerical Frameworks for Leaching and Competitive Sorption-Desorption in Subsurface Environments under Intense Rainfall Using Maximum Likelihood-Optimised Kinetic and Equilibrium Approaches

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Heavy rainfall can lead to the intense leaching of agrochemicals in the subsurface environment, increasing the risk of groundwater contamination [1]. The transport and eventual fate of multiple compounds in soil and consequently in groundwater are largely governed by competitive sorption-desorption mechanisms. These mechanisms are influenced by several key factors, including the soil physical and chemical characteristics, the concentration ratios of the interacting compounds, and the flow conditions. This study introduces a numerical framework for the inverse estimation of dispersion and competitive sorption-desorption parameters by integrating multi-component solute transport with sorption-desorption models under both kinetic and equilibrium conditions. Using a maximum likelihood algorithm [2], the framework accurately simulates agrochemical leaching, retardation, and removal, particularly under rapid transport conditions such as those induced by high-intensity rainfall events. Results indicate that in multicomponent leaching of agrochemicals, sorption-desorption and reactive transport processes of compounds strongly influence one another, leading to reduced overall sorption and retardation. This interaction causes a slight decline in the total sorption capacity. The specific characteristics of the porous media, such as mineral presence, play a critical role in enhancing sorption affinity, limiting desorption, and resulting in greater retardation and pronounced tailing effects. Under high flow rate conditions, a twofold increase in the concentration ratio between competing compounds can reduce sorption affinity by up to 10%. Additionally, elevated flow rates cause less than 3% rise in desorption and a decrease of approximately 20% in sorption capacity.

[1] https://wrap.warwick.ac.uk/id/eprint/187745/

[2] doi: 10.1029/2023WR034655.

# Applied Smouldering to Treat PFAS from Sewage Sludge

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Wastewater treatment plants (WWTPs) are critical infrastructure needed to mitigate environmental harm from pollutants. However, emerging pollutants in sewage sludge pose several risks and treatment challenges. Per- and polyfluoroalkyl substances (PFAS) are notably problematic due to their complexity and ubiquity in sewage sludge. Unfortunately, many WWTPs do not fully treat these compounds. Thousands of PFAS varieties are used in many modern materials – from fire-fighting foams, to cosmetics, to food wrappers. PFAS contamination poses urgent environmental risks due to PFAS' toxicity and strong persistence in the environment. There is a need for novel technologies to destroy PFAS from sewage sludge. Applied smouldering is a novel thermal treatment technology that can treat high moisture content (MC) WWTP sludge (up to 80% MC, wet mass basis) in a self-sustaining manner. Smouldering is a flameless form of combustion that propagates in a porous fuel – and can be harnessed to drive efficient waste treatment. Recently, this technology has shown strong efficacy in treating PFAS-contaminated sludge. This presentation will overview fundamental aspects of smouldering treatment – which are often governed by porous media characteristics – along with recent experimental results that further explore applied smouldering for PFAS treatment in sewage sludge.

# 4D Study of Groundwater Remediation using Nanotechnology, a Pore-scale Study

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Groundwater remediation is a pressing issue globally. In Southeast England, over 75% of public water supply comes from groundwater (Chalk aquifer), while almost 37% of Brazilian cities are supplied exclusively by groundwater. Groundwater is susceptible to contamination in regions where a pollutant source, such as industry, is present.

This work analyses a synchrotron imaging dataset to study reactive transport in porous media. The reaction under study is between zero-valent iron nanoparticles (nZVI) and trichloroethylene (TCE) – a dense non-aqueous phase liquid (DNAPL). DNAPL entrapment within porous medium (host aquifer) poses a significant challenge for groundwater remediation. Nanoremediation uses reactive nanoparticles to promote in-situ remediation of groundwater, however, the process is not optimised, mainly due to the limited insights in pore-scale processes. The studied dataset was obtained via X-ray micro-tomography imaging (X-ray micro-CT) at the Diamond Light Source. It allows for 4D (3D + time) study of the processes happening at pore-scale.

Through analysis of this dataset, we visualised and quantified TCE decomposition with temporal resolution of less than a minute, as well as propagation of gas, produced during the reaction within the sand pack. Pore-scale phenomena, observed during the experiment, included TCE decomposition and remobilisation by gas. This is in line with the previous study performed by Pak et al. (2020).

Segmentation of greyscale images was performed using deep learning algorithms (U-net) in Dragonfly, with further processing and visualisation in Avizo.

Additionally, laboratory-scale column experiments were conducted to study the nanoparticle transport in porous media at a larger scale. These column experiments provide new insights in the pattern of nZVI propagation at high concentrations within the studied columns, enabling us to correlate the findings with the observations made in the imaging dataset.

# Heavy Metal Bioaccumulation and Remediation within Aquatic Ecosystems

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Heavy metals contamination in aquatic ecosystems is a significant environmental concern leading to severe human health implications. This study aims to investigate the significance of heavy metal contamination in river systems and their potential effects on aquatic organisms with a potential remediation technique identified. A series of lakes, within the Attenborough Nature Reserve (ANR), UK, was used as a model system to analyse a 15-year hydrological and meteorological dataset to identify the dominant trends and statistical correlations which may have driven historical pollution levels of copper (Cu) and zinc (Zn). Multiple regression, time series analysis, and ANNs were compared to identify the most accurate model to predict metal concentrations in freshwater lakes based on different abiotic parameters. Subsequently, the potential for bioaccumulation within the invasive bivalve Corbicula fluminea tissue was examined within a series of laboratory-scale mesocosm experiments. The results indicated that the degree of bioaccumulation was proportional to the heavy metal concentrations in the aquatic phase. Removal of Cu and Zn from aqueous solutions using ground coffee waste and a mixture of rice husk biochar and coffee waste was also investigated to remove harmful metallic ions (e.g., Cu and Zn) from wastewater by a fixed bed, column adsorption study where the adsorption equilibrium was achieved around six hours.

# Oral and Flash Presentations

## Session 3

## Flow, transport and reactive processes across multi-scales in porous media – I

# The UK subsurface microbial limits database: a screening tool for safe geological storage

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The activity of microbes in sites used for the geological storage of carbon dioxide ($CO_2$) or hydrogen ($H_2$) has the potential to affect injection or storage (e.g. consumption of stored fluids, production of contaminants, blockage of flow paths, corrosion). As part of the MOET (Managing the Offshore Energy Transition) project, a tool has been developed to aid microbial risk assessment at potential storage sites. This describes the potential for UK's subsurface storage units to support microbial activity. It includes over 850 offshore and 35 onshore storage units covering saline aquifers and oil and gas fields. Risk of microbial activity based on temperature, salinity, pH, porosity, permeability, pressure and sulphate concentration data are provided. Key risk parameters are combined to give an overall risk rating. ~12 % offshore units received a high-risk rating for microbial activity. ~23% offshore units were given a low-risk rating. Further investigation is recommended for the remaining units to fully assess the likelihood of significant microbial activity occurring. An interactive interface allows individual units to be investigated. Together, this provides useful information for preliminary assessments of microbial risks and the suitability of specific sites for $H_2$ and $CO_2$ storage.

# Porous Microscale Current Collectors for Next-Generation On-Chip Energy Storage

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With the rapid growth of the Internet of Things, the key trends in microelectronics are clear - miniaturization, flexibility, and integration are leading the way. Various microelectronic devices, including wearables, implants, micro-robots, and micro-sensors, have made significant advances and are set to become essential parts of our everyday lives. These tiny devices excel in complex tasks such as data processing and wireless signal transmission, paving the way for major innovations in areas like health monitoring, medical diagnosis, and disease treatment. However, powering these devices seamlessly requires an efficient energy supply unit. Our research is dedicated to developing microscale batteries, known as micro-batteries, with a special focus on 3D porous electrode designs to boost energy storage performance within the limited space of microscale devices. We particularly emphasize planar device configurations, which organize electrodes in an interdigitated electrode (IDE) pattern on the same substrate, resulting in a flat, efficient structure. This design offers significant benefits, such as improved control over critical battery properties like internal resistance and ionic diffusion distance, all without needing a separator. Most importantly, it provides a practical solution for reducing battery size and integrating them seamlessly with on-chip microelectronic devices. The processing and precise loading of energy materials onto porous microelectrodes are critical to optimizing charge storage performance. Our research centers on designing advanced 3D porous current collectors and utilizing electrodeposition and Microplotter techniques to specifically and selectively manipulate energy materials on these collectors.

# Mixing in Underground Hydrogen Storage: The Role of Mechanical Dispersion and It's Influence On Site Selection

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In underground hydrogen storage, mixing between Hydrogen and cushion gas could present a problem to the recoverability of working gas and may be a controlling factor in subsurface reactions. The conventional modelling approach focuses mainly on diffusion as the primary mixing process, while little attention is paid to dispersive mixing. Using the finite element simulator COMSOL this work focuses on assessing the relative magnitude of transport between the two processes, where molecular diffusion is shown to be subordinate to mechanical dispersion. The evolution of the model is studied over a range of conditions relevant to potential UK UHS reservoirs to highlight the core sensitivities and inform future site selection. Necessary adjustments should be made when considering implementation of mixing processes in numerical models, with much more attention being given to studying dispersion.

# Exploring The Effect of Hysteresis and Heterogeneity on Hydrogen Storage Efficiency in Saline Aquifers

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To meet global net-zero targets by 2050, low-carbon energy options like hydrogen are essential. Underground hydrogen storage (UHS) in saline aquifers offers promising seasonal storage potential due to their availability. However, scaling UHS presents challenges related to reservoir heterogeneity, hysteresis, and flow dynamics. This study investigates the effects of geological heterogeneity and hysteresis on hydrogen storage performance through numerical simulations.

Two-dimensional formations were modelled, simulating injection and production in four 30-day cycles with permeability ranging from 2.5 to 500 mD. The Sequential Gaussian Simulation (SGS) method was applied to establish spatial variation, with a 100×800 grid layout. An observation well at the model centre monitored gas breakthrough, and injection ceased upon detection to minimise hydrogen losses.

Operational conditions were constrained by fracturing pressure and minimum bottom-hole pressure. Relative permeability and capillary pressure curves were constructed using experimental hysteresis data (Lysyy et al., 2022) to capture both primary drainage and secondary imbibition. Flow rates were optimised to stabilise pressure while preventing early gas breakthrough.

The results revealed that permeability anisotropy significantly affects recovery. Flow-aligned anisotropy (0°) produced high water cuts and low recovery, while perpendicular anisotropy (90°) showed better recovery but large pressure fluctuations. Omni-directional and 45° configurations offered balanced outcomes in terms of pressure and water cut.

In conclusion, the study underscores that hysteresis, heterogeneity, and anisotropy orientation play a critical role in optimising hydrogen recovery and reservoir integrity in saline aquifers under cyclic operations.

# A staged investment and development approach for cost reduction in underground hydrogen storage: The Long Clawson Field, UK.

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Underground Hydrogen storage (UHS) within depleted hydrocarbon reservoirs offers a promising mechanism for large scale energy storage, enabling the effective integration of green energy (wind and solar). High initial CAPEX associated with UHS, as well as limited production capacity or low demand may initially restrict the amount of $H_2$ available for storage, making this relatively new technology potentially unattractive as a financial investment. One way to reduce CAPAX and increase stakeholder interest is by starting with a small-scale project, but with the option to upscale the size of the storage project once a successful start proves technical feasibility. In this study, the Long Clawson (LC) Field serves as a case study to assess the UHS potential of a small-scale onshore oilfield. This study analyses the effectiveness of developing a small scale UHS operation within a single stratigraphic unit of the LC Field, leaving the option for further expansion into neighbouring units. Leveraging a readily available history-matched black-oil reservoir model with site specific data, this study utilises the complex structural geology of the field to isolate $H_2$ within a particular layer enabling efficient H2 storage at low capacities. An ever increasing cushion gas to working gas ratio is required to provide maximum storage capacity as a result of connectivity between layers from reservoir faulting. A CO2 CG injection strategy was developed to reduce pressure dissipation and $H_2$ cushion gas requirements. CO2 cushion gas injection into upper formations was shown to reduce $H_2$ CG requirements, avoiding gas mixing issues, while maintaining future upscaling potential.

# Extending Vertical Equilibrium Modelling for Three-Phase $CO_2$–$CH_4$–Brine Flow

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The transition to a low-carbon future requires widespread deployment of carbon capture, utilization, and storage (CCUS) technologies, particularly geological storage of $CO_2$ in saline aquifers and depleted hydrocarbon reservoirs. Depleted gas reservoirs offer advantages such as proven containment, data availability, and existing infrastructure. However, the presence of natural gas complicates $CO_2$ injection due to complex fluid interactions, necessitating compositional simulations that are computationally intensive.

To overcome these limitations, vertical equilibrium (VE) models provide a computationally efficient alternative by simplifying three-dimensional flow into a two-dimensional framework. This study presents a three-phase VE model for simulating $CO_2$, methane, and brine flow using a black-oil formulation. While miscibility between $CO_2$ and methane is not captured, the model effectively represents key displacement dynamics with reduced complexity.

The model assumes incompressible rock and brine, compressible $CO_2$ and methane, and operates under isothermal conditions. Density and viscosity variations are computed using the Peng–Robinson equation of state and approximated via Taylor series expansions to enhance efficiency.

Simulations were conducted to evaluate the model's performance across various reservoir configurations and injection scenarios. Results showed that the VE model successfully captured buoyant migration, phase segregation, and plume evolution observed in the detailed compositional simulations while the runtime reduced by over 100 times.

In conclusion, the proposed VE framework offers a practical balance between accuracy and efficiency, making it suitable for reservoir screening, optimisation, and uncertainty analysis. Though demonstrated for $CO_2$ injection into depleted gas reservoirs, the approach is broadly applicable to other gravity-driven subsurface processes, including energy storage and $CO_2$-enhanced gas recovery.

# Oral and Flash Presentations

**Session 4**

**Porous Media in Health Care**

# Assessment of the safety of repeated microarray patch applications in a minipig model

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Repeated application safety is essential for the clinical translation of microarray patches (MAPs) as a drug delivery platform. This preclinical study assessed the local and systemic safety of three MAP types: hydrogel-forming, dissolving, and implantable, over 28 days in miniature pigs, a translational model with skin characteristics closely resembling human skin. Blank MAPs were applied to the caudal flanks: hydrogel-forming MAPs every three days, and dissolving and implantable MAPs weekly with 48-hour wear time and four-day rest intervals. Skin barrier integrity was evaluated via transepidermal water loss (TEWL), while systemic effects were assessed through plasma inflammatory markers (TNF-α, IL-1β, IgE, IgG, CRP), blood and urine analyses, and welfare assessments. Histopathological evaluation was conducted post-study. MAPs showed robust mechanical performance, with less than 15% needle height reduction and consistent skin insertion. TEWL values remained stable, and no visible skin reactions were recorded. Inflammatory markers and urinalysis results confirmed no systemic toxicity. Histology showed intact skin architecture at all sites. These results demonstrate the safety and biocompatibility of repeated MAP application, supporting their further development as a minimally invasive, long-acting delivery system. This study contributes critical safety data for regulatory advancement towards human trials.

# Smart Powder Injector microneedles: A next-generation platform for porous material delivery into the skin

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Niacinamide (NIA) is a widely used cosmetic active ingredient known for its anti-inflammatory and antioxidant effects. However, its hydrophilic nature (log P = −0.35) limits passive diffusion through the stratum corneum (SC), necessitating advanced delivery strategies. While approaches such as penetration enhancers and liposomes remain hindered by the SC barrier, dissolving microneedles (DMNs) offer a minimally invasive route for intradermal delivery. Conventional DMNs, however, suffer from low drug loading and limited stability due to full polymer encapsulation. This study presents a novel "PowderInjector" DMN platform featuring porous, hollow microneedle structures designed to enhance drug loading capacity and delivery performance. Three designs were evaluated: (D1) traditional DMNs with NIA dispersed in the polymer matrix, (D2) hollow DMNs loaded with NIA powder only, and (D3) hybrid DMNs combining a concentrated NIA shell with a powder-filled hollow core. Mechanical, insertion, and delivery properties were assessed. D3 achieved a threefold increase in NIA loading (~2060 ± 288 μg) over D1, maintained crystalline stability, and demonstrated superior skin flux (272.14 ± 48.20 μg/cm²/h) and dermal deposition (3.778 ± 1.982%) compared to serum. PowderInjector DMNs offer a promising platform for stable, high-capacity topical NIA and porous material delivery with improved performance.

# Molecular Dynamics Based Modelling for Design of Dissolving Microneedle

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Hormones are key in maintaining good mental health (e.g., tackling menopause in women). However, administering hormone through the oral route has drawbacks like enzymatic degradation and unnecessary side effects like thrombosis. This problem can be dealt by transdermal hormone administration through dissolving microneedles (DMN), which is a pain free method with higher patient compliance. The principle behind DMN approach is 'poke and release' which is to pierce the skin with micron size needles and release drug molecules. A DMN array is fabricated with dissolving polymer which in presence of interstitial fluid of skin (after piercing) will allow the diffusion and uptake of hormone in the blood stream. An efficient microneedle array design with appropriate polymer formulation is crucial to delivering the drug in the desired concentration. To explore potential dissolving polymer behaviour and their compatibility with the hormone, all atom modelling is employed. The polymer with best compatibility will make it to continuum scale modelling where a rational DMN design will be modelled using finite element analysis method. This design will be evaluated for phenomena like dissolution, stress and strain relationship, hydrophobic drug diffusion keeping skin microstructures in consideration. In addressing these issues, the presentation will showcase the results from atomic scale modelling and the initial work done in continuum scale model.

# Numerical Investigation of Shear-Induced Cell Injury Using a Novel SPH-Based Biomechanical Model

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Cell damage caused by shear is a key factor in catheter-based surgeries and the formation of pressure ulcers. To investigate this, a Smoothed Particle Hydrodynamics (SPH) model in Abaqus/Explicit was developed to simulate the effect of shear damage on 'cell-soft tissue' porous interfaces. The top cellular layer was modelled using SPH particles (PC3D), and the substrate layers were represented as C3D8R solids. The Normal loading is applied via a rigid indenter with loads varying from 5–20mN. A shear stress element deletion criterion within Abaqus enables the quantification of critical shear thresholds that lead to cell death and the visualisation of how damage propagates. The experimental setup involved indentation testing using a Universal Mechanical Tester with a 1000µm spherical glass probe, applying loads to a monolayer of Human umbilical vein endothelial cells. These were seeded over a 90nm fibronectin layer on a 1mm thick PDMS (polydimethylsiloxane).

The numerical model exhibited a similar trend to experiments. Post-indentation imaging revealed a doughnut-shaped damage pattern with a central ring of living cells surrounded by a zone of cell death. The simulation enhanced our understanding of the shear-induced failure mechanism, resulting in the design of safer biomedical tools and clinical protocols in the future.

# Quality by design guided development of hydrogel-forming microneedles for transdermal delivery of enfuvirtide

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As the first fusion inhibitor of HIV-1, enfuvirtide has been confirmed to be well tolerated and has demonstrated remarkable antiviral activity compared with an optimised background antiretroviral regimen alone [1]. To minimise the 98% incidence of injection site reactions generated from the 90 mg twice-a-day subcutaneous injection of enfuvirtide, novel formulations of chemically crosslinked hydrogel-forming microneedles (MNs) was introduced as a minimally invasive and painless modality for the transdermal delivery of this peptide. To establish a systematic and robust approach for the formulation development, quality by design (QbD) and design of experiment were implemented. For the first time, the potential critical material attributes (CMAs) and critical process parameters (CPPs) of hydrogel formulations were identified and were associated with the critical quality attributes (CQAs) of MNs to ensure the quality targeted product profile (QTPP).

# Numerical Simulation of Hollow Microneedle Patches for Targeted Drug Delivery using a Coupled Free and Porous Flow Approach

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In this study, we report the development of a numerical simulation framework for the controlled transdermal delivery of ibuprofen (IBU) using a tablet-loaded hollow microneedle (HMN) patch. The model integrates pressure-driven, coupled laminar flow through the MN lumen and skin tissue, employing the Beavers–Joseph interfacial condition at the HMN tip and skin interface to represent the transition between free flow (lumen) and porous regions (tissue). For modelling purposes, IBU is loaded into a porous tablet, which, in practice, can increase the shelf life of the drug formulation and provide greater ease of handling. Drug transport in the system is modelled using the convection–diffusion equation for diluted species coupled with a pharmacokinetic component to predict systemic absorption. Parametric analyses have revealed that MN geometry, drug loading, and skin permeability significantly influence delivery efficiency. Notably, an increase in the drug-loaded tablet diameter leads to higher fluid velocity within the tablet, enhancing drug release. Among the key design parameters, the number of MNs and lumen diameter exhibit the strongest effect on drug permeability, with the permeability nearly doubling when the needle count increases four times from 9 to 36. In contrast, the pitch has a relatively minor impact. Inlet pressure emerges as a critical design factor: while higher pressures (e.g., 40 kPa) improve IBU permeability, they also reduce delivery control and compromise pharmacodynamic stability. The results indicate that maintaining moderate pressure levels enables a more balanced and sustained therapeutic effect, supporting the need for optimised delivery parameters tailored to specific drug characteristics and patient safety.

# Incorporating Fluid-Structure Interactions for Modelling of Pyramidal Hollow Microneedles for Transdermal Drug Delivery

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Hollow microneedles (HMNs) have gained significant attention as a potential alternative to traditional hypodermic needles for delivering drugs through the skin. The rational selection of the HMN geometry and materials is essential for balancing the MN's mechanical stability and efficient drug delivery. In addressing this, the current study aims to develop a numerical model for fluid-structure interactions (FSI) in hollow pyramidal-shaped MNs where HMNs made from two polymers (polylactic acid (PLA) and polyglycolic acid (PGA)) and one metal (stainless steel (SS)) are considered. Finite element (FE) simulations have been performed with COMSOL 6.2 Multiphysics to determine the effect of MN design parameters such as wall thickness, pitch, channel diameter, and dual-zone MN structure (different MN lengths) on fluid flow and von Mises stress distribution in the HMNs. The FSI analysis has been conducted for a laminar flow of water-fentanyl mixture as a model fluid. The findings revealed that raising the inlet pressure from 10 kPa to 30 kPa at the HMN entrance increases the flow rate to 0.005 µl/s, velocity 0.003 m/s, and total drug flux by 248.63%. As expected, SS demonstrated the lowest von Mises stress (13,213 $N/m^2$) while PLA and PGA exhibited a decrease in the stress level as the HMN wall thickness increased. Increasing the MN pitch from 400 µm to 1200 µm reduced skin pore pressure by 72% and enhanced drug concentration by 11.4%. The dual-zone MN arrangement, combining shorter and longer needles, improved the HMN penetration and led to a 90.8% increase in overall flux. These findings provide a foundation for optimising HMN designs, ensuring a balance between mechanical stability and improved transdermal drug diffusion for clinical applications.

# Oral and Flash Presentations

## Session 5

## Manufacturing Technologies for Porous Media

# Industrial Scale Production of Metal-Organic Frameworks for Carbon Capture

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Promethean Particles

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Metal-organic frameworks (MOFs) are an exciting class of crystalline porous materials, which exhibit high uptake capacities for a range of adsorbates, such as H2O, CH4 and CO2. MOF-based technologies have struggled to span the gap from academic research to large-scale industrial application, often due to inherent limitations in the scale-up of traditional batch processes; these include reproducibility issues with increasing production scale, and/or the high cost of manufacture.

Promethean Particles overcome these manufacturing limitations by using a continuous-flow approach to MOF synthesis. Our range of proprietary continuous-flow reactors facilitate the cost-effective scale-up of different MOF syntheses, while maintaining high product quality. Through rapid prototyping at lab-scale (g/hr synthesis), scalable MOF synthetic procedures are developed to utilise mild reaction conditions and raw materials that are low cost and abundant to source at large scale. Our reactor technology has enabled the successful demonstration of multiple MOF compositions, firstly at lab scale (g/hr), pilot (kg/hr), and then production scale (currently at 100s kg/hr with a view to increase further). An example of a MOF that has been upscaled using our continuous-flow process is a mixed metal UTSA-16 structure, which this presentation will detail.

Promethean's high throughput flow reactors have enabled the production of industrially-viable volumes, thereby facilitating pilot scale demonstration of MOFs in real world applications. This presentation will also describe the successful manufacture of 50 kg of UTSA-16 MOF, and its implementation as an adsorbent in a pilot scale carbon-capture unit, where it retained its structure and performance after exposure to real flue gas.

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# Compressive response of aluminium foams under high strain rates

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Aluminium foams are highly effective at absorbing energy under compressive loads while also offering considerable weight reduction compared to their solid metallic counterparts, with applications in the civil engineering, maritime, nuclear and defence industries. In this study, the compressive response of a set of specimens comprising aluminium foam cores sandwiched between steel cover plate is investigated, with the applied strain rate varied from 0.1 - 500 mm / min. Key mechanical properties including initial linear stiffness, plastic proof strength, plateau strength and impact energy absorption capacity are discussed. Digital Image Correlation results are also described that show the magnitude and location of localized stress concentrations within the walls of aluminium foam prior to the onset of initial cell wall buckling and later collapse of the foam matrix. The dependency of these various results on strain rate is described, with mathematical relationships suitable for inclusion in conventional numerical models also proposed.

# Oral and Flash Presentations

## Session 6

## Applications of Particle and Porous Media in Varied Applications

# Driving Sustainability in Electrochemical Water Treatment: A Life Cycle Lens on Electrode Material and Coating Selection for degradation of p-aminosalicylic acid in water.

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The pressing demand for sustainable wastewater system has spotlighted electrooxidation (EO) as a robust and promising approach. However, the environmental trade-offs associated with production of electrode material and method of coating remain underexplored. The present study provides a holistic Life Cyle Assessment (LCA) of combination of active and inactive anode material —BDD, Ti/PbO2 and Ti4O7, aiming to bridge the gap between the electrochemical performance and environmental sustainability. The LCA study was conducted by incorporating the coating techniques, electrode synthesis, energy consumption and emissions. The scale-up study was complemented by correlation analysis and Monte Carlo simulation to identify the dominant factors and variability respectively. Results reveal BDD as more environmentally favourable option, exhibiting the lowest impact across all the impact categories. In contrast Ti/$PbO_2$ exhibited a resource strain over 10 times greater than BDD due to use of toxic lead and high energy consumption during the electrodeposition process. Energy payback Ratio (EPR) and Raw Material Circularity Index was also calculated to further quantify the sustainability of EO process. By coupling quantitative uncertainty analysis with environmental modeling, this study advances a rigorous, systems-level approach for sustainable material selection in electrochemical processes.

# Sustainable Synthesis of Nanocellulose via Fenton Oxidation Using Iron Oxide Nanocomposites: A Green Approach for Biomass Valorization and Environmental Impact

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This work demonstrates a green and effective method for the synthesis of nanocellulose from biomass utilising a Fenton-like oxidation process. An iron oxide nanocomposite served as the catalyst, while hydrogen peroxide ($H_2O_2$) was the oxidising agent. The process aims to convert lignocellulosic waste into marketable nanocellulose without employing harsh chemicals. To optimise the reaction, we adjusted two key factors: $H_2O_2$ concentration and reaction duration. We conducted several tests to determine the impact of $H_2O_2$ concentration (20-30%) and reaction duration (3-12 hours) on nanocellulose yield and characteristics. The iron oxide nanocomposite effectively catalysed the breakdown of $H_2O_2$ into reactive hydroxyl radicals, enabling selective delignification and cellulose defibrillation. The resulting nanocellulose was characterized using SEM, FTIR, XRD, HPLC, TGA, and TEM. The results demonstrated the successful elimination of lignin and hemicellulose, resulting in crystalline cellulose nanofibers. Higher $H_2O_2$ levels and longer reaction times were shown to help break down cellulose, however too much of either resulted in its breakdown. The work demonstrates that iron oxide nanocomposites might be employed in Fenton-based green nanocellulose production. This is a low-cost and ecologically friendly approach to convert biomass into high-value nanomaterials that may be employed in a variety of applications.

# Predicting Core Exposure in Stimuli-Responsive Polymer Particles: Combination of Experimental and Simulation Insights

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The tailoring of design architecture of stimuli responsive polymer nanoparticles or polymer grafted nanomaterials is crucial for their applications in drug delivery, imaging as well as oil recovery and other potential fields. The segments of the polymer chain control the surface chemistry under variable environmental conditions and thus is very important to understand and predict the surface behaviour in advance to minimize trial and error. Furthermore, the usability of the core shell architecture is convenient when the core is protected by the shell even after payload release on response to the changes in the environment. Unintended exposure of charged polymer segments on the particle surface otherwise will result in non-selective binding of opsonins and rapid excretion from the body [1]. Additionally, in delivery and imaging applications, in living cells, the charged core if exposed and present in the surface, can induce severe toxicity [2]. Using, controlled synthetic technique, our multidisciplinary approach of combining experimental results with dissipative particle dynamics (DPD) simulations under different stimulus will create and develop a library of responsive particles to prove the concept and create a model to predict the core behaviour of the nanoparticles. This approach will create a synergy between the theory and the experimental techniques to reduce trial and error approach for designing state-of-the-art stimuli responsive polymer particles for potential applications in biomedical and oil industry.

Reference

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# Spontaneous imbibition in underground hydrogen storage in saline aquifers.

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This study experimentally investigates hydrogen–brine displacement in Bentheimer sandstone, focusing on spontaneous imbibition and its role in underground hydrogen storage in saline aquifers. Two displacement steps are considered: (1) spontaneous imbibition, where gas remains connected and capillary pressure ($P^c$) decreases, and (2) brine flooding, where disconnected gas experiences negative $P^c$.

Experiments were performed using high-resolution micro-CT imaging (3.1 µm/voxel) under 4 MPa and 23°C. A water-wet porous plate mimicked aquifer conditions during repeated drainage to establish irreducible water saturation, followed by incremental $P^c$ reduction during spontaneous imbibition. After reaching $P^c = 0$, pressure was held for 48 hours to observe Ostwald ripening before brine injection.

Spontaneous imbibition caused significant gas snap-off below $P^c = 5$ kPa, displacing over 40% of the initial gas, with residual gas saturation at 0.51. After storage, large disconnected clusters reconnected across the sample. Brine injection further reduced gas saturation to 0.43. In situ contact angle measurements averaged 40°, confirming water-wet conditions. The low interfacial curvature (~1 kPa) and pore occupancy analysis indicated preferential displacement from narrow pores, with gas trapped in larger ones. These results highlight the significant role of spontaneous imbibition in gas displacement and its importance in capillary pressure–saturation modelling.

# Activated Porous Carbon extracted from Lignocellulose-based Bio-waste Materials working as a Superior Electrode Material for High-Performance Supercapacitor

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Rechargeable energy storage technologies are in high demand in the current context. Committed to developing cost-effective energy storage solutions utilising ecologically sustainable technology, a high-temperature controlled heating method has produced activated porous carbon in an inert atmosphere by the KOH activation of bio-waste materials. This study presents the synthesis and electrochemical assessment of activated porous carbon (APC) generated from citrus peel fibre waste (CPFWs) via a two-step KOH-assisted high-temperature thermal activation process. The resultant carbonaceous structure demonstrates a substantial specific surface area (811.8 $m^2g^{-1}$), a small average pore diameter (~1.81 nm), and a hierarchical micro/mesoporous configuration, facilitating effective ion transport and improved double-layer charge storage. In a three-electrode setup utilising a 2 M KOH electrolyte, the APC electrode exhibits a remarkable specific capacitance of 565.2 F $g^{-1}$ and exceptional cyclic stability (~98% retention over 10,000 cycles), resulting in an energy density of 21 Wh $kg^{-1}$ at a power density of 5000 W $kg^{-1}$. The APC was utilised in a symmetric device with a non-aqueous ionic liquid gel electrolyte (PVA–$EMIMBF_4$–DMSO) to increase the operational voltage and improve energy density. The device functioned reliably within a 4 V range, achieving an exceptional energy density of 851 Wh $kg^{-1}$ and a power density of 26 kW $kg^{-1}$, with a retention rate of 90.8% after 10,000 cycles. These findings highlight the feasibility of biomass-derived APCs as high-performance, scalable electrode materials for advanced electrochemical energy storage systems with improved voltage windows and energy metrics.

# Oral and Flash Presentations

## Session 7

## Porous Media in NetZero and Energy Applications

# The Architect in the Pores: Water's Role in Aminosilane grafting for Carbon Capture

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Amine-grafted adsorbents are considered promising for carbon capture, yet their performance can be significantly improved. This study explores how water addition influences the grafting of (3-aminopropyl)triethoxysilane (APTES) onto silica supports to enhance sorbent properties. Using $^{29}Si$ cross-polarisation magic angle spinning nuclear magnetic resonance (CPMAS NMR) spectroscopy, the research challenges the assumption that water simply increases surface silanol content. Instead, results from NMR and Brunauer–Emmett–Teller (BET) analyses show that water facilitates the hydrolysis of ethoxy groups in APTES, promoting faster and more uniform condensation reactions with surface silanol groups. This leads to enhanced diffusion of APTES and greater bonding efficiency, as supported by the observed reduction in $Q^4$ sites (fully condensed silica), which are transformed into reactive silanol groups during water-mediated hydrolysis. A novel hybrid kinetic model combining the Weber–Morris intraparticle diffusion and pseudo-second-order chemisorption (WM–PSO) frameworks revealed that water-assisted grafting significantly improves intraparticle diffusion and balances chemisorptive interactions. This dual-mode model accurately captures the transition from diffusion-limited to chemisorption-controlled uptake, providing a more precise tool for evaluating and optimizing adsorbent performance. These mechanistic insights explain previously observed advantages of wet grafting, including enhanced $CO_2$ adsorption, faster sorption kinetics, improved thermal stability, stronger interaction strengths, and better regenerability. The improvements are attributed to the formation of uniform siloxane networks through water-facilitated condensation of hydrolysed APTES. Overall, the study underscores the pivotal role of water in tailoring silica surfaces and supports the rational design of durable, high-performance sorbents for scalable carbon capture aligned with net-zero goals.

# Monitoring CO2 Sequestration in Basalt and Silicate Porous Media Using Low-Cost Electrical Sensors

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The urgent need to find solutions to the problem of climate change by reducing world carbon emissions to net zero by 2050 has led to rigorous research on carbon capture and sequestration (CCS). The injection of liquid or supercritical CO2 into geological formations can lead to unforeseen geochemical and mineralogical changes which could possibly jeopardize the CCS process. Hence, a reliable $CO_2$ monitoring is critical for carbon capture and sequestration. Popular methods like electromagnetic surveys and seismic are very productive and effective but costly and deficient in early detection. This study proposes a low-cost electrical sensor approach to monitor geoelectrical changes during $CO_2$ injection in silicate and basaltic media. The high reactivity of basalts promotes rapid $CO_2$ mineralization, alters fluid conductivity and enhances sensor sensitivity. This study will explore the effect of pressure, temperature, pH and salinity, and develop predictive models to assess leakage risks in reactive formations. The results aim to support the development of scalable, early-warning CCS monitoring frameworks for myriad geological settings. Finally, this work will contribute to safer, more cost-effective CCS deployment and advances global efforts to prevent the problem of climate change through secure subsurface CO2 sequestration.

# From Biomass to Biochar: X-ray micro-CT Comparison of 3D Pore Structures in Brown Algae

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Biochar is a carbon rich solid material derived mainly from the thermal decomposition of biomass in inert environment. Brown algae (seaweed) are a promising non-lignocellulosic biomass feedstock for biochar production due to their rapid growth, seasonal availability, and rich elemental composition. Pak et al. (2023) demonstrated that pyrolysis of brown algae biomass resulted in the formation of physical properties such as porosity and surface area which are essential for the application biochar for water treatment. However, the structural evolution of algal biomass during pyrolysis remains poorly understood, particularly at the pore scale.

This study for the first time investigated the microstructural transformation of brown algae biomass into biochar using high-resolution X-ray μCT. Four species of brown algae biomass namely Laminaria digitata (LD), Himanthalia elongata (HE), Pelagic sargassum (PS), and Saccorhiza polyschides (SP) were pyrolyzed at 600°C and imaged at 1.4μm resolution. Through image segmentation and pore network modelling we show that pyrolysis resulted in significant microstructural changes across all alga types. Porosity increased from as low as 0.005 (raw biomass) to 0.389 in the biochar samples which is a significant increase of up to 5,540%. Pore size distribution broadened post-pyrolysis, indicating the formation of more heterogeneous and accessible pore networks. Surface area increased significantly, and pore connectivity, evaluated via coordination number, increased across all samples, indicating more interconnected pore structures essential for fluid flow and mass transfer. The pore network models confirmed that pyrolysis enhances macrostructural complexity, transforming isolated pore pockets into more continuous porous frameworks. These findings demonstrate that X-ray μCT effectively captured the internal 3D structure and quantified critical porous properties of algae-derived biochar.

Pak, T. et al. (2023) 'Biochar from brown algae: Pro

# Porous Gold-PANI Microelectrodes for Advanced On-Chip Micro-Supercapacitors

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Miniaturizing energy storage devices is vital for powering modern on-chip technologies. High-performance micro-scale devices like micro-supercapacitors are essential for their high-power density, rapid charging, and long cycle life. However, there is also a need to increase areal energy over a limited device footprint, presenting challenges associated with processing smart electrodes in on-chip device structures. In this context, we introduce highly porous gold (Au) interdigitated electrodes (IDEs) prepared by dynamic hydrogen bubble technique as current collectors for micro-supercapacitors, employing polyaniline (PANI) as the active material. These proposed porous Au IDEs based symmetric micro-supercapacitors (P-SMSCs) demonstrate an extraordinary boost in charge storage performance (187% enhancement in areal capacitance at 2.5 mA) compared to conventional flat Au IDEs based counterparts, despite using the same amount of time active materials loading. As a result, our P-MSCs exhibit areal capacitance of 60 mF/cm2, peak areal energy density of 5.44 $\mu Wh/cm^2$ and areal power of 2778 $\mu W/cm^2$, surpassing most SMSCs reported to date. Our study is thus directed towards developing high-performance SMSCs by advancing the development of highly porous micro-scale planar current collectors, ensuring efficient utilization of micro-electrodes, and achieving maximum possible capacities within the constraints of the limited device footprint.

# Oral and Flash Presentations

## Session 8

### Flow, transport and reactive processes across multi-scales in porous media – II

# Compact, Fully Analytical Solution to the Non-equilibrium Richards Equation for 1D Horizontal Flow

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Experimental saturation profiles showing non-monotonic behaviour under monotonic boundary conditions have led to the development of various non-equilibrium versions of Richards equation. Two of the most common include the dynamic capillary pressure model of Hassanizadeh and Gray (HG) and the effective water content model of Barenblatt. While travelling wave solutions to the HG model can produce non-monotonic behaviour in the saturation profiles, the model Barenblatt however does not. Travelling wave solutions were initially developed over 20 years ago but surprisingly very little has been done in developing any other type of an analytical solution. There seems to only be the similarity reduction of the HG model by King and Cuesta in 2006 for 1D horizontal flow. When a slight variation of the similarity reduction of King and Cuesta is taken along with the diffusivity D, conductivity K and the relaxation function tau, all being power laws of saturation, a straightforward fully analytical compact solution exists when their three different powers are related through a simple algebraic equation. Interestingly there are regions in this parameter space where this solution is non-unique, having both a stable and unstable branch.

# Arsenic oxidation by Fe-rich minerals and field evidence from Assam, India

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Arsenic (As) contamination in groundwater is a major environmental concern, especially in redox-dynamic porous aquifers. The mobility and toxicity of arsenic (As) are strongly dependent on its speciation and interactions with reactive iron (Fe) minerals associated with pore networks. However, the mechanisms of As oxidation by Fe-rich mixed phases remain elusive under dynamic environmental conditions.

We investigated how redox cycling of nontronite (NAu-2), a Fe(III)-rich smectite clay, induces As(III) oxidation under anoxic, circumneutral conditions. Native, chemically reduced, and reoxidized forms of NAu-2 exhibited distinct Fe redox states, as confirmed by Mössbauer and XAS analyses. Reduced and reoxidized nontronite promoted substantial abiotic oxidation of As(III) to As(V), unlike the native form, indicating that redox cycling enhances mineral reactivity.

Field sampling across 60 wells in Assam, India, revealed elevated As concentrations in groundwater associated with Fe-rich phases. Sites with high As also hosted arsenic-tolerant microbial taxa, suggesting coupled biogeochemical controls.

Together, these findings demonstrate that redox-active Fe minerals embedded in porous media can transform and immobilize As through coupled structural and biogeochemical pathways. This work provides mechanistic insight into subsurface As dynamics with implications for contaminant modeling and redox-sensitive remediation.

# Hierarchical Flow and Mechanical Performance in Termite Nests: A Micro-CT-Based Multiscale Study

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We present a numerical framework to characterize the coupled mechanical and flow properties of termite nests using micro-CT imaging. The study focuses on nests from Macrotermes species in Senegal and Guinea, as reported by Kamaljit Singh et al. High-resolution micro-CT scans were used to reconstruct the internal architecture of the nests, enabling extraction of a multiscale pore network. This network was used to evaluate ventilation capacity and thermal buffering through pore-scale flow modeling, while the solid phase was analyzed to compute mechanical stiffness and strength. The results reveal how the hierarchical structure of the nest contributes to both its mechanical integrity and passive climate control. Our framework offers insights into biologically optimized porous systems and their relevance to sustainable design in engineering.

# Impact of capillary pressure heterogeneity on $CO_2$-brine flow through porous media at core scale

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Centimeter- and sub-centimeter-scale geological heterogeneities exert a significant influence on two-phase flow of supercritical carbon dioxide and brine in subsurface reservoirs. These heterogeneities manifest as variations in capillary pressure (capillary pressure heterogeneities) which complicate the determination of representative flow parameters for reservoir simulation. A common method for estimating representative properties is through core plug measurements. However, due to a limited understanding of heterogeneity relevance at the sub-core-plug scale, most core analysis workflows are designed for homogeneous plugs, with little guidance on how to adapt these methods to heterogeneities samples. In this study, we employ the commercial two-phase flow simulator CMG IMEX to examine the effects of capillary pressure heterogeneity on fluid flow at sub-core scale. By constructing idealized geometric representations of heterogeneous rock sample, we isolate the impact of capillary variability within simplified end member scenarios. This approach facilitates an evaluation of different heterogeneity types while reducing the computational demands. Our findings reveal that capillary pressure heterogeneities alone can account for a substantial portion of the observed variability in relative permeability across heterogeneous samples. These results highlight the importance of accurately characterizing capillary pressure distributions and offer a viable framework for improving flow predictions in geologically systems.

# Computational modelling of an incompressible fluid at the interface with a porous medium

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In this talk, we present a computational framework to model an incompressible fluid at the interface between a free-fluid region and a porous material. The approach, called Interface Control Domain Decomposition (ICDD) method, has been developed considering the Stokes and the Darcy equations to represent the macroscopic behaviour of the fluid in each subregion.

Differently from the common approach that imposes the so-called Beavers-Joseph-Saffman conditions at an ideal interface between the fluid region and the porous medium, the ICDD method introduces a thin overlapping transition region where the fluid regime changes rapidly but continuously. The velocity and the pressure of the fluid are matched on the boundary of the transition region by solving an ad-hoc minimisation problem.

To validate the ICDD method, we compare its solution with the one obtained by numerically solving the Stokes equations at the microscale also inside the porous medium. This numerical study permits to identify the optimal width and location of the overlapping region. Moreover, for a homogeneous isotropic porous medium, it shows that the ICDD solution approximates the microscale Stokes solution at order ε, ε being the ratio between the micro and the macroscale.

Reference

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# Pore network modeling of drying-induced salt precipitation

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Evaporation-driven precipitation of solids in porous media is critical in processes like soil salinization and damage of heritage structures due to salt crystallization. These are inherently multiscale phenomena, affected by pore-scale heterogeneity while causing impact at macroscopic scales.

We introduce a computationally efficient pore network modelling framework for simulating precipitation at pore-scale resolution across macroscopic domains. To model evaporation, vapor diffusion is solved using a fictitious pore network representing free space above the porous material. Drying is modelled by air invasion into pores determined by local evaporation rates and capillary entry pressures. Salt transport is governed by diffusion and an advection model where flow is computed using effective pressure differences between pores. Salt precipitates in pores when the concentration exceeds saturation level. Clogged pores inhibit precipitation but still permits diffusive transport allowing oversaturated solution to diffuse to adjacent pores driving further precipitation. Model predictions are compared with experimental results of sodium sulfate crystallization in glass bead packs, reproducing the observed increase in salt deposition deeper within the medium at higher concentrations. This framework offers a scalable and efficient platform for investigating drying-induced precipitation which can be further extended to multiphase reactive transport scenarios relevant in carbon sequestration and hydrate formation.

# Two-phase flow in a model of rough fracture: A novel computational method for interface dynamics

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Given the external conditions such as the pressure head, the position of the interface between two fluids in a disordered porous or fractured medium has multiple equilibria, leading, even in the quasistatic limit of infinitely slowly changing external conditions, to history dependence (hysteresis) and associated energy dissipation due to Haines jumps between the equilibria. An imperfect Hele-Shaw cell (with an aperture randomly varying in space) provides a simple model system in which these phenomena (in the quasistatic limit and beyond) can be studied, promoting understanding of multiphase flow in a rough fracture, as well as providing insights into more complex, 3D porous media. However, even in this simple model the evolution of the interface is nontrivial due to nonlocality brought about by the resulting fluid flow. We present a novel spectral approach for computing the interface evolution in such a system, based on the Fourier expansion of the interface shape at each time step, confirming its accuracy via comparison to the much more computationally costly numerical solutions of the Stokes equations. Using our approach, we find that, even though an individual Haines jump can be a complex, multistage process, macroscopic pressure-saturation cycles follow a simple model combining viscous and "dry friction" dissipation, providing a promising step towards an upscaled model of flows in rough fractures.

# A continuum viscoporoelastic approach to modelling hydromechanical peatland development

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Recent modelling efforts have advanced significantly in describing the complex hydrological and ecological dynamics governing peatland evolution. Coupling these with mechanical models has further revealed intricate interactions between fluid flow and solid deformation processes. In this work, we present a novel, mathematically rigorous continuum formulation incorporating viscoporoelastic principles, which replaces traditional layered approaches. By re-formulating ecological, hydrological, and mechanical processes to capture dynamic peatland properties over short temporal scales, our model can accurately simulate rapid responses to extreme climatic events, including droughts and wildfires. This capability is essential for predicting peatland behaviour in the face of increasingly frequent and severe weather events driven by climate change.

# Poster Presentations

# Multi-scale Characterization of $H_2$ Storage in Carbonate Reservoirs

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Hydrogen storage in carbonate rocks presents unique challenges that must be addressed to accelerate the energy transition, including the effect of heterogeneity, microporosity, wettability, and the dynamic interaction of micropores and macropores with H2 during its injection and withdrawal. Most of the available research on flow dynamics use proxy fluids which cannot be directly extrapolated to an H2 system. It is particularly difficult to address the complexity of H2 flow dynamics in multi-scale carbonates due to the low spatiotemporal resolution of micro-CT scanners; thus, the lack of research.

To bridge the gap, pre-characterization work was done prior to high-resolution synchrotron imaging to develop a null hypothesis and highlight regions of interest. A carbonate mini-plug from the Estaillades formation was imaged in 3D during two cycles of H2 injection and withdrawal at 100 bar and 50 C. We find that microporous phases act as barriers during drainage and increase the tortuosity of flow paths unless their capillary entry pressure can be exceeded. During imbibition, they may increase the connectivity of the overall system, enhance brine flow and affect the residual saturation distribution.

# From Bench to Bedside: Assessing the Mechanical Integrity of Additive Manufactured Porous Polymers under simulated in vivo conditions

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Porous media mechanics enables engineers and healthcare professionals to effectively utilise new, novel, innovative materials for medical applications. This includes tissue engineering and the design of biomedical devices such as bone scaffolds. Over the last 20 years, Additive Manufacturing has been integrated into medicine as a key technology which offers the ability to produce porous and patient-specific implants. This study aimed to compare the changes in ultimate tensile strength (UTS) of two such materials, polylactic acid (PLA) and Nylon, with exposure to sliding wear and bodily fluids.
Samples were prepared in line with ASTM D638 Type V geometry and tested under two wear conditions: 2N for 400 cycles (n=5 samples) and 5N for 400 cycles (n=2 samples) after being soaked for 4 weeks in bovine serum. Samples were tested for tensile strength following ASTM D638 and wear properties under ASTM G133 Standards in both dry and soaked conditions to replicate inside the human body.
Nylon consistently maintained a higher UTS and greater wear resistance than PLA in all test conditions due to its porous structure, resulting in higher lubricating properties. Whilst PLA is used widely in medical devices due to biocompatibility and biodegradable characteristics, this study highlights that Nylon is a promising alternative.

# Impact of Modified Rice Husk Biochar on the Physicochemical Properties of Wastewater-Irrigated Soil and Functional Traits of Beetroot

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The present study investigates the effects of rice husk biochar, applied at different doses (15, 20, and 30 t/ha), on wastewater-irrigated soil in its simple form and after modification with $KMnO_4$. The analysis focused on evaluating the impact of biochar on beetroot plant growth, metal reduction, soil enzyme activities, and various biological parameters. Application of both simple and modified biochar improved soil physicochemical properties, including pH, soil organic carbon (SOC), total nitrogen (TN), and other essential minerals, compared to the control. A dose-dependent decrease in all measured heavy metals was observed, with modified biochar showing greater efficacy than simple biochar. At the highest dose (30 t/ha) of modified biochar, metal concentrations in beetroot roots were reduced by 81% (Cd), 80% (Ni), 56% (Zn), 80% (Cr), 61% (Co), and 72% (Pb) relative to the control. Furthermore, the application of biochar, especially in its modified form, significantly influenced plant functional traits. The reduction in metal availability was associated with decreased production of oxidative biomarkers and modulation of antioxidative enzyme activity. The highest fresh biomass yield was recorded at 15 t/ha of modified biochar. Overall, the appropriate dose of modified biochar can be a promising strategy for reducing food chain contamination.

# Photo electrochemical swing carbon capture and release

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The substantial release of greenhouse gases has been a major driver of global warming and climate change. Carbon capture and storage (CCS) is recognized as a key strategy for decarbonizing energy systems. However, current CCS technologies are often energy-intensive and costly, limiting their widespread application. This research explores a novel photo-electrochemical carbon capture approach using photo-responsive sorbents activated by sunlight. These sorbents incorporate functional $CO_2$ capture sites, photo-switchable units, and a support structure, forming porous materials capable of reversible $CO_2$ adsorption and release. Inspired by the concept of an artificial tree, $CO_2$ is captured under visible light (450 nm) and regenerated using ultraviolet (UV) radiation (365 nm), though a visible-light-only process will also be studied. Sunlight, being a renewable and readily available source, enables low-cost, energy-efficient regeneration and supports the goal of net-zero emissions. The material will be investigated for its performances and properties that include showing great stability, high CO2 capture capacity, and also excellent fatigue resistance for various number of cycles at ambient conditions. This technology enables carbon capture at both point sources and dispersed emission sites, offering flexibility through its decentralized design. It can be globally applied by adapting to various locations and needs, making it a versatile solution.

# Decentralised water leak detection using the LSTM autoencoder and decision fusion

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Water distribution networks (WDNs) globally lose over 126 cubic meters annually due to leakages. This causes significant economic losses exceeding USD 39 billion and poses public health risks through potential contamination ingress. Existing data-driven leak detection methods often suffer from high false alarm rates, are unable to detect incipient and abrupt leaks, primarily catering to burst leakages and have centralised computation bottlenecks. This research proposes a decentralised leak detection methodology employing Long Short-Term Memory (LSTM) autoencoder with temporal persistence filtering and decision-level majority vote fusion across pressure sensors. The methodology integrates feature engineering and the Fourier transformation to capture temporal and seasonal patterns. In addition, the methodology proposes a novel dynamic threshold to distinguish leak from non-leak. Evaluation was performed on the L-Town benchmark dataset using readings from pressure sensors. Results demonstrate precision of 100%, recall of 99%, and an F1-score 99%, with zero false positive rate. Furthermore, abrupt leaks were detected immediately, while incipient leaks were identified within an average delay of 5.47 hours from their onset. These results demonstrate the model's capability for accurate, timely, and interpretable leak detection in real-world WDN monitoring.

# Biocementation by natural microbial communities to strengthen coastal assets

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The microbial production of carbonates has been used for many geotechnical applications. Most commonly, this involves addition of the bacterium Sporosarcina pasteurii to induce carbonate precipitation via breakdown of urea (urease pathway). This produces ammonium and carbonate ions. The release of ammonia from bacterial cells causes a pH increase and calcium carbonate precipitation if calcium ions are subsequently added. To explore the use of this in extending the lifespan of coastal defence assets we compared the behaviour of S. pasteurii to the microbial community present in coastal sediments. Using batch experiments we showed that the main prerequisites for carbonate precipitation (elevated pH and conductivity) occurred after one day with S. pasteurii and after two to three days by stimulation of the natural microbial community. DNA sequencing revealed that the proportion of bacteria belonging to the genus Sporosarcina increased in the natural community and are likely responsible for precipitation. Column tests have demonstrated that the natural community is capable of solidifying beach sands within a few days. Geotechnical strength tests are currently being carried out on samples. Overall, our results show that stimulating natural communities in a beach environment is a viable alternative to adding model organisms to natural systems.

# Environmental factors controlling biogeochemical activity in two model hydrogenotrophic thermophiles under simulated reservoir conditions.

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The biochemical fate of hydrogen injected into porous subsurface geological formations during underground hydrogen storage (UHS) depends on the interplay of competing microbial metabolic pathways (sulphate reduction, methanogenesis and acetogenesis) whose rates are governed by local reservoir conditions. The aim of this study is to improve our understanding of the environmental factors - such as cell density, rock mineralogy, microbial species, brine chemistry, pressure and temperature – that control hydrogenotrophy in depleted hydrocarbon reservoirs.

Experiments are conducted in a high-pressure, high-temperature bioreactor to achieve simulated reservoir conditions of 65°C and 100 bar. Inoculum from batch cultures of the methanogen Methanothermobacter thermoautotrophicus and sulphate reducer Desulfofundulus Kuznetsovii is added to brine and is injected into the bioreactor with hydrogen.

This parametric study will systematically explore how hydrogen consumption varies when environmental characteristics are altered. The evolution of gas headspace over time will be measured using a portable mass spectrometer. Aqueous sulphide concentrations are to be determined through the methylene blue colorimetric assay. Cell counts will be monitored through the quantification of functional genes via qPCR. Findings from these experiments will enhance the predictive accuracy of reservoir biogeochemical models and provide input parameters for microbial flow and imaging experiments.

# Book of Abstracts

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