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Book of Abstracts

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Advancing porous media science across energy, environment, and materials

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DISTINGUISHED LECTURE

Kimberly-Clark Distinguished Lecture

Professor Lyesse Laloui · EPFL, Lausanne, Switzerland

9th Annual Conference on Porous Media · Heriot-Watt University, Edinburgh

KIMBERLY-CLARK DISTINGUISHED LECTURE

Carbon dioxide injection into deep aquifers: a geomechanical perspective

Prof. Lyesse Laloui

EPFL, Lausanne, Switzerland

Carbon capture and storage (CCS) in deep geological formations is a key strategy for reducing atmospheric CO₂ emissions and mitigating climate change. However, the successful and safe implementation of CO₂ injection into deep aquifers requires a comprehensive understanding of the geomechanical and multiphase flow responses of the subsurface.

This lecture will explore the pore-scale to reservoir-scale challenges and opportunities associated with CO₂ sequestration, focusing on reservoir integrity, caprock stability, and reactive transport processes. By integrating experimental studies, numerical modelling, and field data, we will examine the complex interactions between fluid injection, pore pressure evolution, two-phase flow, and rock deformation within heterogeneous porous media.

The discussion will highlight recent advances in understanding and predicting thermo-hydro-mechanical (THM) processes triggered by CO₂ injection. Additionally, we will explore the role of permeability evolution and wettability effects in storage security. The development and evaluation of analytical and computational modelling approaches will be presented as essential tools for reliable risk assessment and process optimization.

By providing a multiscale perspective, from microstructural effects to large-scale reservoir behaviour, this presentation aims to foster cross-disciplinary discussions and contribute to the development of robust and sustainable CCS solutions, aligning with key challenges in porous media research, geomechanics, and subsurface engineering.

ORAL PRESENTATIONS

Session 1

Multiphase Phenomena

INVITED LECTURE

Transient and steady-state multiphase flow experiments: fluctuation analysis, and the measurement of the Onsager coefficients

Dr Marcel Moura

PoreLab, The Njord Center, Department of Physics, The University of Oslo, Norway

In this talk, we explore experimental approaches to characterising transient and steady-state porous-media flows, with particular emphasis on identifying different dynamical states and on the information contained in steady-state fluctuations.

Using experiments with simultaneous injection of two immiscible fluids into a quasi-two-dimensional porous medium, we analyse saturation dynamics and temporal correlations. We show how these fluctuations can be connected, through fluctuation–dissipation relations, to the measurement of Onsager coefficients governing the coupled transport of the two phases.

These coefficients are central to emerging non-equilibrium thermodynamic descriptions of multiphase porous-media flow. Our approach links spontaneous fluctuations to macroscopic transport behaviour and provides a new experimental route for probing the physics of steady-state multiphase flow.

Co-authors and affiliations

Dick Bedeaux¹, Ryan T. Armstrong², Signe Kjelstrup¹

¹ PoreLab, Department of Chemistry, Norwegian University of Science and Technology, Norway

² School of Civil and Environmental Engineering, The University of New South Wales, Australia

CONTRIBUTED TALK

The Influence of Carbonate Secondary Porosity on Hydrogen Storage

Mohammed Al Mandhari^{1,2}, Andreas Busch¹, Kamaljit Singh²

¹ The Lyell Centre, Heriot-Watt University, UK

² Institute of GeoEnergy Engineering, Heriot-Watt University, UK

mzaa2000@hw.ac.uk

Hydrogen energy is expected to play a significant role in the energy transition, with geological storage poised to be one of the few economically viable options for enabling a large-scale hydrogen economy. However, there is a critical lack of research in H₂ storage in carbonate rocks, particularly on the role of secondary porosity in residual trapping. This knowledge gap is critical to address as the nature of carbonate pore systems are not considered in regional site selection assessments. To bridge this gap, lab-based X-ray micro-CT scanning was employed to study three carbonate rock samples with bi-modal pore size distributions and peaks ranging from the nanometre-scale to the millimetre-scale during two cycles of drainage and imbibition at reservoir conditions (10 MPa and 65 °C). During drainage, H₂ pore occupancy pre-dominantly lies in the largest pores with microporous phases acting as flow barriers. During imbibition, we find that microporous phases enhance brine flow, affect phase connectivity and the residual saturation. In the limestone sample, this is evidenced by the increase in residual saturation around an intragranular microporous-rich band. In the chalk sample, the vugular pores connected to the lesser permeable micropores are associated with an increase in residual H₂ saturation due to bypass trapping; however, partial H₂ recovery is observed where the vugular pores locally interface with more permeable microporous phases. Finally, the dolomite sample characterised by moldic porosity displays adverse recovery patterns and pronounced hysteresis due to its heterogeneous distribution of surface roughness, aspect ratio and pore geometry.

CONTRIBUTED TALK

Frictional fingering in a gravity field

Antoine Dop¹, Maud Viallet^{2,3}, Knut Jørgen Måløy³, Bjornar Sandnes⁴

¹ PoreLab, University of Oslo, Norway

² ENS de Lyon, France

³ University of Oslo, Norway

⁴ University of Swansea, UK

antoine.dop@fys.uio.no

Frictional fluids in a Hele-Shaw cell display a great variety of pattern formation processes when invaded by air, as a result of viscous forces, capillary forces and friction forces. The case of frictional fingers, when viscosity can be neglected, has been thoroughly studied, including in a stabilizing gravitational field. We are investigating the unstable case through a combination of numerical simulations and experimental methods. We show that by tilting the cell, the growth of the pattern is biased towards the top, such that we observe a transition from a self avoiding random walk to a single vertical channel. We propose ways to quantify the bias in the resulting pattern introduced by the gravitational field, including a variation in the pattern morphology. Moreover, our experiment allows to study both the unstable and stable cases in a single run, the latter being of interest when attempting to quantify the relative importance of gravity forces in the problem, helping us to determine a key parameter of the simulations: the noise in the initial grains distribution.

CONTRIBUTED TALK

Reduced-Order VE Modelling of Fault-Mediated CO₂ Leakage in Stacked Reservoir Systems

Ahmadreza Shojaee², Hariharan Ramachandran², Saeed Telvari², Uisdean Nicholson², Ahmed ElSheikh², Andreas Busch¹, Norshida Bt Mohsin³, Florian Doster²

¹ The Lyell Centre, Heriot-Watt University, UK

² Institute of GeoEnergy Engineering, Heriot-Watt University, UK

³ PETRONAS, Malaysia

a.shojaee@hw.ac.uk

CO₂ storage in faulted, vertically stacked aquifer systems requires rapid modelling tools that can screen uncertain fault and reservoir scenarios while preserving controls on plume migration. Existing vertical-equilibrium fault-leakage models provide efficient estimates of leakage from a target storage reservoir but treat leaked CO₂ as a loss from the model domain. This limits their ability to assess secondary containment and the fate of leaked CO₂ in overlying formations. We present an extended reduced-order vertical-equilibrium framework for fault-mediated CO₂ leakage in stacked reservoirs. Reservoir intervals are represented as active VE layers separated by sealing units, while faults are described as conservative donor–receiver leakage pathways across the seals. The caprock is not modelled as an active flow region, but its thickness defines the leakage-path length. Gas transfer is inserted as coupled source/sink terms in the multiphase mass-balance equations, so CO₂ leaving a deeper layer is added to a shallower layer. The leakage driving force is formulated using pressure excess in both donor and receiver reservoirs, allowing pressure build-up and CO₂ accumulation in upper layers to affect subsequent leakage. The method is benchmarked against a sloping-aquifer fault-leakage case. For capillary entry pressures of 0, 0.05 and 0.1 bar, the extended model closely reproduces the original leakage-rate and cumulative-leakage responses while retaining leaked CO₂ within the stacked system. The added capability captures plume evolution in the overlying reservoir, enabling assessment of secondary trapping, up-dip migration and possible re-leakage. The approach remains computationally efficient and suitable for early-stage screening of faulted CO₂ storage sites.

ORAL PRESENTATIONS

Session 2

Digital & Data-Driven Modelling

INVITED LECTURE

Multi-scale Dynamic Imaging of Subsurface Porous Rocks: Linking Pore-Scale Processes to TWh-Scale Energy Storage and Geological Waste Disposal

Dr Lin Ma

Senior Lecturer, The University of Manchester, UK

Subsurface porous rocks underpin a wide range of technologies required for the energy transition and long-term environmental protection, including geological CO₂ and H₂ storage, subsurface thermal energy storage, geothermal energy, and geological disposal of radioactive and other wastes. These systems operate at field scales of metres to kilometres and, in the case of energy storage, may ultimately provide TWh-scale capacity. Yet their performance, efficiency and long-term integrity are governed by processes occurring within pores, mineral interfaces and fractures over length scales from nanometres to centimetres. Bridging these spatial and temporal scales therefore remains a fundamental challenge.

Multi-scale, time-resolved and four-dimensional imaging provides a means to directly observe the evolving thermal, hydrological, mechanical and chemical (THMC) processes that control subsurface rock behaviour. Examples include deformation and fracture development under confining pressures; fluid invasion, multiphase flow, diffusion and adsorption; mineral dissolution, precipitation and interfacial reactions under reactive fluids; and structural evolution over temperatures ranging from near-ambient conditions to several hundred degrees Celsius. These observations demonstrate how apparently local processes—such as pore-throat blockage, fines migration, fracture activation, mineral reaction, adsorption and surface-controlled transport—can reorganise connected pore and fracture networks and ultimately alter permeability, storage efficiency, injectivity, deliverability and sealing performance.

The key challenge is therefore no longer simply to obtain higher-resolution images, but to establish quantitative links between dynamic pore-scale processes and reservoir- or repository-scale performance. Future developments require chemically resolved 4D/5D imaging under realistic pressure–temperature–chemical conditions, integration across spatial and temporal scales, physics-informed image-based modelling, and validation against core- and field-scale observations. Such approaches can provide the mechanistic basis needed to predict how interacting pores, fractures and mineral interfaces collectively control the capacity, efficiency and long-term integrity of TWh-scale subsurface energy storage systems and geological waste repositories.

CONTRIBUTED TALK

Bridging Sub-Wavelength Microstructures to Continuum Responses via a Multiscale Computational Framework for Acoustic Wave Propagation in Porous Media

Arun Sridhar¹, Ali Ozel¹, Mohamed Shadi²

¹ Institute of Mechanical, Process and Energy Engineering, Heriot-Watt University, UK

² Institute for Infrastructure and Environment, Heriot-Watt University, UK

ass2009@hw.ac.uk

Predicting acoustic wave propagation in heterogeneous porous materials is computationally prohibitive when the macroscopic domain and the acoustic wavelength substantially exceed characteristic pore dimensions. To address this strict scale separation, this work presents a novel multiscale computational framework bridging mesoscale simulations, homogenisation, and continuum acoustics. Highly porous polycaprolactone (PCL) is employed as a representative physical system. To this end, we propose using Dissipative Particle Dynamics (DPD) to generate representative PCL microstructures and extract their frequency-dependent viscoelastic responses. The resulting bulk modulus constructs a homogenized continuum representation capturing the effective complex acoustic parameters. Macroscopic acoustic propagation is subsequently modelled in the frequency domain using the complex-valued Helmholtz equation, enabling efficient prediction of sound transmission and attenuation (1-6 kHz) without explicitly resolving pore structures. To rigorously validate this newly proposed DPD-driven methodology, predictions are evaluated against solutions of the full heterogeneous complex Helmholtz equation computed directly on explicitly resolved pore geometries. Analysing these field-based error metrics confirms the accuracy of the effective-medium approximation in this regime, establishing a verified and computationally tractable route for linking mesoscale porous dissipation to macroscopic acoustic performance.

CONTRIBUTED TALK

Front-Aware and Locally Conservative PINNs for CO₂–Brine Displacement Fronts

Henglai Zhai¹, Jefferson Gomes¹

¹ School of Engineering, University of Aberdeen, UK

r02hz23@abdn.ac.uk

Reliable forecasting of geological CO₂ storage requires accurate prediction of the CO₂–brine displacement front, because its position and sharpness control breakthrough, swept volume, and trapping. Standard physics-informed neural networks (PINNs) are attractive mesh-free surrogates for two-phase Darcy flow, but their spectral bias smears sharp saturation fronts, causing delayed breakthrough and excessive spreading. This work develops a front-aware, locally mass-conservative PINN for sharp CO₂–brine displacement in a quarter five-spot configuration. The method combines three components. A multi-scale Fourier saturation representation improves resolution of high-gradient features. A mesh-free local finite-volume loss, evaluated on randomly sampled control volumes, regularizes phase-wise mass conservation. A front-aware data term concentrates supervision within the moving front band rather than distributing data loss uniformly over the domain. The architecture is assessed through staged ablations and a four-seed leave-one-out protocol using metrics for global error, front-contour displacement, front width, breakthrough timing, plume-area classification, and local mass imbalance. The results show a separation of roles rather than a uniform gain from every component. The spectral representation primarily governs global accuracy; front-aware supervision improves front placement and breakthrough prediction; and the conservation term improves local mass balance with a modest front-band accuracy cost. Compared with a vanilla PINN at matched training budget, the proposed models consistently sharpen the plume front, reduce front-contour error, improve breakthrough timing, and reduce false-negative plume area. These findings indicate that front-localized learning and local conservation constraints complement aggregate L₂ error for reliable data-driven forecasting of geological CO₂ storage.

CONTRIBUTED TALK

Screening of Large Covalent Organic Frameworks Databases for Urea Removal from Water using Molecular Simulations and Machine Learning

Maryam Zarghamidehaghani¹, Maria Grazia De Angelis²

¹ University of Sheffield, UK

² Institute for Materials and Processes, University of Edinburgh, UK

m.zarghamidehaghani@sheffield.ac.uk

Efficient removal of urea from spent dialysate is a pivotal step toward the realization of wearable artificial kidneys. Covalent organic frameworks (COFs), with their tunable porosity and chemical versatility, represent a promising class of adsorbents for this purpose. In this work, high-throughput molecular simulation insertions were used to rank 993 COFs from the CORE-COF database for their infinite dilution urea binding strength and ideal urea/water selectivity, indicating COF-C6, EB-COF:Cl, COF-F6, and OH-TPB-BPTA-COF as the best candidates. The analysis of CORE-COF descriptors revealed that oxygen-to-carbon ratio (O/C), carbon fraction (Cfrac), and pore limiting diameter (PLD) are the dominant predictors of urea adsorption. The simulated urea binding strength was used to train and benchmark several ML models, using a nested cross validation. The Random Forest (RF) model was the one with the best performance ($R^2_{\text{train}}=0.92$, $R^2_{\text{test}}=0.62$), although its accuracy is less satisfactory for the frameworks with high urea adsorption, that are underrepresented in the dataset. Improved performance in this regime will likely require additional training data targeting these rare structures and/or more informative interaction-sensitive features, which are still a challenge for COF structures. Using the best-performing RF model, we rapidly screened a larger dataset of 69840 hypothetical COFs (hCOFs), which has limited feature-space overlap with CORE-COFs, thus representing a stringent test. Although the model systematically overestimates the hCOFs urea binding strength calculated from simulations, it allows to identify clear chemical patterns that most top hCOF candidates have, such as amide linkers and dia/hcb topologies. The combined simulation–ML strategy here proposed offers a scalable workflow to accelerate the discovery of optimal COFs for urea separation and dialysate regeneration in wearable artificial kidneys.

ORAL PRESENTATIONS

Session 3

Uncertainty & Decision Support

INVITED LECTURE

From Uncertainty to Decisions: Optimising Monitoring Strategies for CO₂ Storage

Dr Michael Liem

Co-founder of Storra Dynamics, Zurich, Switzerland

Geological CO₂ storage, like any other subsurface operation, is inherently affected by geological uncertainty. Horizon topography, fault compartmentalisation, the presence and continuity of thin low-permeability layers, absolute and relative permeability distributions, and other uncertain parameters can significantly influence pressure evolution and plume migration, and thus overall storage performance. Decisions should therefore be based on the full range of plausible outcomes rather than on a single most likely scenario.

This talk presents an uncertainty-aware workflow that connects ensemble-based reservoir simulation, probabilistic risk analysis and monitoring design. By analysing the ensemble, the key drivers of uncertainty in storage performance and risk can be identified, helping to prioritise modelling effort and additional site characterisation. The same probabilistic framework can then support optimisation of storage-site design, for example well placement and injection rates, to improve expected storage performance while reducing expected risk. It also provides quantitative input to the risk assessment required for permitting. Finally, candidate measurement, monitoring and verification (MMV) strategies can be evaluated by how well they detect the CO₂ plume and reduce uncertainty in decision-relevant risk metrics, which provides a robust and quantitative basis for monitoring design.

Ultimately, the goal is not to predict one future as accurately as possible, but to make good decisions despite uncertainty. By integrating uncertainty quantification, risk assessment, storage design and monitoring, the framework supports safe and cost-efficient development of CO₂ storage sites.

CONTRIBUTED TALK

A Compositional Vertical Equilibrium Model for CO₂ Storage in Depleted Gas Reservoirs

Saeid Telvari¹, Hariharan Ramachandran¹, Gang Wang¹, Florian Doster¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

st4014@hw.ac.uk

Decarbonizing energy systems will rely in part on carbon capture and storage, including geological storage of CO₂ in depleted gas reservoirs. These reservoirs are attractive because they have extensive data from past production, retain usable infrastructure, and have held gas over geological time. Residual methane in these fields makes CO₂ injection more complex than storage in saline aquifers, where the working system is essentially CO₂ and brine. Injected CO₂ mixes with the methane-rich residual gas, changes the composition of the gas phase, and creates density contrasts that can drive flow within the reservoir. The model treats the system as two phases and three components: water in the liquid phase, and CO₂ and methane as mixed components of a single mobile gas phase. The primary variables are gas pressure at the datum, CO₂ mass fraction in the mobile gas, and water-column height. Component mass conservation and Darcy's law are integrated vertically into reduced equations for water, CO₂, and methane. Gas density and viscosity depend on pressure and composition, and the gas flux includes a lateral density-driven term. The formulation also tracks immobile residual gas trapped in the water leg, with composition fixed at trapping, and a hydrostatic reconstruction links the datum to phase pressures and lateral fluxes. The earlier model in this line of work was immiscible, representing CO₂ and methane as separate phases in distinct vertical zones. The present work replaces this with a compositional VE formulation, motivated by cases where CO₂-methane interaction, residual-gas remobilisation, and convective mixing are better represented by tracking composition than by separate layers.

CONTRIBUTED TALK

When Well Logs Are Not Enough: Stratigraphic Feature Engineering for Predicting Permeability-Aware Clusters in Carbonates

Victor Souza^{1,2}, Vasily Demyanov¹, Daniel Arnold¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

² Petrobras, Brazil

vp4005@hw.ac.uk

In pre-salt carbonates, facies classifications often struggle to explain permeability variability, since distinct facies can show similar porosity–permeability patterns. This makes them less effective for predicting flow behaviour and complicates geologically consistent history matching. To overcome this, we follow a data-driven approach where Self-Organizing Maps and Random Forest are used to define permeability-aware clusters that remain geologically meaningful, reflecting variations in rock constituents. However, the difficulty lies not only in defining meaningful clusters, but also in propagating them as continuous logs along wells, which is challenging but necessary since reservoir modelling requires continuous vertical information that sparse core data alone cannot provide. Cluster differences are mainly related to variations in carbonate constituents rather than significant changes in mineral composition and are therefore weakly expressed in conventional log responses. To address this, we use a dataset comprising 26 Brazilian pre-salt wells, 926 core samples, and a suite of well logs. Each well is treated as a vertically structured system, where stratigraphic position becomes a key component of the prediction. Rather than relying solely on raw log values, we generate stratigraphic features, including vertical gradients and multi-scale moving-window statistics. An ensemble of tree-based models is then used to predict cluster logs along the well. Results show that incorporating stratigraphic structure improves both prediction consistency and geological realism. More importantly, the study demonstrates that generation of continuous facies logs depends on capturing vertical patterns, rather than relying solely on pointwise log responses, highlighting the key role of stratigraphic context in petrophysical workflows.

CONTRIBUTED TALK

Propagating Fracture-Scale Uncertainty to Network-Scale Predictions: An AI-Assisted DFN Workflow

Sarah Perez¹, Florian Doster², Ahmed ElSheikh², Uisdean Nicholson², Andreas Busch¹

¹ The Lyell Centre, Heriot-Watt University, UK

² Institute of GeoEnergy Engineering, Heriot-Watt University, UK

S.Perez@hw.ac.uk

Predicting flow through fractured rocks requires linking information across scales, from heterogeneous fracture-scale properties to network-scale behaviour. A major challenge is that fracture permeability is both uncertain and strongly affected by modelling assumptions, while discrete fracture network (DFN) simulations commonly rely on simplified deterministic constitutive laws.

We present an AI-assisted workflow for propagating fracture-scale permeability uncertainty to DFN-scale flow predictions. At the fracture scale, aperture maps are processed by a U-Net-based surrogate that predicts spatially distributed permeability together with its local predictive uncertainty. These heterogeneous permeability fields are subsequently mapped onto fracture grids associated with the corresponding mechanical aperture maps and embedded within a mixed-dimensional PorePy DFN model. The resulting framework enables uncertainty in local hydraulic properties to be propagated through network connectivity, fracture intersections, and pressure-driven flow.

The approach is first used on synthetic fracture networks to quantify the resulting variability in network-scale effective permeability. The analysis shows that fracture-scale uncertainty can produce substantial changes in the predicted DFN response, while conventional cubic-law representations yield effective permeabilities outside the uncertainty range obtained from the AI-informed permeability model. To reduce the computational cost of repeated DFN simulations, we construct a second-order Hermite polynomial chaos expansion of the network response. Using a 1000-realisation Monte Carlo simulation as reference, we show that the PCE reproduces the resulting distribution of effective permeability while requiring substantially fewer full DFN evaluations.

The resulting framework combines probabilistic AI-based fracture modelling, DFN simulation and reduced-order uncertainty propagation, providing an efficient route towards uncertainty-aware and probability-based predictions for larger fractured systems.

ORAL PRESENTATIONS

Session 4

Engineering & Manufacturing

INVITED LECTURE

The critical role of multiscale porous materials in the performance of electrochemical devices

Dr Daniel Niblett

Senior Research Fellow, Newcastle University, UK

Electrochemical devices are used for energy storage (batteries), transformation (electrolyser) and utilisation (fuel cells). They involve separating redox reactions in two-regions, often separated by an ion-conducting membrane with the charge conservation fulfilled by an external difference in electrical potential between the anode and cathode.

However, the majority of these materials are porous in some way and involve transport processes occurring across multi-scales: stacks (m), cells (cm), reactant supply channels (mm), porous transport layers (μm) and catalyst layers (nm). Small changes to one of these layers is directly coupled to others and may have integrated effects.

In this talk, I will show our research into modelling and manufacturing of fuel cell components, testing new flow fields as well as how permeability affects cell performance at scale. I will also introduce how porous media properties are key for the operation of our patented alkaline membraneless electrolyzers and how for anion-exchange-membrane electrolysis, catalyst layer design can be investigated and optimised using traditional volume-averaged coupled electrochemical and two-phase flow modelling. To conclude, demonstration of some of our operando X-ray computed tomography results will be shown to highlight our recent visit to Diamond Lightsource for AEM water electrolyser imaging.

CONTRIBUTED TALK

Flow in packed columns of microplastic fibre-granular particle mixtures

Yukie Tanino¹, Hamed Movahedi², Kadhim Gawwam¹, Yamamah Ali Alghurabi¹, Isobel Hermiston¹, Adamada Joel¹

¹ School of Engineering, University of Aberdeen, UK

² School of Biological Sciences, University of Aberdeen, UK

ytanino@abdn.ac.uk

Subsea pipelines are widely used to transport oil and gas. These pipelines are typically made of carbon steel coated on the outside with polymer or concrete for insulation and corrosion protection. It seems plausible that, under certain conditions, polymer coatings may degrade over time and be released into the environment as microplastic debris. Many gaps in knowledge remain about both the degradation of polymer coatings and the impact of the resulting debris. Here we focus on the impact of microplastic contamination on hydraulic properties under conditions relevant to buried pipelines, i.e., where the microplastic debris is released into trench backfill. We present laboratory measurements of water permeability in packed columns of polyethylene fibres mixed with laboratory models of backfill material. We consider three model backfill materials (glass beads, sand, and soil) and fibre concentrations ranging from 0 to 5 wt%. The results may have important implications for a wide range of engineering applications, including decommissioning, temporary plugging of fractures in petroleum reservoirs, and composite manufacturing.

CONTRIBUTED TALK

Do Physics-based Constraints Matter? Evaluating Neural Network-based Surrogates for Constitutive Modelling

Farah Rabie¹, Daniel Arnold¹, Helen Lewis¹, Vasily Demyanov¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

f.rabie@hw.ac.uk

Neural network surrogates are increasingly recognised as computationally efficient alternatives to classical constitutive models in finite element (FE) simulation. Physics-based neural networks provide a principled way to embed domain knowledge directly into data-driven models. Among these, thermodynamics-based artificial neural networks (TANNs) enforce the First and Second Laws of Thermodynamics within the surrogate architecture, ensuring physically consistent material responses across diverse loading scenarios. We explore the practical integration of trained TANNs into FE workflows through different coupling strategies within a commercial solver. These range from fully embedded native implementations to loosely coupled methods that interface with externally hosted Python-based networks. Weak coupling provides the most favourable balance between flexibility and runtime efficiency, without compromising predictive accuracy. A complementary implementation in an open-source FE framework further demonstrates the portability of these methods across simulation environments. We compare the predictive performance of TANNs and purely data-driven neural networks, highlighting the trade-off between physical consistency and accuracy. While TANNs do not universally outperform data-driven models in predictive accuracy, they consistently exhibit greater physical consistency. For surrogate modelling, this is critical where physical consistency and interpretability must be balanced with predictive performance. Across all evaluations, we consistently observe that model performance is primarily driven by the diversity of the training dataset, regardless of whether physics constraints are imposed. This highlights the need to prioritise data design as a first-order consideration in surrogate modelling research.

CONTRIBUTED TALK

Quantification of steady state evaporative heat flux of natural porous media using an optical method

Pahan Wijayabandara¹, Jack Panter¹, Stefano Landini¹

¹ School of Engineering, Mathematics and Physics, University of East Anglia, UK

m.wijayabandara@uea.ac.uk

Evaporative coolers are widely used for HVAC in hot and dry climates, and electronics cooling. While recent advances in wick design have focused on engineered, additive manufactured models, Jute has been extensively researched and largely used as a natural wick for evaporative cooling. However, the characterisation of such natural porous media wicks and highly engineered wicks in a comparable platform has received limited attention. This work employs an optical method to precisely quantify quasi-steady evaporative heat flux of a 3D printed synthetic wick, a Natural Porous wick and a hybrid structure. Findings show that the measurements distinguish between each other and establishes the Jute based wick structure as a viable baseline with a 2819 Wm^{-2} heat flux for engineered wick optimisation in passive cooling applications.

ORAL PRESENTATIONS

Session 5

Energy Transition & Geoenergy

INVITED LECTURE

Hydrogen farming in subsurface

Dr Aliakbar Hassanpouryouzband

Chancellor's Fellow, The University of Edinburgh, UK

Exploration for commercially viable natural hydrogen accumulations within the Earth's crust, here compared to 'foraging' for wild food, holds promise. However, a potentially more effective strategy lies in the in situ artificial generation of hydrogen in natural underground reservoirs, akin to 'farming'. Both biotic and abiotic processes can be employed, converting introduced or indigenous components, gases, and nutrients into hydrogen. Through studying natural hydrogen-generating reactions, we can discern pathways for optimized engineering. Some reactions may be inherently slow, allowing for a 'seed and leave' methodology, where sites are infused with gases, nutrients, and specific bacterial strains, then left to gradually produce hydrogen. However, other reactions could offer quicker outcomes to harvest hydrogen.

A crucial element of this strategy is our innovative concept of 'X' components—ranging from trace minerals to bioengineered microbes. These designed components enhance biotic and/or abiotic reactions and prove vital in accelerating hydrogen production. Drawing parallels with our ancestors' transition from hunter-gathering to agriculture, we propose a similar paradigm shift in the pursuit of hydrogen energy. As we transition towards a hydrogen-centric energy landscape, the amalgamation of geochemistry, advanced biology, and engineering emerges as a beacon, signalling a pathway towards a sustainable and transformative energy future.

CONTRIBUTED TALK

Exsolution, Evolution, and Hysteresis of CO₂ Nanobubbles in Water-Saturated Sandstone

Andreas Busch², Amirsaman Rezaeyan¹, Gernot Rother³, Zaid Jangda², Hannah P. Menke⁴, Kamaljit Singh⁴

¹ The Lyell Centre, Heriot-Watt University, UK

² Department of Civil, Environmental and Geomatic Engineering, ETH Zürich, Switzerland

³ Neutron Scattering Division, Oak Ridge National Laboratory, USA

⁴ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

a.busch@hw.ac.uk

Understanding the nucleation, growth, and persistence of CO₂ gas phases in water-saturated porous media is critical for predicting fluid transport, trapping efficiency, and integrity in geological CO₂ storage. Gas exsolution under depressurisation remains poorly constrained at the nano- to micro-scale, where capillarity, confinement, and surface chemistry strongly influence phase behaviour. Here, we investigate CO₂ exsolution from water saturating a clay-rich sandstone using small-angle neutron scattering (SANS) under realistic reservoir conditions, providing direct, in situ insights into gas phase evolution within the pore space. Experiments were conducted at the EQ-SANS instrument (Oak Ridge National Laboratory) using a pressure cell, with cyclic depressurisation from 12 to 0.7 MPa at 50 °C. The pore fluid was a contrast-matched H₂O–D₂O mixture (68:32 vol.%; scattering length density $4.17 \times 10^{10} \text{ cm}^{-2}$), CO₂-saturated at 12 MPa prior to controlled pressure reduction, so that scattering arises from exsolved CO₂ nanobubbles. The data reveal nanoscale heterogeneities consistent with CO₂ clusters and nanobubbles forming in pores between 5 and 200 nm. Although phase diagrams predict exsolution near 8 MPa, it is only observed at ~2.4 MPa. Progressive loss of scattering from pores smaller than ~15 nm suggests preferential disappearance of nanobubbles in the smallest pores, potentially driven by Ostwald ripening. Pressure cycling highlights partial reversibility and persistent gas features, indicating hysteresis relevant to cyclic injection. These findings demonstrate SANS can resolve nanoscale CO₂ exsolution in complex geomaterials, constraining pore-scale and continuum models and informing assessments of CO₂ mobility, trapping, and leakage risk in clay-rich formations and caprocks.

CONTRIBUTED TALK

Operational Strategies to Reduce the Impact of Mixing in Underground Hydrogen Storage

Sam Marchbank¹, Ian Molnar¹, Mark Wilkinson¹, Katriona Edlmann¹, Niklas Heinemann²

¹ School of GeoSciences, University of Edinburgh, UK

² Faculty of Earth Sciences, University of Barcelona, Spain

s2267401@ed.ac.uk

Underground Hydrogen Storage is a burgeoning technology aimed at alleviating the discrepancy between renewable power generation and consumption. To maintain productivity and reduce capex much attention has been paid to the injection of a separate "cushion gas" to prime the reservoir before initial hydrogen injection. Mixing of the hydrogen and cushion gas in the subsurface can result in hydrogen losses, reactions, and impurities in the produced gas stream, so quantification of this mixing effect is paramount to understanding the risks associated with UHS. This study uses reservoir scale numerical modelling to assess ways in which mixing can be lessened by manipulating well completions, initial injected blend, injection rate, and more. It is shown that hydrogen plume geometry plays a major part in storage efficiency, which can be controlled with a longer well completion and higher injection rate. Additionally, quick initial cycling or a blended H₂-cushion gas injection can promote the creation of a mixed layer or "cocoon" around the plume, insulating it from the effects of dispersion and gravity segregation. This study aims to inform reservoir engineers in the creation and management of a UHS storage site based in the North Sea.

CONTRIBUTED TALK

Neuro-Algebraic Digital Twin for Critical State Analysis of Mine-Water Geothermal Systems

Oleksandr Letychevskyi¹, Adetomiwa Aderemi², Vasily Demyanov², Elli-Maria Charalampidou²

¹ School of Mathematical and Computer Sciences, Heriot-Watt University, UK

² Institute of GeoEnergy Engineering, Heriot-Watt University, UK

O.Letychevskyi@hw.ac.uk

Abandoned mine workings are a proven low-enthalpy resource for geothermal production and thermal storage. Mine water flow is governed by a complex interaction of the residual coal-seam geometry, backfill volume and rheology, and the heterogeneous surrounding rock mass. The controlling subsurface properties – petrophysical, thermal and mechanical (pillar strength, fracture and fault stability) – and the mine topology that couples stress, flow, connectivity and heat transfer are all highly uncertain. Quantifying this uncertainty, and its impact on system development and safe operating margins, demands an ensemble of model realisations spanning plausible subsurface scenarios. Current modelling capabilities and computational cost limit the number of full-field scenarios that can be simulated to de-risk operational strategy. The UK Geoenergy Observatories (UKGEOS, Glasgow) provides extensive geological characterisation and dynamic well-monitoring data. This makes a case for a data-driven digital twin (DT) to replicate subsurface behaviour while assimilating live monitoring. We propose to create a DT for mine-flow geothermal systems to study, monitor sensor data, predict and prevent critical states. The hybrid DT comprises of an AI component and a physics-based algebraic model that captures governing equations of the coupled rock–fracture–fluid–thermal–mechanical system. The physics model generates normal, transitional and critical scenarios that train the AI; while the AI analyses real-time sensor streams to predict potentially hazardous states, while observations continuously refine the model. Predicted states are evaluated in the algebraic model, which then proposes mitigation strategies such as adjusting pumping rates, limiting pressure, or suspending operations to avert events approaching critical conditions.

CONTRIBUTED TALK

Graph Neural Network Surrogates for Heat Transport in Fractured Geothermal Reservoirs

Reza Najafi Silab¹, Hannah P. Menke¹, Florian Doster¹, David Egya², Julien Maes¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

² PETRONAS UK Research & Technology Centre

rn2038@hw.ac.uk

Simulating fractured geothermal reservoirs is expensive, and workflows like optimization, uncertainty quantification, and real-time control require thousands of forward runs. We present a graph-network surrogate that predicts the transient thermal response of fractured geothermal doublets directly on the embedded fracture graph, at a small fraction of the cost of full simulation. Training data are generated with thermal-hfm, a non-isothermal embedded discrete fracture module for the MATLAB Reservoir Simulation Toolbox, which provides a dataset of doublets spanning a fractured-reservoir population. Fractures enter the network as discrete nodes coupled to the matrix through the same non-neighboring connections used by the simulator, so the surrogate operates on exactly the discretization the physics is solved on rather than on a resampled image. A physics-aware algebraic multigrid (AMG) coarsening, seeded by streamline time-of-flight and by a local-density-normalized sampling that preserves fracture cells, lets a hierarchical message-passing and attention model resolve the fracture-dominated flow paths that control thermal breakthrough while remaining tractable on large graphs. The model predicts the cooling-fraction field autoregressively over a fifty-year horizon. Trained on a fixed fracture-density population, it reproduces the simulated temperature evolution with a full fifty-year rollout error of approximately 1 K, and recovers the breakthrough timing and near-well thermal decline that matter for geothermal operation.

ORAL PRESENTATIONS

Session 6

Biological & Soft Systems

INVITED LECTURE

Drying of a soft sponge

Prof. Christopher W. MacMinn

Professor of Engineering Science, University of Oxford, UK

Many porous materials shrink upon drying (i.e., upon drainage). This shrinking occurs via two different mechanisms: (1) deswelling, or osmotic collapse of the solid structure, and (2) capillary compression, or mechanical compression of solid structure by capillary suction during drainage. Many materials, such as clay, wood, and cellulose, feature a multiscale porous structure that is subject to capillary compression of the macroscopic porous skeleton and, simultaneously, deswelling of the skeleton itself. As a result, the roles of these two different mechanisms of shrinking can be difficult to disentangle. We do so here by studying the simultaneous action of deswelling and capillary compression in cosmetic sponges, which are soft, open-cell polyurethane foams with a fine macroscopic pore structure (pores $\sim 10\text{-}100\text{ }\mu\text{m}$). These materials shrink substantially during drying, with a fully dry sponge occupying about half the macroscopic volume of a fully liquid-saturated sponge. However, the evolution of these materials during drying is non-monotonic: As the liquid content decreases, a sponge first shrinks, then expands dramatically, and then finally shrinks to its dry state. We use experiments and modelling to show that this nontrivial evolution is a direct consequence of the different roles of capillary compression and deswelling during drying.

CONTRIBUTED TALK

Impact of Grain Size on Bacterial Attachment–Detachment Dynamics in Packed Columns of Uniform Spheres

Hamed Movahedi¹, Cecile Gubry-Rangin¹, Paul Hallett¹, Yukie Tanino²

¹ School of Biological Sciences, University of Aberdeen, UK

² School of Engineering, University of Aberdeen, UK

hamed.movahedi@abdn.ac.uk

The transport and retention of bacteria in porous media is of great importance in a wide range of subsurface systems, especially in soils and groundwater. Bacterial migration affects nutrient cycling, pathogen dispersal, and soil ecosystem stability, and is also important for controlled microbial transport in applications such as bioremediation and enhanced oil recovery. In this study, bacterial transport and retention behaviour was explored using *Pseudomonas putida* as a model organism, a gram-negative soil bacterium that is ubiquitous in soil and widely used in bioremediation. Packed columns of uniform glass beads of two diameters (0.3 and 1 mm) provided different pore sizes and surface areas to explore bacterial attachment, detachment, and breakthrough behaviour. Bacterial suspensions were injected under different flow rates and ionic strengths to investigate the coupled hydrodynamic and chemical controls on transport. The results show that different regimes of transport and retention exist between the two grain sizes under the same hydrodynamic and chemical conditions, indicating a strong dependence of bacterial mobility on the geometry at the pore scale. These differences are observable in the different breakthrough behaviour and retention dynamics, indicating a transition in the dominant attachment–detachment mechanisms with changing pore size. The findings provide insights for improving predictive models of bacterial migration in soil and contribute to the development of more reliable frameworks for subsurface bioengineering and environmental applications. Our next step is to explore the impact of microplastics on adhesion and pore clogging.

CONTRIBUTED TALK

Fluid-structure Interactions in Central Conducting Lymphatic Anomaly

Jessica Johnson^{1,2}, Howard A. Stone³, Sarah E. Sheppard², Johannes Weickenmeier¹, Christopher W. MacMinn¹

¹ Department of Engineering Science, University of Oxford, UK

² National Institutes of Health

³ Princeton University, USA

jessica.johnson@ndm.ox.ac.uk

The human lymphatic system is a vascular network responsible for bodily fluid homeostasis and immune system response. The central lymphatics facilitate the uptake of excess fluid from organs and tissues (via peripheral lymphatic vessels) and divert it back to bloodstream. Vascular malformations, particularly those of the lymphatic system, are a rare cause of circulatory disorders. Central conducting lymphatic anomaly (CCLA) is a complex and progressive congenital disorder that is characterized by structural abnormalities in the central lymphatic vessels, the thoracic duct and cisterna chyli. The presence of a structural malformation in such vessels often leads to functional irregularities in fluid transport. Common clinical presentations in pediatric patients diagnosed with CCLA include severe breathing difficulty and chest pain, resulting from excessive fluid accumulation. Mathematical models of lymphatic fluid-structure interactions in both healthy and diseased states can elucidate the role of flow and potentially the source of malfunction in the progression of complex lymphatic anomalies. Here, we introduce a network model of the lymphatic system, adaptable to a myriad of congenital disease states. We investigate the relationship between adverse lymphatic fluid transport and abnormal lymphatic vessel structure in patients with CCLA. These findings will help bridge the knowledge gap between the initiation of the pathogenesis during embryonic development and the life-threatening clinical presentations observed postnatally, ultimately improving quality of care and aiding in surgical interventions.

CONTRIBUTED TALK

Developing a Novel Dual-Contrast Workflow for the Non-Destructive Pore-Scale Imaging of Biofilms in Porous Media using X-ray μ CT

CJ Jones¹, Andreas Busch², Jim Buckman¹, Kamaljit Singh¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

² The Lyell Centre, Heriot-Watt University, UK

cj2026@hw.ac.uk

The successful deployment of underground hydrogen storage (UHS) requires a comprehensive understanding of the biogeochemical risks posed by hydrogenotrophic subsurface microbial communities. These risks include hydrogen consumption, biomethanation, reservoir souring, and petrophysical alterations. While X-ray micro-computed tomography (μ CT) is effective for investigating multiphase flow in rock-hydrogen-brine systems, standard μ CT workflows are incompatible with biologically active systems. Conventional chemical dopants (e.g. potassium iodide) dissociate into ions raising the salinity of the liquid phase whilst generating aggressive reactive oxygen species by the activity of iodide ions, compromising cell viability and altering natural biofilm architecture. Here, we evaluate the performance of iohexol (IXL) as a non-ionic, low-osmolality liquid phase contrast agent. Cytotoxicity and metabolic effects were independently assessed in batch cultures (0–6% w/w IXL) using the methanogen *Methanothermococcus thermolithotrophicus* and the sulphate-reducing bacterium (SRB) *Desulfofundulus kuznetsovii*. To provide a secondary contrast signal associated with the biofilm phase, we leverage dissimilatory sulphate reduction by *D. kuznetsovii*, which generates H_2S that instantaneously reacts with free ferrous iron in the liquid phase to form highly attenuating ferrous sulphide (FeS). Pilot μ CT scans of growth-medium-saturated grain columns inoculated with *D. kuznetsovii* reveal the formation of distinct new structures after a 4-day incubation period relative to a sterile control. SEM imaging of colonized grains confirms the proliferation of *D. kuznetsovii* across mineral surfaces, alongside mat-like structures representing a dehydrated extracellular polymeric matrix. EDX elemental mapping shows that iron and sulphur are co-located within these mats, corroborating that the new high-attenuation features identified through μ CT represent biofilm architecture.

ORAL PRESENTATIONS

Session 7

Reactive & Environmental Systems

INVITED LECTURE

Radionuclide transport and retention in environmental systems: an experimental and radiochemistry perspective

Prof. Katherine Morris

Professor of Environmental Radiochemistry, The University of Manchester, UK

Environmental radiochemistry is a wide-ranging discipline which underpins significant national programmes in nuclear- power, -clean-up and disposal, -forensics and -defence. Accidental releases of radionuclides to shallow subsurface environments and planned disposal of radioactive wastes means that understanding and predicting radionuclide transport in these systems is essential. In this talk I will briefly frame these national programmes, discuss the dedicated facilities and associated expertise needed to perform experimental work in these systems, and highlight the experimental approaches. I will then look at some relevant case studies using column and lysimeter experiments to explore radionuclide transport in complex environmental systems, typically undertaken within the Radioactive Waste Disposal and Environmental Remediation National Nuclear Under Facility at the University of Manchester. Finally, I will highlight new work between experiment and modelling researchers to highlight opportunities for collaboration.

CONTRIBUTED TALK

Imaging Fracture Dominated Flow Pathways in Low Permeability Mine Water Lithologies

Elli-Maria (Elma) Charalampidou¹, Mohammad Madankan², Nikolay Kardjilov³, André Hilger³

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

² Research Centre for Carbon Solutions (RCCS), Heriot-Watt University, UK

³ Institute for Electrochemical Energy Storage, Helmholtz-Zentrum Berlin, Germany

ec10@hw.ac.uk

A good understanding of subsurface dynamics is essential for appraising the potential of shallow mine heat energy within future decarbonised energy systems. Fluid migration and lithological controls on flow pathways were investigated using UKGEOS Glasgow GGC01 drill core samples, focusing on interlayered sandstones and mudstones. Our experimental approach combines X-ray tomography and Neutron tomography, two complementary non destructive imaging techniques with different sensitivities and resolutions. X-ray tomography (3D) has highlighted the lithological differences, depositional textures, and both natural and laboratory-induced fractures within the tested samples. Several samples have shown clear visualisation of individual seams or networks of seams - defined by low-density material. Neutron tomography (3D) has shown fluid distribution, indicating that these low-density seams absorbed more water during flow experiments. Similar behaviour has been observed in isolated patches of low density material. To capture dynamic fluid movement, we conducted high-speed neutron tomography (4D) during flow experiments on samples containing laboratory-induced fractures. The results demonstrate that fracture permeability dominates matrix permeability in these low-permeability lithologies. Both natural and induced fractures significantly accelerate waterfront displacement. When fractures intersect more permeable features - such as channels, layers, or zones enriched in organic matter - they enhance saturation of these domains. These findings have direct implications for mine water system modelling. The observed coupling among fractures, lithological heterogeneity, and fluid pathways provides valuable insight into how water movement and thermal conductivity may interact across contrasting subsurface materials.

CONTRIBUTED TALK

Novel Sorbents for Remediation of Crude Oil and Refined Product Spills in Aquatic Systems

Alamin Khamis¹, Christine Switzer¹, Mark Stillings¹, Ondřej Mašek²

¹ Civil and Environmental Engineering, University of Strathclyde, UK

² UK Biochar Research Centre, School of GeoSciences, University of Edinburgh, UK

alamin.khamis@strath.ac.uk

Oil spills to surface water bodies cause significant harm to human health and the environment. In oil-rich regions like the Niger Delta in Nigeria, spill response is further complicated by the relative remoteness of spill locations and potential clandestine activities that contribute to their occurrences. Cost-effective, low-technology, and effective remediation strategies are crucial to mitigate adverse effects on local communities and ecosystems. This research explores the efficacy of sorbents derived from readily available agricultural waste to remediate oil spills. Agricultural wastes included wheat, barley, and rapeseed straws; rice husks; softwood; and potato and banana peelings. A subset of each waste was converted to biochar under slow pyrolysis conditions. The wheat, rice husks, and softwood were reference materials from the UK Biochar Research Centre and crude oil from the Tern oilfield near Shetland, UK (34° API) was used. Liquid-liquid extraction and solvent extraction methods were developed to measure uptake of each waste and biochar in oil-only and oil/water systems. Previous studies established uptake capacities of 200 – 1500% in oil-only systems. This work explores oil-water systems and the effects of water and biochar properties on oil uptake. Both raw and biochar sorbents demonstrated significant oil and water uptake. Generally, the biochars outperformed the raw materials for oil uptake, although some water uptake was observed, too. Uptake seemed to relate to material porosity and hydrophobicity. Further work is underway to assess the resilience of these sorbents under increasingly complex environmental conditions typical of oil spills in Nigeria and worldwide.

CONTRIBUTED TALK

Applied Smouldering systems for carbon-negative waste treatment

Tarek Rashwan¹, Fatemeh Khodaparastan¹, Abby Conroy¹, Phil Renforth², Christine Switzer³, José Torero⁴, Katherine Dobson³

¹ Faculty of Engineering, University of Nottingham, UK

² Institute of Mechanical, Process & Energy Engineering, Heriot-Watt University, UK

³ University of Strathclyde, UK

⁴ Department of Civil, Environmental and Geomatic Engineering, University College London, UK

tarek.rashwan@nottingham.ac.uk

Applied smouldering systems are emerging as an energy-efficient form of thermal treatment for challenging wastes such as sewage sludge and contaminated soil that are otherwise problematic in incinerators and other conventional treatment systems. Moreover, waste smouldering systems often exhibit lower carbon footprints than conventional waste incineration. Despite these benefits, the sustainability of waste smouldering can be improved by curbing carbon emissions. Applied smouldering systems harness a flameless form of slow, low-temperature combustion in porous media, where the porous media properties must enable sufficiently high reaction and oxygen delivery rates. These properties are often achieved through intentionally mixing wastes with a rigid mineral porous media – typically coarse-grained sand. However, other materials may be used to achieve these properties and other environmental benefits. Ultramafic rocks found in mine tailings waste contain high concentrations of calcium and magnesium minerals that can be used to mineralise carbon dioxide as carbonates. However, ultramafic rock carbon mineralisation is inhibited by hydroxyl groups bound between the carbonate-forming minerals. These hydroxyls must be liberated prior to carbonisation, e.g., by thermal activation, where the rocks are heated to release the hydroxyls as water vapour. This project explores how ultramafic rock thermal activation can be integrated in waste smouldering systems. As the amount of carbon mineralisation from the rocks may exceed the amount of carbon emissions released during waste smouldering, this method has the potential to yield carbon-negative waste treatment systems.

POSTER PRESENTATIONS

Poster Abstracts

POSTER PRESENTATION

MULTIPHASE PHENOMENA

Towards reliable numerical simulations of trapped gas dissolution and growth in porous media: A Volume of Fluid based approach

Shamim Karimi¹, Dr. Julien Maes¹, Dr. Hannah Menke¹, Dr. Jacqueline Mifsud¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

mk3031@hw.ac.uk

This contribution describes an improved formulation for Volume-of-Fluid(VOF)-based modelling of mass transfer, providing a more robust basis for pore-scale simulations relevant to geological CO₂ sequestration and H₂ storage, including Ostwald ripening. VOF is an efficient, mass-conserving single-field method for simulating two-phase flow, that can be extended to mass transfer problem using the Continuous Species Transfer (CST) approach. However, the unified VOF-CST formulation introduces significant modelling challenges. A first challenge concerns the definition of the diffusion coefficient in cells that contain both phases. The common approach blends gas and liquid diffusivities using their volume fractions [1]. For cases where the trapped gas is compositionally pure, simulations show that this blending leads to an incorrect interfacial diffusive flux and a spurious resistance at the interface, so that accurate results are obtained only on finer meshes. A second problem is that the VOF method does not represent the interface as a geometrically sharp surface but smears it over several cells. In standard formulations, the relative velocity between phases is assumed to be zero and is replaced by an artificial interface-compression term to limit this smearing. However, in mass-transfer problems the relative velocity between phases is physically non-negligible, and neglecting it leads to additional numerical diffusion, particularly when a compositionally pure trapped gas phase grows. We revisit the VOF-CS equations under the assumption of a compositionally pure trapped gas with zero concentration gradient in the gas phase. This allows the derivation of a conservative effective diffusion coefficient for interfacial cells, for which the appropriate value is shown to be the liquid-phase diffusivity rather than a volume-fraction-weighted average. Implemented in GeoChemFoam [2], this closure reduces interfacial mass-flux errors and, together with a suitable numerical scheme, matches an analytical dissolution solution on relatively coarse meshes. The interface-compression term is then modified to be consistent with the problem physics and boundary conditions, which keeps the interface sharper, reduces numerical diffusion, and improves the predicted evolution of trapped-gas volume and mass transfer. With these improvements, the model can now accurately capture diffusive exchange between neighbouring gas droplets, enabling the simulation of Ostwald ripening in which one droplet progressively dissolves into another.

[1] J. Maes and C. Soulaine. A unified single-field Volume-of-Fluid-based formulation for multi-component interfacial transfer with local volume changes. *Journal of Computational Physics* 402 (2020): 109024 <https://doi.org/10.1016/j.jcp.2019.109024>

[2] <https://github.com/GeoChemFoam> DOI:10.5281/zenodo.11354428

POSTER PRESENTATION

MULTIPHASE PHENOMENA

Limits of Capillary Pressure-Based Equations of State for Confined Hydrocarbon Mixtures

Saeid Tayebi¹, Mahmoud Jamilahmady¹, Antonin Chapoy¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

mt2116@hw.ac.uk

Accurate modelling of fluid phase behaviour in nanoporous media is essential for unconventional tight and shale reservoir engineering purposes. While many frameworks rely solely on integrating capillary pressure (P_{cap}) via the Young-Laplace equation into vapor-liquid equilibrium (VLE) calculations, this assumption requires critical evaluation. This study couples P_{cap} with a modified Peng-Robinson equation of state (PR-EoS) using a novel two-stage numerical solver. The framework combines Successive Substitution (SS) for stable initialisation with a Trust-Region (TR) algorithm for accelerated convergence. This hybrid architecture mitigates severe non-linear instabilities, successfully bypassing trivial state tracking and cubic root-extinction anomalies near the phase boundaries. The model replicates some key macroscopic trends observed in the reported experimental data, predicting bubble point suppression and upper dew point (P_{dew}) elevation in pore sizes below 100 nm. However, it uncovers a fundamental physical limitation for heavier hydrocarbon mixtures: the P_{cap} -included model predicts a decreasing P_{dew} shift as mixture molecular weight increases, directly contradicting experimental data behaviour where heavier mixtures exhibit larger shifts. Following an extensive investigation, this discrepancy is attributed to the highly non-linear changes in interfacial tension and phase envelope alterations under pressure-decoupled states. Ultimately, this work demonstrates that while integrating P_{cap} reproduces basic experimental trends, it cannot comprehensively map confined fluid physics. It underscores that capturing the complete thermodynamic reality of nanoporous spaces requires expanding the framework to incorporate explicit fluid-wall interaction parameters. Therefore, attempts have been directed to introduce a pore-wall fluid surface force term in the PR-EoS with some promising results.

POSTER PRESENTATION

MULTIPHASE PHENOMENA

Comparison of Phase-Behaviour-Guided and Conventional CO₂ Huff-and-Puff Injection Methods for Enhanced Gas-Condensate Recovery and CO₂ Storage in Various Permeability Rocks

Usman Abdulkadir¹, Mahmoud Jamiolahmady¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

ua2009@hw.ac.uk

Gas-condensate (GC) reservoirs represent a significant source of natural gas. Hydrocarbon recovery from such assets declines markedly when reservoir pressure falls below the dew-point pressure (P_{dew}), resulting in retrograde condensate dropout. This condensate banking reduces gas relative permeability, restricts near-wellbore flow, and impairs multiphase displacement in porous media. Carbon dioxide (CO₂) injection has emerged as a promising recovery technique, as it favourably alters GC-phase behaviour, enhances fluid mobility, and offers the additional benefit of geological CO₂ storage. This study evaluates the performance of a newly proposed CO₂ Huff-and-Puff (HnP) injection strategy compared to that of the conventional CO₂-HnP approach across three reservoir rocks with varying permeability. Compositional simulations were conducted using the CMG-GEM simulator, constrained by experimentally measured PVT-and-coreflood data, to better capture CO₂-GC interactions and multiphase flow behaviour. The results indicate that injecting CO₂ at the Maximum Liquid Drop-Out (MLDO) pressure as proposed by the new method, substantially improves condensate recovery and CO₂-storage efficiency, while requiring approximately five times less injected CO₂ than the conventional HnP process, which aims to increase the reservoir pressure higher than the reservoir fluid's P_{dew} . This enhanced performance is attributed to stronger phase-interactions and more effective fluid mobilisation achieved by operating near the MLDO-Pressure. Although the recovery performance of the new CO₂ injection strategy declines with decreasing permeability, it consistently surpasses that of the conventional strategy across all examined rocks. These findings underscore the importance of integrating phase behaviour and multiphase flow characterisation to optimise CO₂-assisted GC recovery and geological CO₂ storage.

POSTER PRESENTATION

MULTIPHASE PHENOMENA

MRI Observations of THF Hydrate Formation during Injection in Porous Media

Khadijeh Zare¹, Jim Hall², Robert Morris², Seyed Shariatipour¹, Lucas Goehring², Ran Holtzman³

¹ Research Centre for Fluid and Complex Systems, Coventry University, UK

² School of Science and Technology, Nottingham Trent University, UK

³ Institute of Environmental Assessment and Water Research, Spanish National Research Council, Spain

zarek@coventry.ac.uk

Gas hydrates are crystalline compounds formed by water and guest molecules under suitable thermodynamic conditions. They naturally occur in marine sediments and permafrost, predominantly as CH₄ hydrates, while CO₂ hydrates may form during geological carbon storage and potentially influence subsequent injection processes. Hydrate formation modifies the pore structure of porous media, affecting porosity, fluid transport, mechanical stability, and further hydrate growth. However, the dynamic evolution of pore structure and fluid distribution during hydrate formation remains poorly understood due to the limited availability of time-resolved experimental observations. In this work, we investigate the effect of tetrahydrofuran (THF) injection rate on hydrate formation within glass bead packs saturated with deionized water. Compared with CH₄ and CO₂ hydrate systems, THF hydrate forms at atmospheric pressure, enabling direct investigation of hydrate dynamics under controlled conditions using time-resolved Magnetic Resonance Imaging (MRI). The obtained 4D datasets capture hydrate development and fluid redistribution within the porous medium, revealing that injection rate and pore structure strongly influence hydrate growth patterns and the evolution of flow pathways. Hydrate formation progressively reduces fluid-filled porosity, demonstrating a direct relationship between hydrate saturation, pore space reduction, and flow restriction.

POSTER PRESENTATION

DIGITAL & DATA-DRIVEN MODELLING

thermal-hfm: An Embedded Fracture Module for Geothermal Reservoir Simulation in MRST

Reza Najafi Silab¹, Hannah P. Menke¹, Florian Doster¹, David Egya², Julien Maes¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

² PETRONAS UK Research & Technology Centre

rn2038@hw.ac.uk

Embedded discrete fracture models simulate fractured reservoirs efficiently without conforming meshes. We present thermal-hfm, a module for the MATLAB Reservoir Simulation Toolbox (MRST) that treats standard EDFM and projection-based EDFM (pEDFM) within a single non-isothermal model, so conductive fractures and low-permeability barriers are represented consistently in two and three dimensions. Fracture-matrix and fracture-fracture conduction, advection, and molecular diffusion are carried on the same non-neighboring connections as fluid flow, and the corresponding transmissibilities update with a pressure- and temperature-dependent water equation of state. The module is built as an extension of the geothermal and hybrid-fracture components of MRST, which keeps it aligned with the upstream toolbox and makes it straightforward to extend to brine transport and well-driven doublets. We verify the implementation against discrete-fracture reference solutions and against standard EDFM, and we demonstrate a geothermal doublet showing thermal breakthrough through the fracture network. The projection-based path recovers barrier and conductivity-contrast behavior that standard EDFM misses, at a computational cost close to EDFM. The module is intended as an open, extensible basis for non-isothermal fractured-reservoir studies, and we show one such extension: using thermal-hfm to generate training data for a graph-network surrogate that predicts thermal breakthrough directly on the embedded fracture graph.

POSTER PRESENTATION

UNCERTAINTY & DECISION SUPPORT

Multiparameter Sensitivity Analysis of CO₂ Storage in Saline Aquifers: Effects of Reservoir, Operational and Brooks-Corey Flow Parameters

Effiong Asuquo¹, Mahmoud Jamiolahmady¹, Hashem Monfared²

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

² Schlumberger

ea2036@hw.ac.uk

Geologic storage of carbon dioxide (CO₂) in saline aquifers is one of the promising ways of mitigating global anthropogenic carbon footprint. However, prediction of CO₂ plume evolution and long-term trapping mechanisms remains highly uncertain due to the complex interactions between reservoir properties, injection strategy and multiphase flow behaviour. This study presents a comprehensive multiparameter sensitivity analysis for quantifying the relative influence of pertinent geological, operational and constitutive-flow parameters on the CO₂ storage performance. Series of numerical simulations were conducted using the Eclipse300-CO2STORE module coupled with MEPO Multiple Realization Optimizer on a representative model of a section of the Utsira sand of the North-Sea Sleipner field. One variable at a time and Latin Hypercube-based experimental designs were employed, respectively, to evaluate single and multiparameter uncertainties associated with horizontal permeability, permeability anisotropy, injection rate, continuous and intermittent injection schedules, diffusion–dissolution processes, and the Brooks-Corey relative permeability and capillary pressure parameters (K_{rgmax} , K_{rwmax} , S_{gr} , S_{wr} , N_g , N_w , λ and Pe). Storage performance was assessed using mobile, immobile and dissolved CO₂ as well as average field pressure inventories. The parameter importance was quantified through multiparameter sensitivity metrics. The results demonstrate that horizontal permeability and permeability anisotropy strongly influence plume migration, whereas Brooks-Corey parameters control residual trapping efficiency and dissolution behaviour. Operational parameters, particularly injection strategy and injection rate, significantly influence pressure evolution. The study identifies the dominant uncertainty drivers governing storage security and storage efficiency, providing practical guidance for parameter prioritization, history matching and risk-informed design of future geological CO₂ storage projects.

POSTER PRESENTATION

ENERGY TRANSITION & GEOENERGY

Linking Triaxial Cyclic Loading Experiments with DEM Modelling for Long Term Energy Storage Assessment – the impact of sedimentary lithologies

Somieibi Jaja¹, Jinci Chen¹, Robert Valdez II², Audrey Ougier-Simonin², Elli-Maria Charalampidou¹

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

² British Geological Survey, UK

sj4037@hw.ac.uk

Understanding how different sedimentary lithologies respond to cyclic loading is essential for evaluating the suitability of geological formations for subsurface energy storage. Cyclic injection and withdrawal impose repeated stress variations; therefore, the long term mechanical integrity of storage systems depends on how rocks accumulate damage when stresses fluctuate around the crack initiation threshold. This study examines the thermo mechanical response of two sedimentary lithologies subjected to cyclic loading designed to replicate long term operational conditions. Triaxial experiments were performed at 25 MPa confining pressure, representative of field depths relevant to energy storage. Samples were tested dry, with thermal loading from room temperature to 50 °C applied during hydrostatic loading, followed by cyclic loading during deviatoric compression. The number of cycles was scaled to reproduce approximately 30 years of storage operations within a two day laboratory timeframe, enabling isolation of thermo mechanical effects across different lithologies. To complement the experiments, Discrete Element Method (DEM) calculations were conducted using the crack initiation thresholds as input parameters. DEM simulations were calibrated against measured cyclic strain accumulation and stiffness evolution allowing direct comparison between physical and numerical samples. By examining lithologies with differing structural heterogeneity, we assess how microstructural characteristics influence cyclic damage accumulation in both experimental and DEM domains. The combined dataset provides a robust benchmark for improving bonded particle parameterisation and enhancing predictions of brittle damage under repeated loading. Initial results reveal clear lithology dependent trends in cyclic strain accumulation and stiffness degradation, underscoring the importance of rock type in designing mechanically resilient subsurface energy storage systems.

POSTER PRESENTATION

ENERGY TRANSITION & GEOENERGY

Cement-Rock Bond Integrity under Injection-Production Cycling in Underground Hydrogen Storage

Solmaz Abedi¹, Vincent Soustelle², Ismail Hakki Saricam¹, Aliakbar Hassanpouryouzband¹, Katrina Edlmann¹

¹ School of GeoSciences, University of Edinburgh, UK

² TNO, Geoscience and Technology, Netherlands

Solmaz.abedi@ed.ac.uk

Underground hydrogen storage (UHS) in geological formations is considered a promising solution for large-scale, long-duration energy storage. Ensuring the long-term integrity of wellbore systems, particularly cement–formation interfaces that act as primary barriers against fluid leakage, is critical for safe storage operations. This study investigates the effects of hydrogen exposure and cyclic injection–production operations on cement–rock bond integrity under simulated subsurface storage conditions. Composite samples were prepared using Class G cement and two reservoir sandstone analogues representative of North Sea formations: clay-rich Corsehill sandstone and quartz-rich Bentheimer sandstone. Samples were exposed to hydrogen at 70 °C and 18 MPa for 50 days and subsequently subjected to triaxial loading and pore-pressure cycling to simulate operational conditions. Nitrogen-exposed and unexposed sister samples were used as controls. Permeability measurements, fluid sampling, acoustic velocity monitoring, SEM, and post-test micro-CT imaging were used to evaluate interfacial behaviour and integrity. Permeability generally decreased during pore-pressure cycling, with the main reduction occurring during the first cycle ($\approx 30\%$ for cement–Corsehill and $\approx 12\%$ for cement–Bentheimer composites). Comparison with nitrogen-exposed control samples indicates that hydrogen exposure did not produce a significant effect under the investigated conditions. The slower cycling rate shows a relatively greater reduction in permeability over the pore pressure cyclicity. At higher cycle numbers, permeability increased, consistent with dissolution processes indicated by ICP analyses. Micro-CT imaging revealed fractures developing within the cement matrix parallel to the interface consistent with a few visual fractures, suggesting that cement adjacent to the interface represents the mechanically weakest zone. Overall, the results indicate that operational cycling conditions and reservoir lithology exert stronger control on interface integrity than hydrogen exposure under the investigated conditions, highlighting the importance of lithology-dependent interface behaviour for evaluating wellbore integrity in future UHS sites.

POSTER PRESENTATION

ENERGY TRANSITION & GEOENERGY

Decoupling CO₂-Brine Multiphase Flow Dynamics for Finite Conductivity and Leaky Crossflow Faults

Jude Igweajah¹, Mahmoud Jamiolahmady¹, Faisal Al-Thawad²

¹ Institute of GeoEnergy Engineering, Heriot-Watt University, UK

² Saudi Aramco, Saudi Arabia

ji2006@hw.ac.uk

Geological carbon storage requires robust fault containment verification. While prior investigations have demonstrated that two-phase fluid transition zones occurring between dry-out and resident brine regions create a pressure derivative "hump" that can intricately mask the pressure transient analysis (PTA) signatures of sealing faults dependent on the distance to fault and injected volume, this research advances this analytical framework to address a more critical containment risk: finite-conductivity, leaky faults. Standard reservoir simulators frequently oversimplify all leaky faults by modelling them using transmissibility multipliers. This abstraction restricts fluid flow strictly to the cross-fault direction, yielding a transient response that becomes indistinguishable from the multiphase hump. This ignores the potential multiphase flow along the fault. In this work, a numerical framework is utilised to model leaky boundaries either through the conventional transmissibility multiplier approach or as a 3-D volumetric zone with finite conductivity highlighting their fundamental diagnostic PTA signatures. While the former generates a derivative hump that deviates significantly from sealing fault model with increasing transmissibility, the latter generates a characteristic bilinear flow 1/4-slope on the Bourdet derivative, which can be visually decoupled from the transition zone hump. Results also consider cases when PTA signatures of leaky crossflow and finite conductivity faults are indistinguishable, and hence, other techniques are required to identify the correct geological structure affecting the fluid flow for CO₂ containment. By identifying realistic finite-conductivity models using PTA, reservoir engineers can successfully separate the corresponding complex multiphase fluid dynamics and vertical containment integrity from the purely structural crossflow leakage signatures.

POSTER PRESENTATION

REACTIVE & ENVIRONMENTAL SYSTEMS

Comparative Geomechanical and Flow Behaviour of Bentheimer and Corsehill Sandstones Under Hydrogen Storage Conditions

Ismail Hakki Saricam¹, Vincent Soustelle², Solmaz Abedi¹, Saeid Ataei Fath Abad¹, Aliakbar Hassanpouryouzband¹, Katriona Edlmann¹

¹ School of GeoSciences, University of Edinburgh, UK

² TNO, Geoscience and Technology, Netherlands

isaricam@ed.ac.uk

Underground hydrogen storage (UHS) is a promising enabler of Net-Zero energy systems, but its safe implementation depends on understanding reservoir behaviour under cyclic loading. This study evaluates how hydrogen exposure and pore-pressure cycling affect the geomechanical and transport properties of two contrasting sandstones: quartz-rich Bentheimer and clay-rich Corsehill. Core plugs were exposed to hydrogen at 70 °C and 18 MPa for 50 days, with nitrogen-exposed and unexposed samples used as controls. Triaxial and flow tests were carried out before and after cycling under reservoir-relevant stresses and temperatures representative of North Sea conditions. Corsehill sandstone showed an approximately 6% reduction in Young's modulus after five pore-pressure cycles, while Bentheimer remained mechanically stable. No clear hydrogen-specific effect was observed. The stiffness reduction in Corsehill is likely linked to fracture development, grain grinding, and mineral dissolution driven by deionized water. XRD confirmed the absence of swelling clays, ruling out clay expansion as a controlling mechanism. Batch geochemistry and core-flooding results further indicated mineral dissolution. The finer, more angular grain texture of Corsehill likely increased water-rock interaction, accelerating alteration under cyclic effective stress. Despite these mechanical changes, permeability remained largely unchanged in both sandstones after cycling, indicating limited impact on flow behaviour.

POSTER PRESENTATION

REACTIVE & ENVIRONMENTAL SYSTEMS

Nano-scale interactions of radionuclides with Lower Strength Sedimentary Rock (LSSR)

Callum Robinson¹, Karl Kravvi¹, Jingyue Hao¹, Katherine Morris¹, Miguel Gomez Gonzalez², Liam Abrahamsen-Mills³, Aislinn Boylan³, Samuel Shaw¹

¹ Department of Earth and Environmental Sciences, The University of Manchester, UK

² Diamond Light Source, UK

³ United Kingdom National Nuclear Laboratory (UKNNL), UK

callum.robinson@manchester.ac.uk

Globally, electricity from nuclear power has been generated for over seventy years and this has consequently generated intermediate and high-level radioactive wastes. The internationally accepted solution for this radioactive waste is to dispose of it in a deep Geological Disposal Facility (GDF) emplaced 200 – 1000 m deep in a host rock. Potential candidate rock types for GDF emplacement are Lower Strength Sedimentary Rocks (LSSRs) including both the Oxford Clay (OXC) and Mercia Mudstone Group (MMG) formations are of relevance. Currently, knowledge gaps exist relating to radionuclide interactions with these LSSRs which can have associated high salinity groundwaters. In particular, the mechanistic understanding of key processes controlling radionuclide speciation, include sorption to high surface area phases, including clay minerals (e.g. illite) and reduction on the surfaces of redox active phases including sulphides. In this study, we used petrographic thin sections to study LSSR-radionuclide interactions at the nanoscale. Thin sections were exposed to synthetic groundwaters doped with ²³⁸U/Se and reacted under anaerobic and oxic conditions. After 2 weeks of exposure the thin sections were analysed using nano-focus X-ray absorption spectroscopy/X-Ray fluorescence (XAS/XRF) at beamline I14 Diamond Light Source, UK. High resolution (~50 nm resolution), XRF maps were collected to determine the distribution of U/Se, and their association with the other key chemical constituents. Analysis of nano-focus X-ray Absorption Near Edge Spectra (XANES) from select regions were subject to linear combination analysis (LCA) against known standards to quantify the oxidation state of the U and Se adsorbed to the LSSR. This state-of-the-art approach will then be synthesised to determine the key reactions (e.g., adsorption, redox) and geochemical factors that control U and Se transport in the LSSR. Abstract Inclusion Subject to Clearance From NWS

POSTER PRESENTATION

REACTIVE & ENVIRONMENTAL SYSTEMS

Evaluating Feedstocks for Carbon-Negative Waste Treatment using Applied Smouldering

Abby Conroy¹, Fatemeh Khodaparastan¹, Tarek Rashwan¹

¹ Faculty of Engineering, University of Nottingham, UK

enyac9@nottingham.ac.uk

Smouldering is a heterogeneous, flameless, and energy-efficient combustion process that can be used to treat wastes with high moisture contents and/or low volatilities, including sewage sludges and coal tars. These wastes must often be mixed with a rigid porous medium, typically sand, to provide the characteristics necessary for smouldering (e.g., suitable air permeability and surface area for reactions). This porous media undergoes prolonged heating during smouldering. However, sustainability of waste smouldering can be improved by replacing sand with ultramafic rocks. Ultramafic rocks can sequester CO₂ through mineralisation; however, these rocks must be dehydroxylated through prolonged heating above 700 °C to remove structurally bound hydroxyls to increase mineralisation capacity. Heat from waste smouldering may therefore drive ultramafic rock dehydroxylation. This project evaluated the suitability of various wastes from 15 waste smouldering studies. The CO₂ released per kilogram of sand was calculated for each waste, assuming complete conversion of carbon to CO₂, thereby providing a conservative estimate of potential CO₂ emissions. The optimal waste should minimise CO₂ emissions while achieving the dehydroxylation temperature (>700 °C). Estimated emissions ranged from 0.03–0.93 kg CO₂ kgsand⁻¹, with sewage sludge producing the lowest values and coal tar the highest. Despite its low CO₂ emissions, sewage sludge failed to reach 700 °C unless combined with supplementary fuels, e.g., granular activated carbon (905 °C) or sawdust (790 °C). Walnut shells offered a balance between low emissions (0.16 kg CO₂ kgsand⁻¹) and sufficiently high temperatures (766 °C). These findings identify promising wastes for coupling smouldering with ultramafic rock dehydroxylation to enable carbon-negative waste treatment.

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Participant List

Participants are listed alphabetically by surname.

Solmaz Abedi

POSTER PRESENTER

University of Edinburgh

Usman Abdulkadir

POSTER PRESENTER

Heriot-Watt University

Mohammed Al Mandhari

CONTRIBUTED SPEAKER

Heriot-Watt University

Mohammed Aldhuhoori

DELEGATE

University of Edinburgh

Yamamah Alghurabi

DELEGATE

University of Aberdeen

Effiong Asuquo

POSTER PRESENTER

Heriot-Watt University

Dr. Zhenkai (Josh) Bo

LOCAL ORGANISING COMMITTEE

Heriot-Watt University - Halliburton

Prof. Andreas Busch

CONTRIBUTED SPEAKER

Heriot-Watt University

Dr. Ri Cao

DELEGATE

University of Edinburgh

Jinci Chen

DELEGATE

Heriot-Watt University

Dr. Elli-Maria (Elma)

Charalampidou

CONTRIBUTED SPEAKER

Heriot-Watt University

Abby Conroy

POSTER PRESENTER

University of Nottingham

Thomas Crook

DELEGATE

Loughborough University

Dr. Antoine Dop

CONTRIBUTED SPEAKER

PoreLab - University of Oslo

Prof. Florian Doster

LOCAL ORGANISING COMMITTEE

Heriot-Watt University

Dr. Nathaniel Forbes Inskip
DELEGATE

Heriot-Watt University

Dr. Aliakbar Hassanpouryouzband
INVITED SPEAKER

University of Edinburgh

Stuart Holley
DELEGATE

University of Edinburgh

Jude Igweajah
POSTER PRESENTER

Heriot-Watt University

Somieibi Jaja
POSTER PRESENTER

Heriot-Watt University

Dr. Zaid Jangda
LOCAL ORGANISING COMMITTEE

Heriot-Watt University

Jessica Johnson
CONTRIBUTED SPEAKER

University of Oxford - National Institutes of Health

CJ Jones
CONTRIBUTED SPEAKER

Heriot-Watt University

Shamim Karimi
POSTER PRESENTER

Heriot-Watt University

Alamin Khamis
CONTRIBUTED SPEAKER

University of Strathclyde

Prof. Lyesse Laloui
DISTINGUISHED LECTURER

EPFL, Switzerland

Dr. Oleksandr Letychevskyi
CONTRIBUTED SPEAKER

Heriot-Watt University

Dr. Michael Liem
INVITED SPEAKER

Storra Dynamics, Switzerland

Dr. Lin Ma
INVITED SPEAKER

University of Manchester

Prof. Christopher W. MacMinn
INVITED SPEAKER

University of Oxford

Sam Marchbank
CONTRIBUTED SPEAKER

University of Edinburgh

Dr. Jacqueline Mifsud
LOCAL ORGANISING COMMITTEE

Heriot-Watt University

Dr. Ian Molnar
DELEGATE

University of Edinburgh

Prof. Katherine Morris
INVITED SPEAKER

University of Manchester

Dr. Marcel Moura
INVITED SPEAKER

PoreLab - University of Oslo

Dr. Hamed Movahedi

CONTRIBUTED SPEAKER

University of Aberdeen

Reza Najafi Silab

CONTRIBUTED SPEAKER · POSTER PRESENTER

Heriot-Watt University

Dr. Daniel Niblett

INVITED SPEAKER

Newcastle University

Dr. Sarah Perez

LOCAL ORGANISING COMMITTEE

Heriot-Watt University

Sam Pickering

DELEGATE

University of Edinburgh

Dr. Farah Rabie

CONTRIBUTED SPEAKER

Heriot-Watt University

Dr. Hariharan Ramachandran

LOCAL ORGANISING COMMITTEE

Heriot-Watt University

Dr. Tarek Rashwan

CONTRIBUTED SPEAKER

University of Nottingham

Dr. Amirsaman Rezaeyan

DELEGATE

ETH Zurich - University of Edinburgh

Callum Robinson

POSTER PRESENTER

University of Manchester

Ismail Hakki Saricam

POSTER PRESENTER

University of Edinburgh

Dr. Ahmadreza Shojaee

CONTRIBUTED SPEAKER

Heriot-Watt University

Dr. Kamaljit Singh

DELEGATE

Heriot-Watt University

Douglas Smith

DELEGATE

Heriot-Watt University

Victor Souza

CONTRIBUTED SPEAKER

Heriot-Watt University - Petrobras

Dr. Arun Sridhar

CONTRIBUTED SPEAKER

Heriot-Watt University

Davoud Tavakoli

DELEGATE

University of Edinburgh

Dr. Yukie Tanino

CONTRIBUTED SPEAKER

University of Aberdeen

Saeid Tayebi

POSTER PRESENTER

Heriot-Watt University

Saeid Telvari

CONTRIBUTED SPEAKER

Heriot-Watt University

Pahan Wijayabandara
CONTRIBUTED SPEAKER

University of East Anglia

Khadijeh Zare
POSTER PRESENTER

Coventry University

Dr. Maryam Zarghamidehaghani
CONTRIBUTED SPEAKER

University of Sheffield

Henglai Zhai
CONTRIBUTED SPEAKER

University of Aberdeen