The University of Manchester
Department of Chemical Engineering

Chemical Engineering PGR Conference 2025

Event Space in Nancy Rothwell Building, Blended Th1 (GA.056)
and Engineering B Blended Th2 (2B.020)
The University of Manchester
2nd June 2025

Programme

Time	Duration	Nancy Rothwell GA.056	Eng B Blended Th2 (2B.020)
08:30-09:00	00:30	*Registration*	
09:00-09:10	00:10	*Welcome* Prof Phil Martin (HoD) Dr María Pérez-Page (HoPGR)	
09:10-09:20	00:10	*Attendees moving between Lecture Theatres*	
		Oral Session 1 *Chairs:* *Dr Rosa Cuellar-Franca &* *Dr Vincenzo Spallina*	**Oral Session 2** *Chairs:* *Dr James Winterburn &* *Prof Stuart Holmes*
09:20-09:35	00:15	(1) Jiaye Shao (D'Agostino)	(7) Gajanand Verma (Theodoropoulos)
09:35-09:50	00:15	(2) Ling Ai (Holmes)	(8) Ali Karagoz (Li)
09:50-10:05	00:15	(3) Aina Jamal (Parlett)	(9) Camilo Salazar (Ma)
10:05-10:20	00:15	(4) Weilin Chen (D'Agostino)	(10) Dimas Taha Maulana (Babaei)
10:20-10:35	00:15	(5) Mujtba Alnasser (Garforth)	(11) George Cook (PA Martin)
10:35-10:50	00:15	(6) Oday Hakami (Garforth)	(12) Tongke Zhou (Niasar)
10:50-11:40	00:50	*Poster Session 1 and Coffee break (Foyer)*	
		Oral Session 3 *Chairs:* *Dr Lin Ma &* *Dr Mehrdad Vasheghani Farahani*	**Oral Session 4** *Chairs:* *Dr Ashwin Rajagopalan &* *Dr Stephen Flores*
11:40-11:45	00:15	(13) Bjartur Hilmisson (Theodoropoulos)	(18) Fernando Vega-Ramon (D. Zhang)
11:55-12:00	00:15	(14) Mark O'Hanlon (Curtis)	(19) Aristarchos Mavridis (D'Agostino)
12:10-12:15	00:15	(15) Stefano Pretto (Miller)	(20) Lan An (Lee)
12:25-12:30	00:15	(16) Nichakorn Fungprasertkul (Winterburn)	(21) Mehdi Ghasemi (Babaei)
12:40-12:45	00:15	(17) Henrik Wong (de Visser)	(22) Ehsan Vahabzadeh (Niassar)
12:55-14:15	01:20	*Poster Session 2 and lunch (Foyer)*	
		Oral Session 5 *Chairs:* *Dr Claudio Pereira da fonte &* *Dr Carlos Avendano*	**Oral Session 6** *Chairs:* *Dr Antonios Anastasiou &* *Dr Isabel Pazmino Mayorga*
14:15-14:30	00:15	(23) Rebecca Clews (PA Martin)	(29) Fulu Zhou (Carbone)
14:30-14:45	00:15	(24) Rania Al Mozani (Cuéllar-Franca)	(30) Runqi Zhao (da Fonte)
14:45-15:00	00:15	(25) Xiaoyu Huang (Azapagic)	(31) Oleksandr Prykhodko (Rajagopalan)
15:00-15:15	00:15	(26) Roger Bellido Peralta (Nair)	(32) Maria Arias (Avendaño)
15:15-15:30	00:15	(27) Amy Dann (Peeters)	(33) Christopher Ratcliff (Sarkisov)
15:30-15:45	00:15	(28) Benjamin Moore (Pérez-Page)	(34) Zhengguang Liu (Babaei)
15:45-17:00	01:15	*Wine and cheese reception, prizes and final remarks (Foyer)*	

Poster judges

- Dr Marta Falkowska
- Prof Andrew Masters
- Dr Pablo Lopez-Porfiri
- Dr Vijayalakshmi Thangaraj
- Dr Min Hu

Posters

Poster number	Student	Supervisor	Theme
01	Jeffrey Akuoko	Dr Lin Ma	Catalysis and Porous Materials
02	Buthayna Nasser Ali Al Ghafri	Dr Maria Perez-Page	Sustainable Industrial Systems
03	Ahlam Al Hadhrami	Dr Antonios Anastasiou	Advanced Functional Materials
04	Ibtehal Al Houqni	Dr Antonios Anastasiou	Advanced Functional Materials
05	Abdullah Al Rammah	Prof Flor Siperstein	Multi-scale modelling
06	Muna Zayid Khamis Al'ajmi	Dr Vincenzo Spallina	Catalysis and Porous Materials
07	Sara Ali Hosseinzadeh	Prof Aline F. Miller	Advanced Functional Materials
08	Yazen Al-Lami	Dr Xiaolei Fan	Catalysis and Porous Materials
09	Omar Alqusair	Dr Jie Li	Process Integration
10	Munthir Alshammari	Prof Arthur Garforth	Catalysis and Porous Materials
11	Mohammed Alsubeihi	Dr Ashwin K. Rajagopalan	Process Integration
12	Ariyan Amirifar	Prof Kostas Theodoropoulos	Biochemical and Bioprocess Eng.
13	Bengang Chen	Dr Lin Ma	Multi-scale modelling
14	Krzysztof Dziuba	Prof Peter Gardner	Advanced Functional Materials
15	Mohamed Elsharkasi	Prof Rahul Nair	Advanced Functional Materials
16	Sahar Gholami	Dr María Pérez-Page	Sustainable Industrial Systems
17	Abigail Harris	Prof Christopher Hardacre	Catalysis and Porous Materials
18	Yutao Jiang	Dr Christopher Parlett	Catalysis and Porous Materials
19	Deva Kadarani	Dr Robin Curtis	Biochemical and Bioprocess Eng.
20	Saumya Kumar	Dr Laurence Stamford	Sustainable Industrial Systems
21	Wei Liu	Prof Stuart Holmes	Catalysis and Porous Materials
22	Zhengguang Liu	Dr Masoud Babaei	Surface Engineering Systems
23	Zehua Liu	Dr Jie Li	Process Integration
24	Mohammadhadi Mohammadi	Prof Kostas Theodoropoulos	Catalysis and Porous Materials
25	Shivani Pandit	Dr Rosa M Cuéllar-Franca	Sustainable Industrial Systems
26	Maariya Rachid Daud	Prof Alan Dickson	Biochemical and Bioprocess Eng.
27	Dian Rahmawati	Prof Adisa Azapagi	Sustainable Industrial Systems
28	Kimiya Ramezani	Dr Ashwin K. Rajagopalan	Process Integration
29	Jacob Russell	Dr Kathryn George	Advanced Functional Materials
30	Mahtab Shahrzadi	Prof Vahid Niasar	Catalysis and Porous Materials
31	Yuebo Shen	Prof Stuart Holmes	Advanced Functional Materials
32	Sonu Sudhikumar Seena	Dr Lin Ma	Multi-scale modelling
33	Yiqi Sun	Prof Vahid J Niasar	Multi-scale modelling
34	Shuyuan Tan	Dr Robin Curtis	Biochemical and Bioprocess Eng.
35	William Tran	Dr Claudio Pereira da fonte	Multi-scale modelling
36	Konstantina Tsafara	Prof Kostas Theodoropoulos	Biochemical and Bioprocess Eng.
37	Hao Wang	Dr Carmine D'Agostino	Catalysis and Porous Materials
38	Hubertus Warsahartana	Prof Arthur Garforth	Catalysis and Porous Materials
39	Yuhang Yang	Dr Daniel Lee	Catalysis and Porous Materials
40	Vladislav Zurba	Dr Vincenzo Spallina	Process Integration
41	Sneha Thomas	Prof Rahul R Nair	Advanced Functional Materials
42	Mohammad Yousuf Zaman	Dr Ashwin Kumar Rajagopalan	Multi-scale modelling

Oral presentations

Oral Presentation 01

NMR Relaxation Unveils the Promoting Effect of Surface Water Interactions on Photocatalytic Degradation of C_3N_4 in Aqueous Solution

Jiaye Shao and Carmine D'Agostino

Theme: Catalysis and Porous Materials

Solar energy is becoming a widely utilised source of energy due to increasing environmental concerns and demand for cleaner energy. As a result, much effort has been focused on exploring high-efficiency visible-light photocatalysts. In recent years, graphitic carbon nitride (g-C_3N_4), has been extensively studied in recent years due to its 2-D structure and tunable electronic structure. During the synthesis of g-C_3N_4, the condensation degree of the melamine precursor increases with temperature, leading to the formation of products ranging from melem to dimelem and finally to the g-C_3N_4 network. The processing temperature significantly influences the physical and chemical properties of the product. To elucidate this effect, we introduced the nuclear magnetic resonance (NMR) relaxation method. In photocatalytic advanced oxidation processes, water serves as a critical medium for radical generation. The NMR relaxation time ratio (T_1/T_2), as a key indicator of the interaction strength between the catalyst surface and the liquid, effectively describes the reactivity of carbon nitride in dye degradation reactions under aqueous conditions.

Oral Presentation 02

MWCNT-CB Hybrid Conductive Networks for PEMFC Catalyst Layers under Light-Duty Vehicle Operando Conditions : Toward Commercial Deployment

Ling Ai and Prof Stuart Holmes

Theme: Catalysis and Porous Materials

This study presents a MWCNT-CB hybrid conductive network as a catalyst support for PEM fuel cells, targeting light-duty vehicle applications. A mild oxidation process was applied to multi-walled carbon nanotubes (MWCNTs) to introduce oxygen-containing functional groups, improving Pt dispersion and support-metal interaction. The optimal MWCNT-CB ratio (1:1) achieved a balance between electrical conductivity and effective Pt loading. Electrochemical and physical characterization demonstrated enhanced catalytic activity, stability, and durability, meeting U.S. DOE targets under operando conditions. The hybrid structure facilitated a more continuous conductive path and improved three-phase boundary formation, verified by SEM and ECSA retention under accelerated stress tests. These results demonstrate a scalable, high-performance catalyst design suitable for commercial PEMFC deployment.

Oral Presentation 03

Tailored acid sites on silica nanospheres for fructose conversion to 5-hydroxymethylfurfural

Aina Syahida binti Jamal , Dr Jesus Esteban, and Dr Christopher M. A. Parlett

Theme: Catalysis and Porous Materials

5-hydroxymethylfurfural (HMF), derived from lignocellulosic biomass, is recognised by the US Department of Energy as one of the most significant and promising platform chemicals. It is a versatile molecule that can be transformed into various value-added chemicals, including fuels, solvents, and polymer monomers.[1] I have investigated the development of catalysts for 5-HMF production through producing organic acid functionalised supports based on mesoporous silica nanospheres, via surfactant templated synthesis.[2] Characterisation of these includes SEM, TEM and nitrogen porosimetry, with XPS confirming the presence of sulfonic, carboxylic and phosphonic acids and titrations confirming acid site loadings. Catalytic reaction under microwave heating, including within a biphasic system using MIBK and cyclohexanone as the organic phase at different volume ratios, identified that sulphonic acid functionalised silica to be the most active and carboxylic acid to be the more selective. MIBK inclusion elevated fructose conversion and HMF yield, whereas cyclohexanone aided in product recovery from a great partitioning of it into the organic phase.

1. Bicker, M., J. et al., Green Chem., 2003, 5, 280-284.

2. Zhang, K., et al., J. Am. Chem. Soc., 2013, 135, 2427–2430.

Oral Presentation 04

Application of porous materials for sustainable chemical processes

Weilin Chen and Dr Carmine D'Agostino

Theme: Catalysis and Porous Materials

With the rapid growth of the global population and the acceleration of industrialization, natural environments have been increasingly impacted by human activities, particularly in terms of water pollution. Consequently, there is an urgent demand for the development of green, economical, and efficient water treatment technologies. Metal-organic frameworks (MOFs) and covalent organic frameworks (COFs) have emerged as highly promising materials for wastewater treatment due to their ultrahigh specific surface areas, tunable pore structures, and multiple active sites. This project employs green solvent methods to synthesize MOF (UiO-66) and COF (COF-LZU1), as well as their composite materials. A systematic investigation into their performance in removing water pollutants will be conducted, aiming to provide new insights and strategies for the development and application of eco-friendly water treatment materials.

Oral Presentation 05

Catalytic Ethane Dehydrogenation over Metal/ZSM-5 Catalysts

Mujtba Alnasser, Dr Vincenzo Spallina, and Prof Arthur Garforth

Theme: Catalysis and Porous Materials

Background and motivation: Ethylene is globally in high demand as a building block for major polymer products. Ethylene is mainly produced from steam cracking process which is considered a high-intensity energy process with conventional reliance on fossil fuel burners as main source of supplied energy [1]. Consequently, a high release of CO2 is associated with the production of ethylene; a worldwide estimate of 264 million tonnes of CO2 in 2030 ($\sim$ a 33% increase from 2015) [1]. Therefore, investment into a catalytic process to produce ethylene with reduced energy use is critical.

Materials and methods: This work studies the catalytic ethane dehydrogenation over a series of metal/zeolite catalysts prepared via ion exchanged. Fe, Cr and Mo catalysts were wet-impregnated with nominal loadings (5%) on ZSM-5 with varied Si:Al ratios for Fe/ZSM-5 to study support acidity effect on conversion and selectivity towards ethylene. Further investigation on ion-exchanged Fe/ZSM-5 coimpregnating Cr with different Fe:Cr ratio.

Results and discussion: ZSM-5 silica to alumina ratio showed an important factor in the Fe catalyst preparation affecting the catalytic activity and product distribution. Evidently, it catalytically promotes ethane cracking as Fe surface area increased with lowering Si:Al ratio. One of the biggest challenges in the catalytic ethane dehydrogenation process is the carbon deposition that significantly impacts the catalyst activity [2,3].

References:

1. J. Middleton, Decarbonisation of steam crackers, (2021).
2. F. Solymosi, P. Tolmacsov, Conversion of ethane into benzene on Re/ZSM-5, Catalysis Letters 93 (2004) 7–11.
3. A.A. Dergachev, A.L. Lapidus, Catalytic aromatization of light alkanes, Russian Journal of General Chemistry 79 (2009) 1244–1251.

Oral Presentation 06

Low-cost Dip-coated 3D-printed Catalytic Filters for CO Mitigation for Biomass Stoves

Oday Hakami , Amanda Lea-Langton and Prof Arthur Garforth

Theme: Catalysis and Porous Materials

The burning of biomass in domestic stoves contributes to air pollution, impacting air quality, climate, and health[1]. Key pollutants include particulate matter (PM) and carbon monoxide (CO). This study aims to develop a cost-effective Cu-CeO_2 catalyst to oxidise CO into CO_2 while filtering PM. Noble metal catalysts (Pt, Pd, Rh) are highly effective but expensive, necessitating alternatives. Copper (Cu) has shown promise for CO oxidation at low temperatures (<300 °C)[2].

A Cu-CeO_2 catalyst (15 wt.% Cu) was synthesised via wet impregnation, dried, and calcined at 450 °C. It was then coated onto 3D-printed kaolin monoliths of varying heights (20-40 mm) to assess gas hourly space velocity (GHSV) effects. Catalytic performance was tested using a domestic stove with an integrated catalytic chamber, and CO oxidation was monitored via FTIR.

Results demonstrated high catalytic activity, achieving complete CO conversion below 200 °C due to abundant oxygen vacancies[3]. Characterisation revealed a $60\,m^2\,g^{-1}$ surface area, mesoporous structure, cubic crystalline nanostructure (8 nm crystallite size), acidity of 0.15 mmol NH_3/g, oxidisability of 0.16 mmol O_2/g, and a CuO reduction temperature of 184 °C. These findings highlight Cu-CeO_2 as a promising low-cost catalyst for pollutant mitigation in biomass stoves.

References

- He, Chi, et al., Chemical reviews 2019, 119.7, 4471-4568.
- Saqer, S.M., et al., Applied Catalysis B: Environmental 2011, 103:3, 275-86.
- Jeong, D.W., et al., Journal of Industrial and Engineering Chemistry 2015, 27, 35-39.

Oral Presentation 07

Robust Stability Analysis of Koopman-Based MPC Using IQCs

Gajanand Verma, Prof William Heath, and Prof Konstantinos Theodoropoulos

Theme: Multi-scale modelling

Linear Model Predictive Control (MPC) is often preferred for complex nonlinear systems due to its computational efficiency over nonlinear MPC. In this work, we employ a data-driven Koopman operator to lift the nonlinear dynamics into a higher-dimensional linear space, enabling the use of linear MPC. However, since the Koopman operator is inherently infinite-dimensional, a finite-dimensional approximation is required, which introduces unstructured model uncertainty into the system. To ensure closed-loop stability, robust stability analysis becomes critical. We employ the Integral Quadratic Constraint (IQC) methodology to provide robust stability guarantees. The proposed approach is demonstrated through its application to a complex nonlinear large-order tubular reactor system exhibiting Hopf bifurcation for different parameter combinations.

Oral Presentation 08

AI-assisted Process Design: Toward Expert-Level Performance

Ali Karagoz and Dr Jie Li

Theme: Process Integration

Artificial intelligence (AI) or machine learning (ML) approaches have been utilized in various chemical engineering problems ranging from surrogate modeling, property and fault predictions to drug discovery. A new wave of AI applications is growing in chemical engineering using tools and techniques from natural language processing, image processing, and game playing. This creates an opportunity to develop alternative ways to search the solution space for optimal designs and obtain highly accurate AI models that can assist engineers in the early steps of the design procedure. Following the methodology from Nabil et al. (2023), models were pretrained with synthetically generated flowsheets and then finetuned with simulated and optimized ones to obtain a model that can produce high-performance supercritical CO_2 power cycle layouts to be used as a bottoming cycle in natural gas combined cycles. The approach was replicated with LSTM and Transformer architecture to highlight the important decisions and their effects on performance. A novel framework of a two-model approach was formulated to distinguish the comparative performance of alternative flowsheets and use this information to improve the predictive and generative power of AI models with the same dataset. The two-model approach improves the baseline suggestions of a single model from 70% to 90% for high-performance design generation. It shows a better utilization of the data at hand and formulates the design problem in a more domain-appropriate way through a structure-performance relationship compared , similar to reinforcement learning applications without the problems of reward design.

Nabil, T., Noaman, M., Morosuk, T., 2023. Data-driven structural synthesis of supercritical CO2 power cycles. Frontiers in Chemical Engineering 5.

Oral Presentation 09

Subsurface Electrochemical Energy Storage, an Initiative for the Future

Camilo Salazar and Dr Lin Ma

Theme: Subsurface energy systems

The transition to renewable energy sources necessitates the development of efficient and sustainable energy storage solutions. In 2024, the United Kingdom has made significant strides in this direction, with an installed capacity of approximately 16 gW for solar power and around 30 GW for wind energy. However, integrating these intermittent renewable sources into the electrical grid presents substantial challenges, highlighting the critical need for advanced energy storage technologies that can stabilize power output and maintain grid reliability.

Currently, pumped hydro storage (PHS) and compressed air energy storage (CAES) are among the most prevalent grid-scale storage solutions. Despite their widespread use, these technologies face significant limitations, including geographical constraints and high implementation costs. For instance, the UK operates four major PHS plants, with the upcoming Coire Glas project poised to be the largest in 40 years. However, the substantial investment and extended timelines required for such projects underscore the necessity for innovative and rapidly deployable storage solutions.

This project proposes an innovative approach to massive renewable energy storage by utilizing subsurface rocks as natural reservoirs for iron-based flow batteries. This novel solution leverages the unique properties of geological formations and the high efficiency of iron flow batteries, aiming to create a system capable of providing uninterrupted power to a city of 500,000 inhabitants for at least one week. By eliminating the need for extensive surface land and reducing implementation time and costs, this approach holds the potential to revolutionize energy storage, supporting the global transition to renewable energy and enhancing energy security and sustainability.

Oral Presentation 10

Impacts of temperature variation on injectivity in geothermal systems: A coupled thermomechanical and chemical reactions numerical modelling study

Dimas Taha Maulana , Prof. Vahid Niasar and Dr. Masoud Babaei

Theme: Multi-scale modelling

Geothermal energy production is heavily dependent on maintaining well injectivity, which is influenced by reservoir permeability and mineral precipitation. Temperature fluctuations have a significant impact on these parameters, as they induce thermal expansion, alter fracture networks, and promote mineral scaling. However, the combined effects of temperature variations and scaling on geothermal well injectivity remain insufficiently understood. This study aims to investigate the influence of temperature on permeability and mineral scaling mechanisms in geothermal reservoirs using a coupled numerical modeling approach. TOUGH2 and TOUGHREACT simulations were employed to analyze fluid flow, thermomechanics, and geochemical interactions under varying injection temperatures and flow rates. The model was validated against established empirical relationships, including those proposed by Guo et al. (2017) and Siega (2014).

The results indicate that temperature variations significantly influence injectivity trends. Increasing the injection temperature from 30 °C to 70 °C resulted in a 40% improvement in injectivity, while prolonged cold-water injection caused permeability decline due to silica and calcite precipitation. The injectivity index showed variation with initial rock permeability and injection flow rates, with a 20% improvement at higher injection rates (120 kg/s) compared to the baseline ($100\,\mathrm{kg\,s^{-1}}$). Additionally, the Thermo-Scaling K-Change model demonstrated that while initial thermal expansion improved permeability, long-term scaling effects gradually reduced fluid flow.

The model was applied to analyze the performance of an injection well at the Dieng Geothermal Field, Indonesia. The simulation was employed to validate 12 years of measurement data from the injection well. Neglecting scaling effects, the simulation results showed a 71% match with the observed data. In contrast, incorporating scaling effects into the simulation increased the match to 88%, while considering thermo-mechanical effects resulted in a match of 83.4%.

Oral Presentation 11

The Use of Laser-Induced Breakdown Spectroscopy (LIBS) for characterization in underwater environments

George Cook and Prof Philip Martin

Theme: Sustainable Industrial Systems

The British Nuclear Decommissioning Authority, through Sellafield Ltd, is currently engaged in a program to remove radioactive waste from its legacy radioactive storage ponds on the Sellafield nuclear site and elsewhere. Characterization of that waste must occur prior to this. Typically, this would occur via collection of solid and liquid samples followed by lab analysis.

However, this is both challenging (from both a logistical and safety point of view) and costly, and remote, in-situ analysis may offer a much less challenging, safer and cheaper option, whilst also providing an opportunity to undertake analysis for the presence of radionuclides in the waste and the concrete of the walls of the ponds.

This work is aimed at exploring the characterization of both liquids and submerged samples, ideally remotely and with no sample preparation using laser-induced breakdown spectroscopy (LIBS).

LIBS is a pseudo-non-destructive technique which uses a laser pulse focused on a material to convert a small section of the target into a plasma, which then de-excites releasing photons of particular energies which can be collected to ascertain the elemental composition of the material.

Work has begun with laboratory tests using an 'off the shelf' LIBS kit (Applied Photonics LIBS-SCAN 150) into the detection of trace elements in aqueous and high pH solutions with an initial focus on magnesium, cobalt and strontium, in the form of salts. Calibration curves for quantitate analysis of these elements have been produced for these elements using a variety of LIBS peaks for each element. Various data analysis and pre-processing techniques have been applied to attempt to improve the accuracy of analysis. This provides a proof of concept for the use of LIBS for detection of elements of interest in aqueous environments and a basis for further work.

Oral Presentation 12

Dynamics of brine drying and salt precipitation and growth in porous media during CO_2 injection

Tongke Zhou and Prof Vahid Niasar

Theme: Process Integration

Subsurface CO_2 storage in deep saline aquifers, owing to their capacity, containment efficiency, and availability, is a promising strategy to enable the global net-zero target. However, dry CO_2 injection can cause brine evaporation, leading to salt precipitation and potential injectivity loss. Understanding the complex synergic effect of injection parameters and thermodynamics on pore-scale drying and salt precipitation remains a challenge.

In this work, we conducted microfluidic experiments to provide fundamental understanding of evaporation and salt precipitation in two-dimensional porous media. The experiments were conducted under different temperatures and injection rates to shed light on key mechanisms controlling drying and salt precipitation in porous media. The results signify that (i) the residual brine distribution, determined by gas injection rate, significantly controls the evaporation rate and salt distribution, (ii) depending on the injection rate and system temperature, two distinct types of salt crystal structures (single-crystalline and polycrystalline salt crystals) may appear in porous media. The role of capillary backflow, driven by capillary pressure gradients during evaporation, was also elucidated in the context of salt crystallisation processes. This work provides a comprehensive understanding of the fundamental mechanisms of brine drying and salt precipitation, offering insights for optimising CO_2 injection strategies in saline aquifers.

Oral Presentation 13

Optimisation of recombinant protein production in microalgae

Bjartur Hilmisson and Prof Konstantinos Theodoropoulos

Theme: Biochemical and Bioprocess Engineering

Microalgae have been investigated as alternative expression systems for recombinant protein production, with numerous transformation strategies and genetic tools developed for the model microalga *Chlamydomonas reinhardtii*. Despite this growing molecular toolbox, yields of recombinant proteins expressed in *C. reinhardtii* remain too low for industrial adoption of the platform. Alongside synthetic biology approaches, bioprocess optimisation strategies can further drive protein yield improvements. This project aims to optimise the production of recombinant proteins in microalgae through a combination of experimental cultivations and kinetic modelling. Erythropoietin (EPO) was selected as a model therapeutic protein to evaluate the feasibility of the approach: various vector constructs were designed and cloned, including several fusions with the fluorescent reporter protein mCherry, but no EPO-producing transformant cell lines have yet been isolated. Conversely, expression of mCherry was successful and efficient secretion of the protein was confirmed via Western blot. Two transformants, one mCherry-secreting and one non-secreting, were selected for cultivation experiments. Characterisation of the mixotrophic cultivation process was conducted by varying the initial concentration of acetic acid and nitrogen, as well as light intensity. A previously developed kinetic model for cultivation of *C. reinhardtii* was then adapted to additionally simulate and predict the dynamics of mCherry production.

Oral Presentation 14

Characterising the reversible self-association of alpha-chymotrypsinogen: Implications for Protein Formulation Stability

Mark O'Hanlon and Dr Robin Curtis

Theme: Biochemical and Bioprocess Engineering

Under certain solution conditions, protein molecules tend to cluster due to attractive, non-specific interactions. This clustering is known as protein aggregation. The deposition of proteins in any aggregate form is a characteristic feature of many degenerative diseases, most notably Alzheimer's and Parkinson's. Protein aggregation is also a major challenge in the formulation of protein therapeutics, as even small amounts can reduce efficacy or trigger immunogenic responses. The transient nature of protein-protein interactions and the various aggregate complexes that can form present significant challenges when studying and characterising protein aggregation. This study focuses on a specific aggregation pathway called reversible self-association (RSA), where protein monomers associate transiently to form small, reversible oligomers. We investigate RSA in a globular protein, alpha-chymotrypsinogen, aiming to understand how its oligomeric state is influenced by solution conditions. Using light scattering, analytical ultracentrifugation, small-angle X-ray scattering, and viscosity measurements, we characterise how pH and ionic strength modulate RSA by altering electrostatic interactions. These methods allow us to determine the size, shape, and interaction strength of protein species in solution. This multi-technique approach enables us to begin deconvoluting the hydrodynamic and thermodynamic contributions to RSA and supports the development of aggregation-resistant protein therapeutics.

Oral Presentation 15

Self-Assembling Peptide Hydrogels: Moving Towards Sustainable 3D Liver Models in Drug Discovery

Stefano Pretto and Prof Aline Miller

Theme: Advanced Functional Materials

Animal models and animal-derived matrices like Matrigel are increasingly criticized in drug discovery due to ethical concerns and limited relevance to human physiology. Drug-induced liver injury (DILI) remains a leading cause of post-marketing drug withdrawals, often undetected in preclinical testing. This study introduces a reproducible, xeno-free peptide hydrogel (EEFKFEFKFE) as an alternative matrix for hepatic organoid culture and enhanced hepatotoxicity prediction. The hydrogel's structural and mechanical properties were characterized using transmission electron microscopy, FTIR spectroscopy, and rheology. HepG2 cells cultured in 3D within the hydrogel maintained ¿90% viability over 35 days, forming spheroids (∼50) with polarized structures and no necrotic cores, confirmed by F-actin staining. Functional assays showed consistent albumin and urea secretion, indicating stable liver-specific activity. Notably, the hydrogel enabled improved detection of acetaminophen toxicity, with a lower LC_{50} (10 mM) compared to Matrigel (15.8 mM), highlighting enhanced sensitivity. These findings support the use of peptide hydrogels as a scalable, ethical alternative to animal-derived systems. By improving the physiological relevance and predictive power of in vitro liver models, this approach offers a promising platform for safer, more effective drug development.

Oral Presentation 16

Design of Experiment Driven Optimisation of Microbial Conversion of Agri-Processing Waste to Fatty acids.

Nichakorn Fungprasertkul, Dr Peter Martin and Dr James Winterburn

Theme: Biochemical and Bioprocess Engineering

Unsaturated fatty acids are suggested as a primary source of fat consumption for humans by WHO as they can decrease the risk of heart diseases. The most significant by product of rapeseed oil production is rapeseed meal (RSM), with approximately 39 million metric tons per annum produced. *Metchnikowia pulcherrima* is an under-explored oleaginous yeast with potential as a lipid producer by utilizing biomass as a feedstock. The key factors for maximizing the lipid production by *M. pulcherrima* were identified and optimized by using Plackett-Burman design with multiple linear regression model and Box-Behnken design with quadratic model subsequently. *Aspergillus oryzae* was used for RSM hydrolysis (i.e., converting RSM to assimilable molecules for *M. pulcherrima*) in solid-state fermentation (SSF). SSF conditions were optimized by using five-factors Doehlert design with quadratic model. Carbon and nitrogen sources were identified as important factors for lipid production by *M. pulcherrima*. The optimal C:N ratio was at 28.58 (g carbon/g nitrogen). SSF time was identified as the important factor, and the optimal SSF time was at 3 days. M. pulcherrima utilized the hydrolysate and produced unsaturated fatty acids in 500 ml bioreactor which are 60% Oleic acid (C18:1) and 21% Linoleic acid (C18:2) of total fatty acids.

Oral Presentation 17

Selective C–H Abstraction by $[FeIV(O)(N_4Py)]^{2+}$: Efficient Deformylation of 2-Phenylpropionaldehyde Toward Green Catalyst Design

Henrik Pak Hong Wong and Dr Dr Samuel P de Visser

Theme: Biochemical and Bioprocess Engineering

2-Phenylpropionaldehyde (2-PPA) is a phenylacetaldehyde analogue widely used as a flavour and fragrance agent imparting green hyacinth leaf and lilac notes in perfumes and food products. High-valent iron(IV)-oxo species are key intermediates in enzymatic and synthetic oxidations, yet their reactivity patterns with aldehydes remain underexplored. Here, we report that the nonheme iron(IV)-oxo complex $[FeIV(O)(N_4Py)]^{2+}$ (N_4Py) promotes efficient deformylation of 2-phenylpropionaldehyde (2-PPA) and its deuterated analogues via selective abstraction of the aldehyde C–H bond. Kinetic isotope effects measured for -[D1]-2-PPA and aldehyde-[D]-2-PPA (KIE $\approx$ 5–10) confirm that C–H cleavage is rate-determining, ruling out nucleophilic addition or α-C–H activation pathways. Complementary DFT studies reveal that noncovalent -stacking with the substrate's aromatic ring precisely orients the aldehyde for hydrogen atom transfer. This chemoselectivity underscores N_4Py's capacity to harness iron-oxo cores for targeted C–H activation in aldehyde deformylation, expanding the toolkit of nonheme iron catalysts for selective oxidation chemistry. This particular reaction paves the way for greener processes in the pharmaceutical and flavor industries, and informs the design of catalysts that can depolymerize lignin into valuable aromatic building blocks for the chemical sector.

Oral Presentation 18

Hybrid Modelling for the Dynamic Simulation of WGSR and Methanol Synthesis Reaction Networks

Fernando Vega-Ramon , Prof. Christopher Hardacre, and Dr Dongda Zhang

Theme: Catalysis and Porous Materials

Despite the widespread industrial application of $Cu/ZnO/Al_2O_3$ catalysts, there remains a gap in understanding how operating conditions and feed composition govern their catalytic activity and selectivity towards the watergas shift and methanol synthesis reactions. In this context, the complex nature of the underlying reaction mechanisms and the lack of informative data for parameter estimation prohibit the development of conventional kinetic models that can guide process improvements and rational catalyst design. To address these challenges, we propose a hybrid approach that integrates a mechanistic (power law) model backbone alongside data-driven modelling techniques (artificial neural networks) to enhance kinetic model generalisability and predictive capabilities. We demonstrate the construction and application of the hybrid model using spatially resolved kinetic data, where pronounced changes in catalytic activity were observed with respect to temperature, pressure and $CO:CO_2$ feed ratios. The hybrid model exhibits satisfactory predictive accuracy throughout and its confidence intervals are well aligned with the variability in experimental data, indicating its robustness to capturing underlying trends with respect to operating conditions. This work highlights the potential of hybrid modelling frameworks to accelerate kinetic model development for applications in process optimisation and control.

Oral Presentation 19

Low field NMR studies to probe motion and dynamics in rock pore structures

Aristarchos Mavridis and Dr Carmine D'Agostino

Theme: Catalysis and Porous Materials

Carbon geo-storage is a promising approach to substantially mitigate net greenhouse gas emissions, by permanently storing CO_2 in underground reservoirs. The success of such operations would greatly depend on the wettability of the geological formations towards the injected supercritical CO_2, and the brines which would always be present in a porous geological formation. Therefore, having reliable experimental methods to study such systems is of significant importance.

NMR relaxation is a well-established method for studying the behaviour of fluids in porous media. Relaxation time distributions can provide information about the different pore sizes present in the sample, and the ratio between T_1 and T_2 can be useful to assess the strength of interactions between the fluid molecules and the solid surface.

In this work, we are looking at the behaviour of different brine samples, made up of NaCl, KCl, $CaCl_2$ and $MgCl_2$ at various concentrations, confined in different types of porous solids, including metal oxides and rock samples. The results suggest that the interactions largely depend on the type and concentration of electrolytes, and they may vary across different solid surfaces. Furthermore, we are using NMR to investigate how rock samples change after exposure to supercritical CO_2, and we are utilizing simulations to help us better understand the experimental results.

Oral Presentation 20

NMR investigations of insulating Metal-Organic Frameworks for charge storage in supercapacitors

Lan An and Dr Daniel Lee

Theme: Advanced Functional Materials

Supercapacitors, as high-performance energy storage devices situated between conventional physical capacitors and batteries[1]. However, the liquid electrolytes traditionally used in supercapacitors can give rise to safety concerns, particularly due to their flammability[2]. There is thus a strong drive towards solid-state electrolytes, but these are currently limited by ionic conductivity and electrode/electrolyte interfacial contacts. Metal-organic frameworks (MOFs), which are highly porous can be used to bridge this gap. Conductive MOFs and insulating MOFs mixed with conductive additives have been investigated as potential electrode materials[3-5] but insulating MOFs can also be used as electrolyte system, substantially reducing flammability[6]. We use solid-state nuclear magnetic resonance (ssNMR) spectroscopy to investigate two insulating but contrasting MOFs, MFM-300(Sc) and MIL-125(Ti), soaked with $NaBF_4$/diglyme electrolyte. The the measurements reveal that diglyme interacts strongly with the framework of both MOFs. Owing to the more flexible structure, easier formation of defects, and larger pore size of MIL-125(Ti)[7], it can accommodate a greater number of ions moving more rapidly within the pores and get restricted motions of Na+ according to broader line of Na^+ powder pattern. The results of the ssNMR spectroscopy elucidated a quasi-solid-state electrolyte system and provided a theoretical foundation for further enhancing the performance of MOF-based electrolytes.

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Oral Presentation 21

Advanced Design of Mixed Matrix Membranes for Gas Separation

Mehdi Ghasemi, Prof Lev Sarkisov and Dr Masoud Babaei

Theme: Multi-scale modelling

In response to the imperative for developing efficient techniques to capture carbon dioxide (CO_2) from industrial processes, membrane-based gas separation holds significant promise for its cost-effectiveness, safety, environmental benefits, and energy efficiency. Among the wide variety of materials applicable to this technique, polymeric materials have predominantly captured attention for their suitability for large-scale deployment. Despite the successful commercialization of polymeric membranes, they suffer from the permeability- selectivity trade-off. A promising approach to address this issue involves the utilization of mixed matrix membranes (MMMs), formed by integrating porous materials as fillers into a polymer matrix. MMMs leverage the processability of polymeric membranes along with the superior selectivity and permeability of porous materials. In the development of efficient MMMs, several critical factors come into play, including the morphologies of MMMs, types of polymers, filler particle types, particle dispersion, plasticization, and physical aging. Enhancing MMM performance is also achievable through modifications, such as adjusting filler size, shape, and loading, adding additives, and implementing filler surface modifications. In my presentation, I will be discussing a recent finding from my PhD research, which focuses on how geometrically optimized fillers can enhance the performance of designed MMMs for gas separation.

Oral Presentation 22

Microbial Reactions and Transport Interplay in Underground Hydrogen Storage: Impacts on H_2 Loss and Purity

Ehsan Vahabzadeh and Prof. Vahid Niasar

Theme: Subsurface energy systems

Underground hydrogen storage (UHS) in depleted gas reservoirs introduces complex interactions between physical transport, mixing, and microbial reactions. This study presents a sensitivity analysis exploring how microbial reaction rates, injection/withdrawal (I/W) flow rates, and cycle lengths influence hydrogen loss and the purity of withdrawn H_2. A two-phase bio-reactive transport model incorporating methanogenic archaea and sulphate-reducing bacteria was developed and applied across a range of operational scenarios. Results show that while microbial reaction rates have limited impact on total H_2 loss over long storage periods, flow rate and cycle length significantly influence consumption dynamics and spatial distribution of microbial activity. Higher flow rates enhance mechanical dispersion but reduce overall H_2 loss due to shortened cycles. Conversely, longer cycles allow greater cumulative microbial consumption, though relative loss decreases due to more effective substrate mixing in shorter cycles. Methanogenesis dominates over sulphate reduction due to yield differences, but microbial activity overall contributes less than 1% to the reduction in H_2 purity. Mixing and buoyancy are identified as the dominant drivers of impurity. These insights highlight the need to jointly consider operational strategies and subsurface bio-chemical processes when optimizing UHS system performance.

Oral Presentation 23

In-Situ Monitoring of Spent Nuclear Fuel Gas Plenums Using a Combined Spectroscopic Approach

Rebecca Clews , Louise Natrajan, Sean Woodall, and Prof Philip Martin

Theme: Process Integration

As part of the Nuclear Decommissioning Authority's strategy, the majority of the UK's spent nuclear fuel (SNF) inventory is set to be stored in interim containers pending its final disposal. There are two methods currently in operation for this – wet and dry. Dry storage has been widely deployed globally, in countries such as the USA, Canada, and Germany. Although some sites in the UK, such as Wylfa and Sizewell B, have already implemented dry storage for their SNF, the most established technique in the UK, and globally, remains wet storage. Wet storage, however, has limitations for certain fuel types, bringing attention towards dry storage as an attractive alternative.

Currently, there are no mature monitoring techniques for interim SNF dry storage. This project will bridge this gap in knowledge by utilising a combined LIBS (Laser-Induced Breakdown Spectroscopy) and Raman spectroscopy approach to monitor the SNF. The two techniques can be deployed in-situ, with stand-off detection of key chemical species released in the degradation of the fuel and integrity failures of the container. As each species is indicative of different failure conditions, the techniques will provide an insight into the integrity of the SNF and cask without the need for direct intervention.

Oral Presentation 24

Life cycle assessment guided preparation methods for heterogeneous catalysts: The case of $Cu/ZnO/Al_2O_3$ for CO_2 conversion

Rania Al Mozani , Prof. Christopher Hardacre and Dr Rosa M. Cuéllar-Franca

Theme: Sustainable Industrial Systems

Introduction. Global industrialisation and population growth has led to increasing greenhouse gases emissions, including CO_2 emissions, which have contributed to climate change. Various efforts to mitigate such phenomenon include new technologies focusing on the utilisation of CO_2 via conversion into valuable chemicals and fuels such as formic acid, light olefins and methanol. At the centre of such technological innovations lies advances in catalysis to ensure the effective activation and conversion of the very thermodynamically stable CO_2 molecule. Whilst the design and selection of catalysts with respect to their performance, i.e. high yields and conversion, is paramount in the development of such technologies, it is also important to consider the environmental sustainability of their synthesis to avoid burden shifting.

Experimental/methodology. The preparation of catalysts involves several stages that are both material and energy-intensive. In the case of the heterogeneous catalyst $Cu/ZnO/Al_2O_3$, commonly employed in the conversion of CO_2, the synthesis route involves the consumption of metal nitrates, aluminium oxide, solvents, and precipitating agents under specific conditions of temperature and pH. Therefore, this study aims to assess the environmental sustainability of different industrial preparation methods (coprecipitation, deposition precipitation, and wet impregnation) of $Cu/ZnO/Al_2O_3$, a commercial catalyst used for the conversion of CO into methanol and has shown promise for the conversion of CO_2 to methanol, using the life cycle assessment (LCA) methodology. A cradle to gate approach is considered for this work to compare the synthesis of 1 g of $Cu/ZnO/Al_2O_3$ via three commercial preparation methods. Inventory data for catalyst preparations were obtained from literature, Ecoinvent database V3.8, and own calculations. The LCA modelling was performed using LCA for Experts v10.7 and the environmental impacts were estimated according to the ReCiPe 2016 v1.1 method considering a hierarcist perspective.

Results and discussion. The climate change impact results for the three preparation methods—coprecipitation, deposition precipitation, and impregnation—show that coprecipitation exhibits the highest cradle to gate climate change at 31.5 g CO_2 eq./g of catalyst. Deposition precipitation follows with 29.0 g CO_2 eq./g of catalyst, while impregnation has the lowest impact at 2.2 g CO_2 eq./g of catalyst. In addition, hotspots and opportunities for improving the synthesis of this benchmark catalyst are identified in an effort to guide the development of more environmentally sustainable synthesis of catalysts. Finally, to support the decision of selecting the more environmentally sustainable method for the preparation of $Cu/ZnO/Al_2O_3$, a comparative analysis of the catalysts obtained from each method is conducted via N_2O pulse and Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES).

Oral Presentation 25

Sustainability Assessment of Solar Thermochemical Hydrogen Production Technologies in China

Xiaoyu Huang , Dr Harish K. Jeswani and Prof Adisa Azapagic

Theme: Sustainable Industrial Systems

In 2023, global energy-related CO2 emissions reached a record high (37.7 Gt), highlighting the need for low-emission energy sources. Green hydrogen, particularly through solar thermochemical (STC) production, presents a promising alternative. This study evaluates the environmental and economic sustainability of STC hydrogen production in China using solar tower power (STP) across five chemical cycles: sulphur-iodine, hybrid sulphur, three- and four-step magnesium-chlorine and copper-chlorine. Among the cycles, hybrid sulphur and four-step copper-chlorine have the lowest climate change (1044–1389 kg CO2 eq./t H2) and costs (5.5–8 k$/t), outperforming the other cycles, with four-step magnesium-chlorine performing worst in both. Similar trends are observed for other environmental impacts. The STP plant components dominate both the impacts and costs. Compared to conventional methods, all STC cycles achieve 58-95% lower climate change but have higher levelised cost of hydrogen, with the lowest STC cost being 2.3 times that of steam methane reforming with carbon capture. Sensitivity analysis indicates that the environmental and economic performance is strongly influenced by STP efficiency, capacity factor and system lifetime, with regions of high solar irradiance being less affected by these parameters. Combined advancements in STC technologies will be essential for improving the competitiveness of STC hydrogen production.

Oral Presentation 26

Solvent-responsive membranes with molecular sieving capabilities for ethanol-water separation

Roger Bellido Peralta and Prof Rahul R. Nair

Theme: Advanced Functional Materials

Responsive membranes are structures that change their behaviour when exposed to different stimuli. The triggers for the response can range from change of pH to exposure to different solvents and usually impact the molecular sieving capacity of the membrane. However, there is a need to actively change the substance the membrane is in contact with for the change to happen. In this work, we show how a GO:PDDA membrane tunes its ethanol (EtOH) selectivity as we change the concentration of the feed solution. We found that a variation in ethanol concentration in the feed solution of a pervaporation experiment triggers a switch in our membrane. An initially ethanol–selective structure ($\sim$ -38% EtOH rejection) at low alcoholic concentrations flips to being water–selective ($\sim$ 85% EtOH rejection) as the concentration increases, while keeping permeation around the characteristic values for GO membranes ($\sim 2\,\mathrm{L\,m^{-2}\,h^{-1}}$). This means this structure does not require a change of solvent in its entirety to trigger its response, opening the possibility of a continuous working regime in which the membrane adapts to the concentration change and increases or decreases the ethanol selectivity according to the experimental design.

Oral Presentation 27

Dual-Strain Detection of Norovirus GI.1 and GII.4 in Food Samples Using Epitope-Imprinted Polymers

Amy Dann and Prof Marloes Peeters

Theme: Advanced Functional Materials

Norovirus is the leading cause of viral gastroenteritis worldwide, contributing to widespread disease and financial burdens. Proactive on-site testing of high-risk food samples is essential to prevent outbreaks, requiring the development of innovative sensors. We have developed a thermal sensor capable of detecting two norovirus genotypes, GI.1 and GII.4. The sensor uses epitope-imprinted polymer nanoparticles (nanoMIPs) designed from a 10-amino-acid sequence from the GI.1 viral capsid. The nanoMIPs demonstrated favourable detection capability to norovirus GI.1 and GII.4 virus-like particles in buffer solutions, achieving detection limits of 1.53 and 2.28 pg/mL, respectively. The selectivity of the nanoMIPs was evaluated against a panel of similar viruses, including murine norovirus, Tulane virus, and bacteriophage MS2, each of which showed a reduced signal. Notably, the sensor achieved rapid detection (30 min) of norovirus GI.1 and GII.4 virus-like particles in spinach samples while maintaining comparable detection limits (2.19 pg/mL and 2.69 pg/mL) to spiked buffer solutions. The combination of rapid detection time, dual strain recognition, and simple sample preparation makes this thermal sensor a promising tool for on-site testing. Furthermore, the ability to detect multiple strains using a single ligand represents a significant advantage, enabling the development of straightforward systems capable of detection various strains.

Oral Presentation 28

Hydrophilic Polyethersulfone and Two-Dimensional Siloxene Membranes: Pursuing Antifouling Performance for Enhanced Biological Application

Benjamin Moore and Dr Maria Perez-Page

Theme: Advanced Functional Materials

Membranes for biomedical applications face the issue of fouling from biological components, which limits the separation performance. However, at the research stage, they are commonly tested using feed concentrations unrepresentative of real conditions. By developing and testing a membrane under high feed concentrations, analogous to those used during target application, antifouling capabilities can be better assessed. In this work, siloxene, an easy-to-synthesise novel hydrophilic two-dimensional nanomaterial, was successfully incorporated as a filler into a Polyethersulfone (PES) membrane matrix. At optimised filler loadings of 0.15 wt%, the pure water permeance was increased from 75 to 147 LMHBar while rejecting ∼99% of protein model solution, bovine serum albumin (BSA), by achieving high hydrophilicity with a water contact angle as low as 27°. Furthermore, the Flux Recovery Ratio increased from 17% to 62% after siloxene was incorporated, which shows significant improvement in their capability to cope with concentrated biological feeds using an $80\,\mathrm{mg\,mL^{-1}}$ BSA solution, analogous to human blood plasma protein concentration. PES-organosilane-functionalised-graphene oxide, highlighted in the literature for its protein-antifouling properties, was fabricated for comparison, where PES-Siloxene superseded its performance. Novel PES-Siloxene membranes show great potential in biomedical membrane applications based on their substantial improvement over their counterparts.

Oral Presentation 29

Applicability of the Thermodynamic and Mechanical Route to the Young Equation for Rigid and Soft Solids: A Molecular Dynamics Simulations Study of a Lennard-Jones System Model

Fulu Zhou and Prof. Paola Carbone

Theme: Multi-scale modelling

The wetting behavior of a liquid on a solid is typically described by Young's equation, linking the contact angle of a droplet to the interfacial properties involved. Simulations often assume a rigid solid or substitute surface free energy with interfacial tension. In this study, Molecular Dynamics simulations of a Lennard-Jones liquid on a Lennard-Jones crystal are conducted, comparing contact angles from droplet shapes to those predicted by Young's equation using both surface free energy and surface stress. The study examines both rigid and flexible solid surfaces with varying wettability and softness. Results show that while both surface stress and surface free energy yield similar contact angles, they differ in interfacial behavior. Notably, freezing solid atoms can lead to inaccuracies, especially when the liquid packs well at the interface. Ultimately, the study concludes that surface free energy must be used in Young's equation for accurate contact angle predictions, and using surface stress leads to growing errors as the solid becomes softer.

Oral Presentation 30

Dynamics of Confined Bubbles in Shear-Thinning Liquids: Toward Improved Photobioreactor Performance

Runqi Zhao and Dr. Claudio Pereira da Fonte

Theme: Multi-scale modelling

The efficient cultivation of microalgae is crucial for sustainable bioresource production and CO_2 mitigation, yet photobioreactor performance remains limited at high cell concentrations. In particular, cultures exceeding 30 g/L exhibit pronounced shear-thinning behaviour, which significantly alters gas holdup and gas–liquid mass transfer rates. Moreover, such high biomass densities lead to severe light attenuation, reducing the effective light available to individual cells and thus limiting photosynthetic productivity. This study investigates the dynamics of gas bubbles rising through shear-thinning media under geometric confinement, as encountered in flat-panel photobioreactors. Experiments and computational fluid dynamics (CFD) simulations are conducted within a Hele-Shaw cell ($\sim$1 mm gap), representing a simplified 2D confined geometry. A validated numerical model accurately predicts bubble terminal velocities and shapes in Newtonian fluids across a range of bubble diameters. The model is extended to shear-thinning fluids assuming the Ostwald–de Waele rheological model, enabling systematic analysis of the effects of flow behaviour index n and consistency index K on confined bubble dynamics. Results reveal that shear-thinning markedly modifies bubble morphology and rising velocity, with implications for gas–liquid mass transfer. Preliminary experiments in model non-Newtonian fluids (Xanthan gum) support the numerical results. These findings contribute to the understanding of multiphase transport in non-Newtonian media and inform the design of intensified photobioreactors for high-density microalgal cultures.

Oral Presentation 31

Predicting the impact of particle size and shape distributions on filtration performance of crystallized products

Oleksandr Prykhodko , Dr Carlos Avendano and Dr Ashwin Kumar Rajagopalan,

Theme: Sustainable Industrial Systems

Filtration is a crucial downstream step in pharmaceutical, fine chemical, and agrochemical industries, where crystallized products are common. The filter cake's structure, porosity, and permeability impact later steps such as washing and drying. Recent work has experimentally demonstrated how particle size and shape distributions (PSSDs), particularly for needle-like crystals, affect cake structure and resistance, validating a model for cake structure and porosity. However, key metrics like cake resistance and filtration time—vital for industrial optimization—still lack predictive models. This study uses a combined experimental and modelling approach to predict key filtration metrics for needle-like crystallized products based on their PSSD. A two-step modelling framework is proposed: a Monte Carlo model simulates cake formation, followed by computational fluid dynamics modelling in OpenFOAM to simulate fluid flow at steady state. Compared to DEM–CFD, this method lowers computational effort and requires fewer input parameters. The framework was applied to various case studies, examining PSSD attributes like shape, polydispersity, and pressure drop. Experimentally, tailored PSSD populations were generated and analyzed via advanced imaging. Constant pressure filtration tests were conducted using a custom rig and compared to simulations. This work introduces a predictive tool that minimizes experimental reliance, enabling faster and more cost-effective filterability assessments in research and development.

Oral Presentation 32

Modelling the phase behaviour of antibodies

Maria Gabriela Arias Segura and Dr Carlos Avendano

Theme: Multi-scale modelling

Monoclonal antibodies are an important class of therapeutic molecules in the pharmaceutical industry. The formulation of antibody-based products is challenging because concentrated solutions are prone to aggregate or display liquid-liquid separation, which may have a negative impact on the effectiveness of the treatment. Here, computational models can be useful to understand and predict phase separation behaviour. The present work uses two simplified models which consist of a y-shaped "body" made of beads that mimics the shape of antibodies and 'patches' that represent regions involved in intermolecular bonding. The interactions between molecules are defined by the Lennard- Jones potential which is repulsive at short distances and attractive at intermediate distances. We investigate the effect of different patch-patch interactions on the LLPS behaviour of the model antibodies. The direct coexistence method was used in Molecular Dynamics simulations to observe the separation of a protein solution into protein "rich" and "poor" phases at constant temperature and volume. We also studied the second virial coefficient (B_2), which is a parameter that describes the character of the intermolecular interactions and may be used to compare models with similar structure but different interactions. Mayer sampling, a technique based on importance sampling, was used to calculate the B_2.

Oral Presentation 33

Molecular simulation study of stability of MOFs during activation process

Christopher Ratcliff and Prof. Lev Sarkisov

Theme: Multi-scale modelling

Throughout history, and into the present day, porous materials have found extensive use due to their inherent, advantageous characteristics. As such, porous material research has faced continuous pressure to enhance and improve upon existing solutions, primarily resulting in the development of novel classes of porous materials. One such class, metal-organic frameworks (MOFs), has received significant interest due to its modular structure and unparalleled topological diversity, enabling direct-design of structure properties. Substantial research had been spent on designing specialised MOFs, but synthesis has proven very difficult - a significant barrier to industrial application. In particular, for the final stage required to functionalise a MOF, known as activation, leftover solvent must be entirely extracted. Unfortunately, during activation, MOF structures have a propensity to collapse, breaking down the crystal structure and becoming amorphous. This has become known to the community as the phenomenon, activation-collapse. Initial work has suggested collapse may be caused by strong capillary forces exerted on to the framework during phase transition of guest-solvent molecules, but, due to limited research, little fundamental information is known. In this talk, I will review the progress I have made thus far in exploring the effect using a simulation-based methodology, and discuss the unexpected behaviour which has arisen from our simple model.

Oral Presentation 34

Isopropanol-Acetone-Hydrogen chemical heat pumps for improved heat recovery from geothermal resources, A case study in China

Zhengguang Liu and Dr Masoud Babaei

Theme: Subsurface energy systems

This study focuses on geothermal energy utilization through multi-objective optimization of Isopropanol-Acetone-Hydrogen chemical heat pump (IAH-CHP). In this paper, IAH-CHP coupled with medium-low temperature geothermal heat source simulation was constructed. China, the world's largest carbon emitter, was used as a case study to highlight environmental benefits. Comparative analysis was conducted between carbon emissions and investment of chemical heat pumps with other common heating equipment in different buildings. The results show IAH-CHP system has higher initial investment costs, however, their CO_2 emissions are significantly lower. The results of multi-objective analysis demonstrate the system can operate under a Pareto (multi-objective) optimal scheme. Under this plan, the levelized cost of heat (LCOH) is only 0.12 USD/kJ, and the carbon emissions are as low as 4.97 tons/year with a coefficient of performance (COP) of 7.4. Compared with a single-objective optimal solution, 8.12 tons of carbon emissions and LCOH of 0.15 USD/kJ could be achieved. Applying IAH-CHP system to China to replace original coal-fired heating solution can achieve annual carbon emission reduction of more than 5 million tons in areas with medium and low temperature heat sources.

Poster presentations

Poster 01

Enhancing Low-Temperature Serpentinization for Hydrogen Production: Catalytic Role of Awaruite and Chromite

Jeffrey Akuoko and Dr Lin Ma

Theme: Catalysis and Porous Materials

Serpentinization of ultramafic rocks generates hydrogen gas, offering a potential clean energy resource. While hydrogen production is most efficient at elevated temperatures (250–350°C), low-temperature serpentinization—more typical of near-surface environments on Earth and Mars—is limited by slow reaction kinetics. This study investigates the catalytic potential of awaruite (Ni_3Fe) and chromite in enhancing serpentinization at lower temperatures. We apply thermodynamic modeling using PHREEQC, coupled with molecular dynamics simulations in LAMMPS, to explore the kinetic and atomistic mechanisms underlying mineral-catalyzed hydrogen generation. By integrating geochemical modeling with atomistic insights, this research aims to clarify the role of these minerals in accelerating serpentinization reactions. Ongoing simulations are expected to yield insights with valuable implications for sustainable hydrogen production on Earth and for models of planetary geochemistry relevant to Mars and other ultramafic-rich environments.

Poster 02

Fabrication of Membranes using Green Solvents

Buthayna Nasser Ali Al Ghafri and Dr Maria Perez-Page

Theme: Sustainable Industrial Systems

Membrane filtration has been proposed as an energy-efficient method for pharmaceutical wastewater treatment, leading to a growing demand for polymeric material and the requirement for petrochemical derived solvents for their fabrication. To enable sustainable membrane production routes, this research aims to predict the suitability of green solvents throughout complementary approaches: The COSMO-RS and Hansen Solubility Parameters (HSP) to compute the molecular interaction and polymer solubility, respectively, plus experimental validation. 146 potential solvents were classified using the CHEM21 guide as green, hazardous, and problematic for the thermodynamic evaluation for polyethersulfone membrane fabrication. Density Functional Theory calculations were performed on the PES oligomers to establish a proxy to represent the physicochemical properties of the polymer chains. Computed activity coefficients at infinite dilution at 298K and 323K revealed a proportionality to chain length due to consistent segment-solvent interactions. Results suggest a predictable linear screening trend across molecular sizes, enabling comparison between solvent-PES affinity. HSP analysis and experimental dissolution observations demonstrated concordance with COSMO-RS predictions. Predicted green solvents cyrene and γ-valerolactone were used for the PES membrane fabrication, obtaining membrane morphologies comparable to conventional dimethylformamide solvent. This work helps to establish greener membrane manufacturing protocols that maintain equivalent filtration efficiency while reducing environmental impact.

Poster 03

Sustainable Synthesis of Micro and Nanoparticles in Droplet Micro-Reactors

Ahlam Al Hadhrami and Dr Antonios Anastasiou

Theme: Advanced Functional Materials

This PhD project is focused on the investigation of droplet microfluidic reactors for the sustainable synthesis of solid micro and nano-particles, with potential applications in biomedical engineering, water treatment, catalysis etc. Droplet microfluidics enables precise manipulation of reaction conditions (e.g. concentration gradients, volume of reaction) and continuous synthesis of the particles, resulting in better control and uniformity over their properties, compared to conventional batch synthesis methods. In the first stage of the project the mechanisms and hydrodynamics of droplet formation were studied aiming to optimise internal droplet mixing that is critical for nanoparticle crystal growth. Different geometries have been designed and fabricated using high accuracy 3D printers while the droplet formation was studied using high speed cameras and a μ-PIV system. Preliminary experimental results have, showed that viscosity, flow rate ratios, and orifice dimensions significantly influence droplet size and formation dynamics. Smaller orifices and lower viscosities enhanced shear forces, producing smaller droplets and shorter formation times, while higher viscosities led to more uniform droplets but slower formation rates. A comparison of three correlations from literature revealed discrepancies with our experimental data, leading to the development of a new empirical model that can be used for more accurate prediction of droplet size in multi-inlet geometries. CeO_2 nanoparticles is the first system that is currently examined for the synthesis in the microreactors and an initial comparison with commercial samples is made. The research supports the advancement of scalable and sustainable production of nanomaterials using droplet microfluidics.

Poster 04

Design and Optimization of a Membrane-less Microfluidic Fuel Cell

Ibtehal Al houqni , María Pérez Page and Dr Antonios Anastasiou

Theme: Advanced Functional Materials

Membrane-less microfluidic fuel cells (MMFCs) are gaining attention as promising alternatives to conventional proton-exchange membrane fuel cells (PEMFCs), offering advantages such as simplified fabrication, miniaturisation, and reduced material requirements. However, traditional MMFCs with co-laminar flow suffer from mass transfer losses, CO_2 bubble generation, high-pressure while are not scalable. Considering the well-recognized disadvantages of the membrane in conventional fuel cells and the limitations of the current MMFC, a novel fuel cell is proposed where the functionality of the membrane is substituted by a gas-liquid interface. Our concept relies on the stratified gas-liquid flow that can be achieved in falling film devices. In these cases, a stable gas-liquid interface is formed that prevents fuel crossover and allows the transfer of protons through different mechanisms to occur. In the first stage of the project a 3D-printed prototype is developed and experimentally evaluated using methanol as fuel and oxygen as the oxidant. Wettability studies on hydrophilic and hydrophobic surfaces revealed key flow patterns—corner rivulet, falling film with dry patches, and a complete film flow—depending on flow rate and surface properties. Results indicate that controlling methanol concentration and microchannel width can significantly improve film stability at lower flow rates. The minimum wetting flow rate (MWF) required for achieving a complete film decreased with increasing methanol concentration and was further reduced by decreasing microchannel width, which aligns with previous studies. These findings establish the foundation for the ongoing development of high-efficiency MMFCs.

Poster 05

Limitations of Classical Force Fields for CO_2 Adsorption in MOFs: Toward Quantum Accuracy at DAC-Relevant Pressures

Abdullah Al Rammah , Prof Lev Sarkisov, Dr Ashwin Rajagopalan and Prof Flor Siperstein

Theme: Multi-scale modelling

Adsorbent-based carbon capture technologies are considered a cost-effective approach for mitigating climate change, but current adsorbents lack the performance required for large-scale deployment. Metal organic frameworks (MOFs), with their high tunability and structural diversity, offer significant promise for gas adsorption applications. Molecular simulations provide an efficient means to screen both experimental and hypothetical MOFs, but their accuracy depends on the quality of the force fields used. In this work, we use molecular simulations to screen an anion-pillared MOF database, targeting structures with large CO_2 working capacities. We examine discrepancies between simulations and experimental data at low pressures relevant to direct air capture (DAC), revealing limitations in commonly used force fields for estimating MOF–CO_2 interactions. Our results underscore the importance of conducting simulations at the quantum mechanical (QM) level to gain deeper insight into CO_2 adsorption at low pressures and to establish reliable benchmarks independent of experimental uncertainty for force field validation. We evaluate machine learning interatomic potentials trained on QM data, which offer reduced computational cost compared to density functional theory (DFT), but find they lack transferability and utility for Grand Canonical Monte Carlo (GCMC) simulations. Consequently, we adopt an approach to parameterise force fields directly from DFT calculations.

Poster 06

New Materials for Enhanced Carbon Capture and Utilisation Process

Muna Al-Ajmi and Dr Vincenzo Spallina

Theme: Catalysis and Porous Materials

This research proposes developing an integrated chemical looping process of chemical looping coupled thermochemical CO_2 splitting systems to produce CO-rich gas with in situ CO_2 utilisation. The problem began to alarm when CO_2, the primary residue of fossil fuels, became immediately responsible for global warming, which affects human health and the environment. This project will demonstrate an understanding of synthesising suitable functionalised materials (new catalyst formulations of high entropy perovskites) and report the performance of redox materials in thermochemical CO_2 splitting in terms of types of metal-oxygen carriers in thermochemical cycles, fuel yield, cycle stability, types of reactors, reaction conditions, synthesis method, and critical areas for future research and development. In the preliminary results, this research demonstrated the redox activity of the partial substitution of the perovskite oxide in B-site doped $La_{0.7}Sr_{0.3}Mn_{0.65}Co_{0.35}O_3$ and $La_{0.7}Sr_{0.3}Mn_{0.8}Ni_{0.2}O_3$, comparing it with high-entropy perovskites $SmSrCaMnO_3$ and $SmSrCaLaO_3$ for thermochemical redox cycles using TGA and characterised by SEM and XRD. Furthermore, the effects of temperature, pressure, and types of reducing agents on the production rate in a packed bed reactor were examined.

Poster 07

Development of Peptide-Chitosan Hydrogel Composites for Wound Healing Applications

Sara Ali Hosseinzadeh , Prof Alberto Saiani and Prof Aline F. Miller

Theme: Advanced Functional Materials

Introduction: Infections continue to pose significant challenges in the treatment of wounded tissue. In recent years, wound dressings made from natural polymers have gained popularity due to their anti-inflammatory and antibacterial properties. The materials used for wound dressings must possess moisturizing properties, biodegradability, and mechanical strength. Accordingly, Peptide hydrogels are being considered due to their ability to meet these requirements. The microbial resistance and mechanical properties of peptides can be enhanced by other polymers like chitosan. In this study, we optimized a peptide/chitosan hydrogel to develop an antibacterial hydrogel with improved mechanical properties. The physical and chemical characteristics, release properties, and antibacterial activity were thoroughly investigated.

Method: First, chitosan dissolved in a weak acid solution (0.08 M HCl) and stirred for 24 hours. Then, peptide powder was added to the chitosan solution in different weight ratios (1:1, 1:2, 1:4, and 1:8) to evaluate how these concentrations affect the final properties of the composite. The mixture was stirred until a uniform composite was obtained. Mechanical and viscoelastic properties were assessed using shear rheology. FTIR and UV-VIS spectroscopy were performed to confirm interactions between peptide and chitosan. The antibacterial properties of the composite were tested against Bacillus strains.

Results: The results demonstrate that peptide-chitosan composite hydrogels exhibit enhanced mechanical and antibacterial properties. FTIR and UV spectroscopy show the interaction between peptide and chitosan. Peptide hydrogels containing chitosan exhibited greater storage modules regarding rheology. Furthermore, the peptide-chitosan hydrogel showed a significant reduction in bacterial growth.

Conclusion: The peptide-chitosan hydrogel exhibited significantly enhanced antibacterial properties compared to peptide hydrogel and chitosan hydrogel alone. Future work will focus on further exploring its antibacterial properties and optimizing the hydrogel for potential use in wound healing.

Poster 08

Development of multifunctional catalysts for fatty acid hydrodeoxygenation for biofuel production under mild conditions

Yazen Al-Lami , Dr Jude Allen, Dr Christopher Parlett, Dr Xiaolei Fan

Theme: Catalysis and Porous Materials

The transition to sustainable aviation fuels (SAF) is crucial for reducing carbon emissions in the transportation sector. Our innovative research on fatty acid hydrodeoxygenation (HDO) offers a promising route for converting model bio-oil (e.g., lauric acid) into hydrocarbons in the jet fuel range. Unlike decarbonylation and decarboxylation, in the HDO process, oxygen molecules are removed as water (H_2O), the fatty acid's carbon chain is preserved, and the hydrocarbon yield increases. The research focuses on modifying conventional zeolites to introduce a hierarchical structure with mesopores and micropores, into which preformed Pd nanoparticles were selectively deposited within the mesopores. This design improves metal dispersion and active site accessibility by adding mesoporosity, overcoming the drawbacks of traditional zeolites. The selective deposition of Pd nanoparticles into the mesopores makes the effective conversion of fatty acids into alkanes with preserved carbon chain length possible, enhancing the synergy between the metal and acidic sites. This is essential for promoting the cascade HDO reactions, which include carboxylic acid reduction, alcohol dehydration, and alkene hydrogenation, for converting biomass-derived fatty acids substrates to corresponding alkanes with equivalent carbon chain length as the substrate.

Poster 09

Novel Design Framework for Process Synthesis, Integration, and Intensification

Omar Alqusair and Dr Jie Li

Theme: Process Integration

Achieving sustainable development requires a clearer understanding of resource and product management within processes. This work presents a novel framework for designing chemical processes using phenomena building blocks (PBBs). Unlike traditional methods that rely on predefined unit operations in a top-down approach, this method builds process flowsheets from modular blocks that represent underlying physical and chemical phenomena. The project aims to develop a phenomena-based design framework that produces intensified process flowsheets with minimal emissions. This framework process optimization to minimize total emissions while meeting product requirements, raw material availability, and operational constraints. A case study for ethylene glycol production from ethylene oxide and water is investigated. The design problem is formulated as a nonlinear programming (NLP) model and solved using commercial optimization software. The optimization results show that net emissions can be lowered by around 5% when compared to a non-optimized flowsheet for ethylene glycol production. Simulation and optimization results are compared to evaluate the performance and feasibility of the designs. Furthermore, structural synthesis of these blocks is investigated, which can lead to further reductions in emissions. The proposed framework offers a promising strategy for the development of low-emission, intensified processes that are can be tailored to specific design objectives.

Poster 10

Catalytic Conversion of Light Cut Plastic Derived Oil to High Value Petrochemicals using HZMS-5

Munthir Alshammari and Prof Arthur Garforth

Theme: Catalysis and Porous Materials

Global plastic waste has become a significant environmental challenge due to their persistence and slow degradation, with rising consumption of (413 million tons in 2023), creating serious concerns for waste management. Chemical recycling of plastic waste, particularly through thermal pyrolysis, offers a potential solution by transforming mixed waste plastic to plastic-derived oil (PDO). Commercial process for the direct introduction of PDO is limited due to its varied, source-dependent complex composition, impurity profiles and the scarcity of the research on its upgrading. This study investigates the catalytic cracking of PDO light fraction using a HZSM-5 catalyst with a silica-to-alumina ratio of 80:1 and a surface area of $425\,m^2\,g^{-1}$. The reaction was conducted in a plug-flow reactor at temperatures of 375 °C, 400 °C, and 450 °C, with a weight-to-feed ratio (W/F) of $74.2\,g\,h\,mol^{-1}$. The PDO light fraction, containing hydrocarbons with boiling points below 150 °C, was introduced into the reactor at a constant flow rate of 0.05 L/min, co-fed with argon gas at 100 L/min. Catalytic cracking at 450 °C showed a marked shift in hydrocarbon distribution, favoring the production of mono aromatics and light olefins, indicating a significant potential for upgrading pyrolysis oils into valuable chemical products.

Poster 11

Scientific Machine Learning for Crystallization Processes: A Hybrid Method for Multidimensional Kinetic Models

Mohammed Alsubeihi , Arthur Jessop, Ben Moseley, and Dr Ashwin Kumar Rajagopalan

Theme: Process Integration

Modelling is a useful tool that can benefit process understanding, development, scale-up, and operation. For crystallisation, this often means using population balance equations (PBEs) to describe the evolution of a particle size and shape distribution (PSSD) and the liquid phase concentration over time. Depending on the model formulation, one can account for different physical phenomena, including but not limited to nucleation, growth, and dissolution. Typically, the equations used to model these phenomena are empirical in nature and selected from a set of proposed candidate models. However, traditional numerical implementations face challenges related to computational complexity and model formulation. As more phenomena are modelled, or a more accurate particle representation is used (e.g. extending to multidimensional PBEs), the computational complexity increases. This can become a bottleneck when performing traditional parameter estimation or trying to use the model for model predictive control. The choice of empirical model significantly impacts accuracy, as a given empirical equation may not sufficiently capture the complex kinetics at play. Scientific machine learning (SciML) offers various approaches to address these challenges, enhancing computational efficiency while enabling the discovery of underlying physics and equations from experimental data.

In this work, we build upon a differentiable JAX-based PBE solver[1] that we have developed and combine this with a high-quality dataset that is available to us from a previous dissolution study.[2] Leveraging our computationally efficient and differentiable solver, we investigate traditional and hybrid SciML approaches to learning the underlying dissolution phenomena shown in the experimental studies. We first demonstrate the benefit of our solver by fitting a range of conventional empirical dissolution models using gradient-based optimization. This improves upon previous work[2] by calculating gradients and forward model passes faster using automatic differentiation and the parallel computing capabilities of our solver.[1,3] We then extend this approach by replacing the dissolution model with a neural network and training this hybrid model on the same dataset. By embedding the neural network in our fixed solver, we maintain physical interpretability, prevent the overall model from breaking conservation laws, and better capture the complex kinetics observed in the experiments.

This study demonstrates how hybrid SciML approaches can provide efficient and improved predictive performance when modelling experimental data. It also lays the foundation for further study into how we can better learn using these differentiable hybrid models in the future.

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Poster 12

A Comprehensive study on PHB biosynthesis through kinetic modelling

Ariyan Amirifar and Prof. Konstantinos Theodoropoulos

Theme: Biochemical and Bioprocess Engineering

Plastics present a mounting environmental crisis, with 79% accumulating in ecosystems, only 12% recycled, and 9% incinerated[1]. Additionally, over 95% of plastics are fossil-derived[2], compounding sustainability issues. As a biodegradable alternative, polyhydroxyalkanoates (PHAs)—microbial polyesters—show great promise, with poly(3-hydroxybutyrate) (PHB) being the most extensively studied. However, their industrial uptake is limited by high production costs and low yields. One viable approach is integrating PHB production into biodiesel facilities by using crude glycerol—a low-cost byproduct—as the carbon source[3,4].

Expanding on prior work[3,4], a holistic mechanistic model was developed for PHB production by Cupriavidus necator DSM 545, using glycerol and ammonium sulfate. The model was calibrated on batch fermentations under pH 6.8 and 30% dissolved oxygen, with varying initial carbon, nitrogen, and biomass concentrations. Incorporating five dynamic variables and 33 kinetic parameters, it captures key metabolic behaviour and reveals new physiological insights. Unlike earlier models, it robustly predicts system behaviour across a wide range of initial conditions. Using this model, an optimized fed-batch strategy was designed, resulting in a ∼3-fold increase in PHB titer. Experimental validation of the optimized process is currently planned.

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Poster 13

Micro-scale pore-fracture evolution of deep reservoir rocks (minerals) via in-situ X-Ray CT uniaxial compression

Bengang Chen and Dr Lin Ma

Theme: Multi-scale modelling

Understanding the mechanical response, including the deformation and failure behaviour, of reservoir rocks under subsurface energy storage conditions is crucial for evaluating their integrity and performance. This study presents an in-situ uniaxial compression tests on sandstone samples aimed at investigating the deformation and failure mechanisms relevant to compressed air and hydrogen energy storage systems. High-resolution X-ray CT imaging was employed to capture the progressive development of pore structures and fracture networks under incremental loading conditions that simulate deep subsurface stress environments. Image-based analysis revealed localized strain accumulation, pore collapse, and fracture coalescence, highlighting the critical role of mineral heterogeneity and pre-existing microstructural features in controlling deformation pathways. The results provide insights into the evolution of internal damage zones and the feedback mechanisms between mechanical stress and microstructural features in reservoirs sandstones. These insights contribute to a better understanding of the geo-mechanical behaviour of reservoir rocks and offer valuable implications for the long-term stability of geological reservoirs subjected to incremental loading conditions of subsurface energy storage systems.

Poster 14

Semantic Segmentation of Breast Cancer Pathology using Quantum Cascade Laser Infrared Hyperspectral Imaging and Advanced Deep Learning

Krzysztof Dziuba and Prof Peter Gardner

Theme: Advanced Functional Materials

Microscopic examination of stained biopsies remains standard practice in cancer diagnosis but suffers from subjectivity and limited chemical information. Vibrational spectroscopy offers richer biochemical data, and Quantum Cascade Laser (QCL) based Infrared hyperspectral imaging provides a promising avenue for rapid, high-resolution chemical mapping of tissues. This research utilizes QCL hyperspectral images acquired on a Bruker Infrared Laser Imaging (ILIM) microscope from commercial tissue microarrays of paraffin-embedded human breast cancer tissue sections, covering over 500 tissue cores from approximately 420 patients.

Our primary objective is the semantic segmentation of these high-dimensional QCL images. We aim to differentiate key diagnostically relevant tissue constituents, primarily normal epithelium, normal stroma, cancer epithelium, and Cancer Associated Stroma, using pixel-level ground truth annotations derived from co-registered H&E stained slides, annotated by pathologists on a subset of 170 individual tissue cores. From a computational perspective, this work focuses on developing and evaluating advanced deep learning models for this segmentation task, benchmarking them against established methods like Random Forests and standard Convolutional Neural Networks. Specifically, we investigate:

1. Attention Mechanisms: Integrated within DL architectures, hypothesizing they can automatically identify salient spectral biomarkers indicative of different tissue types within the QCL data, thereby also enhancing model interpretability.

2. Graph Neural Networks: Employed to explicitly model the spatial context and architectural relationships between adjacent pixels or superpixels in the hyperspectral images, capturing tissue structure information often vital for accurate pathological assessment.

Preliminary results have been obtained, and the performance of these models is being rigorously assessed using standard segmentation metrics. This study provides a quantitative comparison of these advanced DL techniques for QCL hyperspectral pathology image segmentation, evaluating their potential for improved accuracy and interpretability in breast cancer analysis and contributing to the clinical translation goals of CLIRPath-AI.

Poster 15

Development of a Novel Graphene Oxide GO-Based Membrane for Hypersaline Wastewater Purification

Mohamed Elsharkasi and Prof. Rahul R Nair

Theme: Advanced Functional Materials

Water scarcity is a pressing global challenge that demands innovative and sustainable solutions to protect the environment and preserve freshwater resources. Hypersaline wastewater pollution exacerbates this issue, with conventional disposal methods harming ecosystems and contaminating available water supplies. To address these challenges, sustainable water practices, including advanced wastewater treatment, significantly improve the availability and quality of water resources. Advanced desalination technologies play a key role in addressing these challenges by conserving freshwater and enabling the reuse of hypersaline wastewater. This study focuses on developing GO-based membrane technologies to enhance efficiency, reduce costs, and improve the feasibility of hypersaline wastewater treatment. By advancing minimal and zero liquid discharge MLD/ZLD strategies, this research minimises reliance on thermal brine concentrators, offering a sustainable and economically viable solution for industrial wastewater management.

Poster 16

Selective extraction of platinum group metals (PGMS) using novel bio-based deep eutectic solvents (DESs)

Sahar Gholami, Dr Carmine D'Agostino; Dr Jesús Esteban, and Dr María Pérez-Page

Theme: Sustainable Industrial Systems

The growing economic importance and finite availability of platinum group metals (PGMs) underscores the need for efficient recovery methods, aligning with sustainability and circular economy principles. Hydrophobic deep eutectic solvents (HDESs) have emerged as environmentally benign alternatives for PGM extraction from acidic leaching solution of metal-bearing waste. In this study, type V HDESs were evaluated as novel extractants for PGM-containing solutions. This research includes the characterisation of solid-liquid equilibrium phase diagrams and physicochemical properties of HDESs (density, viscosity, and thermal and chemical stability) across varying compositions and temperatures. The solvents were tested for Pt(IV) and Pd(II) recovery from acidic solutions, analysing operating parameters including DES composition, shaking time, organic-to-aqueous phase volumetric ratio, acidity, and temperature. The results highlight the remarkable potential of HDESs as cleaner and tunable solvents for PGM extraction, achieving over 90% extraction efficiency for either metal under optimised conditions. Furthermore, adjusting the eutectic components and solution acidity enables precise tuning of metal selectivity, demonstrating excellent selectivity for Pt(IV) over Pd(II).

Poster 17

One Step Reforming of Biogas by Non-Thermal Plasma Catalysis

Abigail Jane Harris and Prof Christopher Hardacre

Theme: Catalysis and Porous Materials

Biogas reforming is a promising strategy to reduce greenhouse gas emissions by converting renewable biogas into syngas, a key intermediate for processes such as Fischer–Tropsch synthesis. However, conventional reforming requires high temperatures (¿973 K) due to the thermal stability of CO_2 and CH_4. Non-thermal plasma (NTP) offers a lower-temperature alternative by activating reactants via high-energy electrons (1–10 eV). This study investigates 5 wt% Ni/γ-Al_2O_3 catalysts under plasma-catalysis conditions, leveraging Ni's affordability and proven activity in thermal reforming. Catalysts were prepared via wet impregnation and tested in a dielectric barrier discharge (DBD) reactor (1.5 mm gap, 20 mm length), powered by an AC high-voltage source. Gas flows (Ar, CO_2, H_2O, CH_4) were fixed at 100 mL/min. Product gases were analysed using online gas chromatography. While -AlO exhibited high initial CH and CO conversion, it deactivated over 700 minutes (conversion drops of 74% and 84%). In contrast, Ni/γ-Al_2O_3 showed stable activity and higher H_2 production ($\sim$28,000 ppm vs. $\sim$22,000 ppm). Both systems produced C_2–C_3 hydrocarbons, but Ni/γ-Al_2O_3 maintained selectivity more effectively. Results suggest Ni sites enhance plasma-catalytic stability by enabling synergistic surface and plasma-phase reactions. Ongoing work aims to elucidate structure–activity relationships across Ni loadings.

Poster 18

Elucidating Active Sites and Reversible Transformation Pathways of Au Catalysts for Base-Free Benzyl Alcohol Oxidation

Yutao Jiang , Dr. Christopher M.A. Parlett and Dr. Carmine D'agostino

Theme: Catalysis and Porous Materials

Gold single atom catalysts (SACs) on CeO_2 represent a transformative breakthrough in oxidation catalysis, yet their deactivation mechanisms under liquid-phase conditions remain poorly understood. Although the Au–O–Ce–Ov (oxygen vacancies) interface is widely recognised as the active site, its stability is compromised by the reduction of Au to metallic Au via sintering, which is possibly reversible base on my current research. Recently, I developed a series of $Au/CeO_2/SiO_2$ SACs that exhibit significant differences in activity for industrially important alcohol selective oxidation, even though they possess identical surface oxygen vacancy concentrations on ceria and similar levels of cationic gold. My preliminary studies reveal that the accessibility of oxygen vacancies, rather than their mere concentration, plays a critical role in dictating the stability of Au SACs. Investigating the true interactions between Au and Ce is crucial for understanding their impact on catalytic activity

Poster 19

Towards Controlling Protein Self Assembly with Biological Ions

Deva Krisna Kadarani and Dr Robin Curtis

Theme: Biochemical and Bioprocess Engineering

Protein self-assembly significantly influences protein stability in both cellular and therapeutic systems. Multivalent biological ions, particularly adenosine triphosphate (ATP), have emerged as potential modulators of protein self-assembly, often attributed to interactions involving the adenine moiety. However, recent research comparing ATP with sodium tripolyphosphate (TPP) using lysozyme models at neutral pH suggests phosphate groups predominantly mediate self-assembly.

This study explores lysozyme behaviour at pH 5, demonstrating similar phase transition patterns induced by ATP and TPP, although ATP promotes more substantial precipitation. Zeta potential measurements indicate both ATP and TPP reverse the lysozyme surface charge from positive to negative, with ATP producing a notably stronger negative charge, reflecting enhanced electrostatic interactions. Correspondingly, the negative values of protein-protein interaction (kD) parameters and second virial coefficient (B_{22}) confirm attractive protein interactions in solutions containing ATP and TPP.

Melting temperature (Tm) analysis further supports the superior affinity of ATP towards native lysozyme conformations, evidenced by higher Tm values compared to TPP. ATP and TPP display similar affinity to lysozyme at pH 7 suggesting that the enhanced affinity of ATP at pH 5 is due to interactions with protonated histidine ($pK_a \sim 6.0$), through pi-cation interactions, and $\pi - \pi$ stacking. The strong binding underscores ATP's distinct role in protein stabilization at acidic conditions.

Poster 20

Examination of Environmental Sustainability and Circularity in Existing and Emerging Electronics

Saumya Kumar , Dr Judith Apsley and Dr Laurence Stamford

Theme: Sustainable Industrial Systems

The growing consumption of electronic devices has led to unprecedented levels of electronic waste (e-waste), creating significant environmental challenges. Addressing these issues is critical to reducing resource depletion, minimizing environmental impacts, and advancing the transition towards a circular economy. Life Cycle Gap Analysis (LCGA) is an interpretation method which builds on Life Cycle Assessment (LCA) to identify environmental losses called "lifecycle gaps" by comparing the impacts of production with the benefits of end-of- life (EoL) recycling. While LCGA highlights limitations in current recycling practices, this research expands the framework by incorporating lifecycle extension strategies such as repair, refurbishment, and reuse. These approaches delay EoL, reduce demand for new production, and lower emissions associated with raw material extraction and manufacturing. The adapted LCGA method aims to quantify environmental savings from extended product lifespans, offering a more complete view of circular economy pathways. Preliminary LCA modelling comparing pyrometallurgical and hydrometallurgical recycling of printed circuit boards shows that pyrometallurgy results in 21% lower climate impacts per kilogram of gold recovered. Although lifecycle extension can delay disposal, efficient recycling will remain essential. Future work will apply the adapted LCGA to assess both lifecycle extension and recycling, informing sustainable e-waste management and supporting global sustainability goals.

Poster 21

Synthesis and Characterization of Pt/rGO Composites as Electrocatalysts in PEMFC Presenting Improved Durability

Wei Liu and Prof Stuart Holmes

Theme: Catalysis and Porous Materials

Catalysts are a vital part of the fuel cell but have limitations in terms of durability and cost. Particle growth and detachment of catalysts are common causes of less satisfactory stability performance of the fuel cell. And noble metals like platinum are expensive, taking up over 40% of the total cost of the PEMFC. Generally, the Pt based catalysts are prepared by reducing the precursor with certain reductants like $NaBH_4$ and ethylene glycol, increasing the overall cost. Based on the theory of galvanic displacement, the Pt(II) precursor can be reduced with the substrate serving as the source of electrons. No external reductant is added. Here an innovative method has been established to deposit Pt nanoparticles on the reduced graphene oxide (rGO) via the galvanic displacement. The rGO acts as the substate and the source of electrons at the same time. Both XRD peaks and SEM images prove the successful reduction and the existence of Pt particles. Benefiting from the strong interaction between rGO and the precursor, the Pt/rGO composites are expected to be durable electrocatalysts in proton exchange membrane fuel cells (PEMFCs).

Poster 22

Isopropanol-Acetone-Hydrogen chemical heat pumps for improved heat recovery from geothermal resources, A case study in China

Zhengguang Liu and Dr Masoud Babaei

Theme: Subsurface energy systems

This study focuses on geothermal energy utilization through multi-objective optimization of Isopropanol-Acetone-Hydrogen chemical heat pump (IAH-CHP). In this paper, IAH-CHP coupled with medium-low temperature geothermal heat source simulation was constructed. China, the world's largest carbon emitter, was used as a case study to highlight environmental benefits. Comparative analysis was conducted between carbon emissions and investment of chemical heat pumps with other common heating equipment in different buildings. The results show IAH-CHP system has higher initial investment costs, however, their CO_2 emissions are significantly lower. The results of multi-objective analysis demonstrate the system can operate under a Pareto (multi-objective) optimal scheme. Under this plan, the levelized cost of heat (LCOH) is only 0.12 USD/kJ, and the carbon emissions are as low as 4.97 tons/year with a coefficient of performance (COP) of 7.4. Compared with a single-objective optimal solution, 8.12 tons of carbon emissions and LCOH of 0.15 USD/kJ could be achieved. Applying IAH-CHP system to China to replace original coal-fired heating solution can achieve annual carbon emission reduction of more than 5 million tons in areas with medium and low temperature heat sources.

Poster 23

Simulation of Post-Combustion CO Capture Using Piperazine Solutions

Zehua Liu and Dr Jie Li

Theme: Process Integration

Post-combustion carbon capture (PCC) is essential for reducing CO emissions from industrial flue gases, playing a key role in retrofitting existing facilities. The conventional approach employs absorption-stripping columns with circulating monoethanolamine (MEA) solutions to separate CO_2. Although widely used, MEA has limitations such as corrosiveness, volatility, and thermal degradation, which have driven the exploration of alternative solvents like piperazine (PZ).

This study presents a simulation of a PZ-based PCC process using Aspen Plus V12.1. Thermodynamic equilibrium constants and reaction kinetics were determined and validated against experimental data. Models were developed for standalone absorbers, standalone strippers, and integrated closed-loop systems. Validation was conducted using pilot plant data reported in the literature.

The mean absolute percentage error (MAPE) was used to assess model accuracy. In standalone stripper simulations, the MAPE for key variables ranged from 0.9% to 3.5%, with an overall MAPE of 2.4%. In closed-loop simulations across 14 case studies, the system achieved a minimum energy consumption of 3.86 MJ/kg CO_2 with a MAPE of 2%, demonstrating both high accuracy and promising energy performance. This work offers valuable insights into amine-based carbon capture processes and establishes a foundation for future simulation and optimisation of CO_2 conversion technologies

Poster 24

Performance prediction of Solid Oxide Cells (SOC) by ex-situ characterisation of electrodes and physical modelling

Mohammadhadi Mohammadi , Dr Masoud Babaei, and Prof Konstantinos Theodoropoulos

Theme: Catalysis and Porous Materials

Achieving the full potential of hydrogen energy requires the use of highly efficient devices for its production and consumption. In-situ and ex-situ characterisation techniques can be applied to differentiate effective designs from less efficient ones. In-situ methods assess cells during operation, while ex-situ techniques analyse individual components. Complementing these techniques, physical modelling aids in understanding cell phenomena and predicting performance. However, models in the literature often require parameter tuning. The robustness of these models improves as more parameters are independently defined. Yet, destructive tests and advanced facilities can only determine some key morphological parameters. This study enhances the characterisation of SOCs. First, a comprehensive dataset of microstructures is generated by the Plurigaussian method, and their morphological parameters are evaluated. Next, a surrogate model is trained to estimate triple phase boundary density and tortuosities from electrode composition and average pore/particle radius. Finally, a physical model is employed to predict cell performance. Results indicate that the ion volume fraction significantly impacts the cell performance. Additionally, reducing particle sizes, especially electron-conductive particles, enhances cell performance by increasing TPB density. An electrode design with finer electron-conductive particles and composition of 60% ion and 20% electron volume fractions can notably improve SOC.

Poster 25

Environmental sustainability assessment of graphene production methods

Shivani Pandit , Prof William W. Sampson, and Dr Rosa M Cuéllar-Franca

Theme: Sustainable Industrial Systems

Graphene, a 2-D material with exceptional properties that surpass those of existing materials, has garnered attention for its potential applications across various industries. The use of graphene can support climate change mitigation solutions by advancing sustainable materials and energy-efficient technologies. This necessitates the development of scalable production methods for large-scale implementation. With increased demand, and the emergence of novel preparation methods of graphene, it is paramount that sustainability aspects be considered at early design stages. Environmental sustainability tools such as life cycle assessment (LCA) can be employed to assess and compare the performance of graphene production methods to understand opportunities for improvement that can lead to more sustainable production practices. However, there are limited LCA studies reported in literature providing insights into the environmental impacts associated with graphene production at large-scale. Using few-layer graphene (FLG) as a representative type of graphene, due to its widespread applications across high-impact industries including concrete, composites, and energy storage, this project aims to compare 'traditional' top-down and novel bottom-up production methods from 'cradle to gate'. This is to identify key environmental hotspots within the selected methods, providing a basis for more sustainable decision-making and optimisation strategies in the development of advanced materials and technologies.

Poster 26

Optimising mRNA therapeutics to enhance mRNA uptake into HEK293 cells

Maariya Rachid Daud and Prof Alan Dickson

Theme: Biochemical and Bioprocess Engineering

Messenger RNA, also known as mRNA, is a single-stranded ribonucleic acid molecule synthesised in the nucleus during transcription. mRNA therapeutics exploit this mechanism by using the host cell's machinery to elicit an immune response. Even though, this process has shown to have promising results, there are still many unknown areas of research. The aim of this project focuses on optimising mRNA therapeutics in mammalian cells. The research that I am currently undertaking involves looking at the uptake of different EGFP mRNA constructs into HEK293 cells. To identify the optimum conditions during the transfection of mRNA different amounts of lipofectamine reagents, different concentrations of mRNA and different time points post transfection were tested using a plate reader. After conducting a thorough analysis, I was able to determine that EGFP fluoresced the highest 48 hours post transfection when transfected with 0.15μl of Lipofectamine MessengerMax. These conditions provided the basis for upscaling experiments to conduct flow cytometry, qPCR and a western blot analysis. The optimisation of the transfection of EGFP mRNA into cells is critical for future research and scientific advancements as it will contribute into improving the efficiency and scalability of mRNA-based therapies including vaccines and gene therapies.

Poster 27

Life Cycle Assessment of Multi-stage Flash Distillation (MSFD) Desalination with Various Potential Energy Sources in Indonesia

Dian Rahmawati , Dr. Harish Jeswani and Prof. Adisa Azapagic

Theme: Sustainable Industrial Systems

Water scarcity is one of the significant world concerns, and freshwater is less than 3% of all water available on earth. Most is locked in glaciers and ice caps, while 30% is groundwater, and only 1% is available on the Earth's surface. Even though groundwater is easily extracted and treated, excessive groundwater extraction causes land subsidence and saltwater intrusion. In Indonesia, several locations experience land subsidence and saltwater intrusion at 3 to 50 m/year rates. The desalination process by multi-stage flash distillation (MSFD) to produce freshwater from seawater can be an option to reduce the dependency on groundwater and surface water. However, no study has evaluated the environmental impact of MSFD, especially in tropical regions. Therefore, this study performs a life cycle assessment of MSFD with various energy sources available in Indonesia. The result shows that MSFD with waste heat as a thermal energy source has the lowest environmental impacts. When waste heat is not enough/available, biogas can be the first option, followed by wood chips. However, several measures should be taken to mitigate the environmental impacts. If solar energy is used, a combination with biogas is preferred over a combination with the current electricity grid.

Poster 28

The Effect of Mixing on the Evolution of Particle Size Distribution of Batch Cooling Crystallization Processes

Kimiya Ramezani , Dr Claudio P. Fonte, and Dr Ashwin Kumar Rajagopalan

Theme: Process Integration

Crystallization is a widely used separation and purification technique in the fine chemical industry to obtain pure solid products. However, designing a reproducible crystallization process remains challenging due to complexities associated with scale-up and crystallizer hydrodynamics. Conventionally, crystallizers are assumed to be perfectly mixed, with uniform liquid and solid phase properties. In reality, they operate under turbulent flow, where spatial variations in turbulence significantly influence key crystallization mechanisms, such as secondary nucleation, ultimately affecting product characteristics. Thus, to improve accuracy and predictability, models must incorporate relevant crystallization physics, including hydrodynamics[1,2]. This study examines the effect of mixing on batch cooling crystallization, a common industrial process. While approaches combining population balance equations (PBE) with computational fluid dynamics (CFD) exist, their use in process design is limited due to the high computational cost of solving PBEs on fine grids[3]. To address this, we develop a hybrid framework coupling CFD with a compartmental modelling approach for solving the PBEs. The framework is automated, robust, and computationally efficient for industrial-scale design. Turbulent flow is modelled using RANS equations in OpenFOAM to capture flow patterns, energy dissipation, and temperature. Compartments are defined using clustering algorithms and PBEs are solved using an in-house solver. Computational experiments highlight the effects of non-uniform mixing on crystallization outcome.

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Poster 29

Novel Approaches to Lithium Isotope Enrichment to Support the Development of Nuclear Fusion Reactors

Jacob Russell and Dr Kathryn George

Theme: Advanced Functional Materials

Nuclear fusion power is a promising avenue for next-generation carbon-free energy production. In terms of fusion energy generation in the coming decades, the dominant fuel mix will be deuterium (D) and tritium (T). Deuterium is relatively easy to acquire and is done regularly. Tritium, however, is incredibly rare, naturally occurring at around 1 atom in every 10^{18} atoms of hydrogen. Additionally, with a half-life of 12 years, tritium is also difficult to stockpile, and hence an alternative source of tritium is required.

The two naturally occurring isotopes of lithium, ^{6}Li (7.5% natural abundance) and ^{7}Li (92.5% natural abundance), can both produce tritium, but the energetics are different. For the preferential breeding of tritium in a fusion power plant, ^{6}Li is the preferred isotope. Solvent extraction via crown ether complexation has been proposed as a method to enrich the ^{6}Li isotope from natural abundance.

This poster presents and compares a number of methods of lithium enrichment in terms of both distribution (D) and isotope enrichment per stage (α). Additionally, analytical techniques used throughout are discussed, compared and contrasted: Inductively Coupled Plasma Mass Spectrometry (ICP-MS), Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) and X-ray Fluorescence Spectroscopy (XRF).

Poster 30

Discrete Particle Model (DPM) of Air-Water Behaviour in Gas Channel PEM Fuel Cell

Mahtab Shahrzadi and Prof. Vahid Niasar

Theme: Catalysis and Porous Materials

CO_2 emissions significantly contribute to global warming and climate change, causing serious problems. Therefore, many countries have pledged to achieve net zero emissions. Reaching this target needs a fundamental attention to energy production strategies, including a substantial increase in the use of renewable energy sources. However, the availability of these sources can fluctuate throughout the year. Hydrogen production from renewable sources, provide a perfect solution, as it can be converted into electricity using fuel cells. PEM fuel cell is an electrochemical device that converts energy stored in hydrogen into electrical energy while producing water and heat as by-products. Therefore, water management plays a decisive role in fuel cells. Due to high computational demand nature of CFD approaches, they may not be ideal for industrial applications. In this study, a simplified gas channel is analysed using discrete-particle model, which reduces computational cost while maintaining acceptable accuracy. Mass conservation equations for water and air, and force balance equations for droplets are considered. A more accurate adhesion force calculation is also implemented, further improving the model's reliability. This study examines the effect of key parameters on water management, including the effect of different GDL contact angle, Reynolds number, pore density and pore diameter.

Poster 31

Water Management Challenges in Low-Temperature PEM Fuel Cells: Implications for Catalyst Development

Yuebo Shen and Prof Stuart Holmes

Theme: Advanced Functional Materials

In low-temperature proton exchange membrane fuel cells (LT-PEMFCs), water management plays a crucial yet often underestimated role in determining system performance and catalyst efficiency. This project explores the interdependence between water transport dynamics and cathode catalyst design, with particular attention to flooding and dehydration phenomena under varying operating conditions. Early-stage investigation has revealed that untreated membrane and non-optimized gas diffusion layers can severely distort electrochemical readings and hide intrinsic catalyst activity. These insights have led to a re-evaluation of testing procedures and system baselines. While long-term goals focus on the design of structured Pt-based nanocatalysts for enhanced ORR performance, current efforts aim to establish a more reliable and controllable environment for catalyst screening. This work forms part of an ongoing study towards balancing material functionality, electrochemical accessibility, and system-level stability in LT-PEMFC applications.

Poster 32

Enhanced Digital Rock Image Super-Resolution Using SR-CBAM-GAN: A Novel Attention-Based Approach

Sonu Sudhikumar Seena and Dr Lin Ma

Theme: Multi-scale modelling

Digital rock imaging is essential for characterizing porous media properties, yet achieving high-resolution imaging at representative scales remains challenging. This study introduces SR-CBAM-GAN, a novel super-resolution framework integrating Convolutional Block Attention Module (CBAM) with Generative Adversarial Networks (GANs) for digital rock image enhancement. The architecture implements dual-pathway attention mechanisms that selectively emphasize geological features during super-resolution. Our framework was evaluated on high-resolution micro-CT sandstone scans (1792 × 1792 pixels, 4.73 μm resolution) from the National X-ray CT Facility at the University of Manchester. Synthetic low-resolution images (448 × 448 pixels, 18.92 μm) were created through 4× downsampling. Quantitative analysis shows SR-CBAM-GAN achieves superior performance with PSNR (39.05 dB), SSIM (0.9691), and normalized cross-correlation (0.9698), representing improvements of 18% in PSNR and 26.2% in SSIM over conventional methods. Comparative analysis against ESRGAN, HAT, and SRGAN confirms that SR-CBAM-GAN offers enhanced preservation of critical geological features. The generator's integrated CBAM modules enable effective feature detection, while the discriminator's cascading CBAM blocks maintain geological authenticity. This research provides a foundation for more accurate petrophysical analysis by enabling superior recovery of sub-voxel microstructural features essential for reservoir characterization.

Poster 33

Multi-region simulation of all vanadium redox flow battery (VRFB) using OpenFOAM: modeling of free flow, porous electrode, membrane regions

Yiqi Sun and Prof Vahid J Niasar

Theme: Multi-scale modelling

Vanadium redox flow batteries (VRFBs) represent a promising technology for large-scale energy storage due to their independent scaling of power and energy capacity, exceptional cycle life, and high efficiency. Computational fluid dynamics (CFD) simulations enable the coupling of multiple regions and multiphysics fields, allowing for simulation of electrochemical and transport phenomena through various parameter settings and flow field designs, thereby significantly enhancing VRFB development. This study presents a comprehensive three-dimensional computational framework for VRFBs using OpenFOAM, implementing a multi-region approach that couples free flow channels, porous electrodes, and membrane regions. The framework addresses cross-regional coupling work in VRFB simulation by developing internal coupling interfaces conditions. We implemented a basic pressure-velocity coupling between channel and porous electrode regions based on the Beavers-Joseph condition and developed initial species transport methods intended to maintain flux continuity across regions. The current model includes simplified representations of convection and diffusion processes and shows good results when compared with selected experimental data. Preliminary simulations provide insights into velocity profiles, pressure distributions, and species transport behaviors. This early-stage computational framework represents confirmation of the feasibility of the model, though further refinement is needed.

Poster 34

Effects of ATP and TPP on Protein-Protein Interactions and Aggregation of rHSA

Shuyuan Tan and Dr. Robin Curtis

Theme: Biochemical and Bioprocess Engineering

Overcharging of proteins by polyvalent anions such as adenosine tripolyphosphate (ATP) and tripolyphosphate (TPP) is an emerging strategy to modulate protein-protein interactions and enhance colloidal stability. However, the underlying mechanisms remain poorly understood. Here, we investigated the effects of ATP and TPP on recombinant human serum albumin (rHSA) under mildly acidic conditions. Zeta potential measurements revealed increased negative net charge on rHSA, indicating overcharging via non-specific electrostatic interactions. Static light scattering (SLS) showed that both anions increase the osmotic second virial coefficient (B_{22}), reflecting enhanced repulsive interactions at low ionic strength. Small-angle X-ray scattering (SAXS) provided effective structure factors (Seff) as a function of scattering vector q, revealing long-range repulsions beyond classical DLVO predictions. Dynamic light scattering (DLS) thermal ramp experiments demonstrated that ATP and TPP elevate the aggregation onset temperature (Tagg), indicating suppressed heat-induced aggregation. Differential scanning fluorimetry (DSF) showed that TPP increases the melting temperature (Tm) at low concentrations due to surface binding, while a slight decrease at higher concentrations suggests additional binding to the unfolded state, indicating a dual mechanism of conformational stabilization. Together, these findings show that polyvalent anions enhance protein colloidal and conformational stability via overcharging, providing insights for stable protein formulation in biopharmaceuticals.

Poster 35

Slipping flow of yield stress fluids in planar porous media

William Tran and Dr Claudio Pereira da fonte

Theme: Multi-scale modelling

Flows of yield-stress fluids through porous media are important to practical applications in many sectors, including energy, environmental engineering, and biomedical sciences. However, despite their importance, the effect of confinement and complex geometry on flow behaviour remains poorly understood, with wall slip and dead zone formation presenting significant challenges when modelling fluid flow. Numerical models have recently been developed for two-dimensional domains, but there remains a severe lack of experimental validation. In this work, we investigate experimentally the pressure drop and velocity distributions of a Carbopol microgel flowing through model planar porous media of varying porosities, which consist of microfluidic Hele-Shaw channels partially occluded with randomly distributed cylindrical pillars.

Experiments were conducted at a range of flow rates using viscoplastic fluids with different yield stress values, under slip and no-slip conditions. Wall slip was controlled by altering the construction material and wall-surface roughness of the microfluidic devices. Velocity distributions were obtained using Particle Tracking Velocimetry of top-view images. We find that the predictions of a two-dimensional network model of the flow do not capture the measured pressure and velocity distributions in the experimental planar porous medium, because it does not account for the effect of confinement from the top and bottom walls. We extend the two-dimensional network model by modelling the pore throats as cylindrical pipes through the use of a hydraulic diameter and achieve promising agreement with experimental data for both the slip and no-slip cases. We investigate the conditions for which this quasi-three-dimensional network model can predict flow channelisation corresponding to paths of least resistance for the no-slip case, enabling the identification of dead zones in the planar porous medium.

Poster 36

Robust Modelling and Optimization of Microalgal Systems for Bioplastics Production

Konstantina Tsafara and Prof. Konstantinos Theodoropoulos

Theme: Biochemical and Bioprocess Engineering

The environmental impact of plastic waste has driven the search for sustainable alternatives, such as polyhydroxybutyrate (PHB), a biodegradable bioplastic produced by microorganisms. Cyanobacteria represent a promising platform for PHB production due to their autotrophic growth, low nutrient requirements, and potential for multi-product generation supporting biorefinery applications. This project investigates PHB production in both cyanobacterial monocultures and co-culture systems with heterotrophic bacteria, aiming to enhance PHB productivity through experimental and modeling approaches. Biomass growth and PHB accumulation will be studied under nitrogen and phosphorus co-limitation, alongside co-product generation. A comprehensive kinetic model will be developed and calibrated using a combination of genetic algorithms and deterministic optimization. To account for data variability and improve model robustness, optimization under uncertainty methodologies will be employed, while structural and practical identifiability analyses will be conducted to ensure reliable parameter estimation. Co-cultivation will be explored as a strategy to exploit synergistic microbial interactions and enhance overall process efficiency. Modeling of interspecies dynamics will inform the design of optimized co-culture protocols. The outcomes are expected to advance modeling and optimization methodologies and contribute to the development of improved cultivation strategies for economically and environmentally sustainable PHB production.

Poster 37

One-pot conversion of fructose to 5-HMF over sulfonated mesoporous silica

Hao Wang and Dr. Carmine D'Agostino

Theme: Catalysis and Porous Materials

In response to the global socioeconomic crisis of crude oil, biomass energy is particularly promising as a green, cheap and renewable carbon source. The conversion of lignocellulosic biomass to 5-hydroxymethylfurfural (HMF), a versatile biomass-derived platform compound to produce hundreds of value-added chemicals which is also listed as one of the top 10 platform chemicals by the U.S. Department of Energy, is of great research interest. This project focuses on the design and synthesis of mesoporous silica supports featuring tunable hydrophobic pore environments and high specific surface areas to facilitate rapid molecular diffusion and maximize accessible active sites. Post-synthetic grafting of sulfonic acid moieties onto the silica framework will generate robust Brønsted acid sites, tailored to promote efficient fructose dehydration in aqueous media. Through systematic optimization of pore hydrophobicity, acid loading, and reaction conditions, the study aims to achieve high HMF selectivity and yield under mild, water-based reaction conditions, thereby advancing biomass-derived chemical production toward practical, green-chemistry applications.

Poster 38

Assessing Inorganic Additives' Role in Deactivating Polymer Hydrocracking Catalysts

Hubertus Warsahartana , Thomas Scott, Dr Edidiong Asuquo, Dr Stephen Edmondson, Dr Christopher Parlett, abd Prof Arthur Garforth1

Theme: Catalysis and Porous Materials

From the comfort of modern textiles, to the protection of sterile equipment in hospitals, plastics play an essential role in modern life. Despite their prevalence, little thought has been given to reclaiming used plastics, and a majority of plastic products end up in landfill. The mechanical recycling industry is growing, but there are limitations to its product quality. Hydrocracking promises a chemical recycling route for mixed plastic waste, converting polymers into fuels and high-value chemicals under moderate conditions (200-380°C, 10-20 bar H_2) using bifunctional metal-acid catalysts. However, post-consumer plastics often contain inorganic additives that can deactivate these catalysts, undermining process efficiency and economic viability.

In this initial study, real plastic wastes (20 g of mixed polyolefins) from mechanical recyclers containing an abundance of heteroatoms (e.g. $CaCO_3$, $Mg_3Si_4O_{10}(OH)_2$, TiO_2, Fe_2O_3) will be converted over a Pt-ZFC (Pt-zeolite formulated catalyst) and H_2 (20 bar at room temperature) in a 300 ml autoclave batch reactor at 360°C. Two experimental campaigns were conducted: Campaign 1 involved hydrocracking of virgin PP, while Campaign 2 used post-consumer plastic waste supplied by Recycle For Future (RFF, Peterborough, UK). For feedstock characterisation, thermal techniques, namely, DSC was conducted to identify the polymers present, while TGA and ashing was done to quantify inorganics and decomposition temperatures. Hydrocracking product distributions were analysed to assess variations in hydrocarbon chain length and cracking behaviour, using GC-MS for liquids, GC-FID for gases, and TGA for solid residue analysis. Catalyst performance was monitored across sequential reaction cycles to evaluate deactivation and fouling, with XRF employed to quantify elemental deposition on the spent catalyst.

Poster 39

High cooperative proton conduction between water and imidazole in an aluminium-based Metal-Organic framework

Yuhang Yang , Prof Sihai Yang and Dr Daniel Lee

Theme: Catalysis and Porous Materials

Proton conductor material plays an important role in the electrochemical energy transfer and storage field. However, the traditional Nafion, which is high-cost, can only work in limited service conditions and cause difficulty in studying mechanisms due to the non-crystalline structure. This paper proposes a novel proton conductor material, Im-MIL-96, based on a metal-organic framework (MOF). Imidazole molecules are anchored to the metal nodes of aluminium-based MOF, MIL-96(Al), by a chemical coordination strategy, which realizes the cooperative optimization of structural stability and proton conductivity. Al-N coordination bonds fixed Imidazole to open Al sites without changing the framework. The proton conductivity Im-MIL-96 (Al) at 90 and 90% relative humidity reaches 2.47×10^{-2} S/cm, comparable to Nafion. Electrochemical impedance spectroscopy, activation energy analysis (Ea=0.87 eV) and solid-state NMR confirm that proton conduction mainly follows the Vehicle mechanism and depends on the synergistic effect of anchored imidazole with dynamic water molecules. In addition, the material maintained a conductivity of 10^{-2} S/cm during 20 hours of continuous testing, demonstrating excellent stability. This study provides a new strategy for the development of efficient and stable MOF matrix conductors.

Poster 40

Deep Learning-Enabled Forecasting of Chemical Looping Processes

Vladislav Žurba and Vincenzo Spallina

Theme: Process Integration

Cyclic processes like chemical looping do not have a normal steady state and therefore require dynamic optimization methods to achieve best performance. One option is to use algebraic, PDE-based models of the process and optimize them. Such models are accurate and powerful, but have a high computational cost. Substitute models based on deep learning methods are proposed in this work and shown to be at least 30 times faster than algebraic while maintaining acceptable accuracy. Training data was obtained from a validated algebraic model implemented in Aspen Custom Modeler. Two different architectures were used to develop the surrogate models — LSTM and Transformers. Direct forecasting, i.e. simultaneous prediction of multiple future timesteps was used due to it's stability and long-term forecasting potential. The Transfomer-based model performed better on most metrics, including accuracy and inference speed. This is directly relevant for improvement of optimal control strategies for chemical looping and other dynamic processes. Additionally, the Transfomer-based model is agnostic towards the number of variables, rendering it much more generalizable compared to the LSTM approach.

Poster 41

Graphene Oxide-based Membranes for Arsenic Removal

Sneha Thomas and Prof Rahul R Nair

Theme: Advanced Functional Materials

In this work, a novel graphene oxide (PGO) nanofiltration membrane was prepared to selectively remove both As(V) and As(III) from water. Our novel coating methodology incorporates polymer in GO membrane through in-situ polymerization during membrane formation. The resulting nanofiltration (NF) membrane exhibits high structural stability and $> 95\%$ long-term arsenic rejection performance. In addition, the membrane maintains performance across a wide pH and pressure range and works in the presence of other heavy metal contaminants. Through the incorporation of polymer, not only has the interlayer spacing of graphene oxide (GO) nanosheets been appropriately regulated but also an improved anti-swelling property has been achieved. The dosage of GO, reaction time with polymer, and mass ratio of polymer to GO have been optimized to achieve a high-performance membrane. Arsenic concentration in ground water is predominantly in ppb levels, and our membrane exhibits excellent arsenic removal performance in varying concentration ranges till 1000 ppb. The resultant PGO membrane has exhibited excellent long-term stability and maintains a steady arsenic rejection which brings down the permeate arsenic concentration always below the specified WHO limit of 10 ppb. Moreover, the rejection mechanism of the PGO membrane is a synergistic effect of charge repulsion and size exclusion which is confirmed by zeta potential and molecular weight cutoff measurements. Results have indicated that PGO could be considered as a promising candidate for simultaneous and selective filtration of As(V) and As(III).

Poster 42

Unveiling the Interplay Between Morphological Crystallisation Process Models and Data

Mohammad Yousuf Zaman , Giovanni Maria Maggioni, and Dr Ashwin Kumar Rajagopalan

Theme: Multi-scale modelling

Mathematical models are essential for understanding, designing, and optimising complex processes. However, a model is only as good as its data; poor-quality or insufficient data leads to non-identifiable models, where parameters cannot be uniquely determined from observations. This results in ill-posed models with high parameter uncertainty, limiting their predictability and practical applicability. Crystallisation, a key purification-separation step in pharmaceutical and agrochemical manufacturing, presents an ideal system to showcase the critical interplay between model and data. This is due to the presence of competing mechanisms (e.g., growth, nucleation, breakage) and challenges in accurately characterising both liquid and solid phases[1].

In this work, we systematically quantify the impact of data on model identifiability and its consequences on model reliability. In crystallisation, a process where the particle size and shape distribution (PSSD) affects product quality and process efficiency, we employ population balance equations (PBEs) to track its evolution with mass balance equations for the liquid phase, forming a system of integro-partial differential equation [2]. To study the influence of data, we simulated batch crystallisation using a PBE coupled with a digital twin that mimics process monitoring tools (e.g., Focused Beam Reflectance Measurement (FBRM), and single-projection imaging such as from microscope, particle vision measurement, or BlazeMetric probes). This approach reflects real-world data limitations while leveraging the digital twin to by-pass resource and time constraints, ensuring a practical and representative study. To investigate key issues related to identifiability and their underlying causes, we conducted a series of carefully selected case studies. Through profile likelihood analysis of the parameters, we examine how different experimental strategies af- fect identifiability and model robustness. Examples include how FBRM struggles to capture the shape of crystal populations, leading to high uncertainty in estimation of growth kinetics, and how single-projection imaging introduces noise, which we quantify through parameter confidence intervals. Additionally, we demonstrate actions to improve identifiability, such as optimising sampling frequency and selecting key experimental variables (e.g., seed mass and PSSD variance). These findings provide practical guidelines for enhancing the predictability and generalisability of crystallisation models[3].

This study highlights the critical role of data quality and experimental techniques in identifiability, offering guidelines to improve model performance. Using a digital twin, we assess the impact of real-world data limitations while avoiding resource constraints. These insights lay the foundation for designing efficient experiments that enhance the practicality and reliability of crystallisation models[1].

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