UNIVERSITY OF BIRMINGHAM | School of Chemical Engineering

ChemEngDayUK&I 2026

Abstract Book

Thursday 16th and Friday 17th April 2026

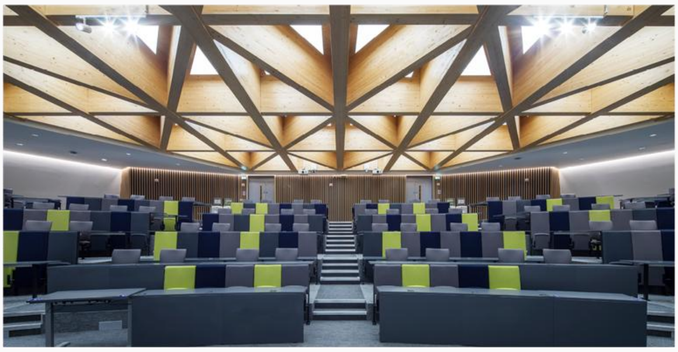
Teaching and Learning Building, University of Birmingham

Contents

About ChemEngDayUK&I 2026

ChemEngDayUK&I 2026 brings together chemical engineering students and educators, researchers and industrialists to discuss advances in chemical engineering research, technology and education. This annual event is proudly hosted in 2026 by the School of Chemical Engineering at the University of Birmingham.

The event features special sessions on Education, Diversity and Inclusion / Athena Swan, AI in the process industries and careers, with invited speakers. Two distinguished plenary speakers further enhance the main conference programme.



Sponsors

Founded in 2001, the Centre for Doctoral Training (CDT) in Formulation Engineering is the longest running CDT in the UK, having been funded by EPSRC through five consecutive grants.

The Centre for Doctoral Training works with Partners from a range of Formulation Industries, including leading food, personal care, pharma and fine chemicals companies, as well as experts in new medicines and therapies. Pioneering the concepts of Formulation Engineering in the UK, the CDT won the University a Queen's Anniversary Prize 'for excellence in Formulation Engineering' in 2011.

The CDT aims to be a world-leading provider of research and training, equipping graduates with the skills needed to manufacture the next generation of sustainable formulated products, spanning numerous industry sectors.

CDT in Formulation Engineering - University of Birmingham

Through their headquarters in Hamburg and UK office in Hampshire, GUNT engineers develop, manufacture, and supply didactic equipment that is designed specifically for teaching in universities, colleges, technical and vocational schools. This gives students a hands-on practical approach to help understand even the most complex principles.

In addition to its broad range of equipment, GUNT has developed innovative tutorial software and web-based E-learning modules, these form a comprehensive range of teaching materials and videos to assist both student and teacher.

Combined with augmented reality, digital acquisition of test results and network capability, multiple users can access real-time data, all of which are designed to complement GUNT’s product range and to meet Industry 4.0 criteria

IChemE

Founded in 1922, the Institution of Chemical Engineers (IChemE) is the UK based and internationally recognised qualifying body and learned society for chemical, biochemical and process *engineers. We exist to advance chemical engineering's contribution for the benefit of society. IChemE is the professional home for over 32,000 members worldwide.*

NETZSCH

Proven Excellence.

Wielding over 60 years of experience, NETZSCH Analyzing & Testing provides top-of-the-line customized solutions in thermal analysis, rheology, the determination of thermophysical properties, and fire testing. Our representative offices around the globe, along with our large subsidiaries in China, Japan, the USA, and Korea, allow us to deliver our unparalleled service and support to customers in academia, industry, and materials testing worldwide.

Used in the fields of polymers, life sciences, energy solutions and electronics – as well as in high-temperature applications such as glass, ceramics, metals, alloys, building materials and inorganics – the instrumentation in our comprehensive portfolio is developed and manufactured in-house, in deliberate collaboration with our customers to ensure their utmost satisfaction.

Technical excellence, innovative technology, uncompromising quality standards and first-rate software make us to one of the world's leading manufacturers in our trade, with exceptional service offerings rounding out our unsurpassed reputation.

For first-class instrumentation and expert service, look no further.
We've got you covered.
NETZSCH.

Surface Measurement Systems
World Leader in Sorption Science

At Surface Measurement Systems, we specialize in the development and engineering of advanced instrumentations and innovative experimental techniques for the physico-chemical characterization of complex solids.

With over 30 years' experience in the field, we have developed a range of groundbreaking gravimetric sorption analyzers that are favored by sorption researchers across the globe. Offering world-class technical & scientific support to our customers, we are always pushing the boundaries of what is possible in sorption science.

Programme

Thursday 16 April 2026

Time	Session	Location
09:00 - 09:45	**Registration and Refreshments**	**Atrium**
09:45 - 10:00	**Welcome & Opening Remarks**	Lecture Theatre 1 (LG18)
10:00 - 10:45	**Plenary Speaker - Marianne Ellis** Session Chair - Liam Grover	Lecture Theatre 1 (LG18)
10:45 - 11:45	**Bioprocessing and Biotechnology** (15 minutes each) **O1 – Simon Attwood** - Process intensification through design: digitally manufacturing biocatalytic reaction systems **O2 - Alexander Brooks** - Identifying biofilm-forming conditions in probiotic bacteria **O3 - Zichen Fan** - Virus-Mimicking pH-Responsive Polymer-Functionalised Lipid Nanoparticles for Effective RNA Delivery and Enhanced Thermostability	Lecture Theatre 1 (LG18)

	O4 - Owen Thomas - Real-time Determination of Monoclonal Antibody Structure During Chromatography Session Chair: Patricia Perez Esteban	
10:45 - 11:45	**Process Modelling, Reactions & Simulation** (15 minutes each) **O5 - Bara Anaya** - Process Compatible Modelling of Bubbling Fluidised Bed Gasifiers for Steam Oxygen Gasification of Waste to Fuel Systems **O6 - Freddie Barter** - A Novel Dimensionless Number for the Characterisation of Densification and Segregation in a Vibrationally Excited Granular System **O7 - Mostafa Delpisheh** - Toward offshore wind to green hydrogen: Multiphysics insights into rotation and magnetic-field induced electrolysis **O8 - Aiden Cranney** - Molecular Insights into Enzyme Selectivity for Terpene Alcohol Esterification in Flower Essential Oils Session Chair - Peter Fryer	Lecture Theatre 2 (102)
10:45 - 11:45	**Healthcare Technologies** (15 minutes each) **O9 - Ben Cassidy** - Development of biomimetic extracellular matrix coatings to improve tissue integration of arteriovenous grafts **010 - Ahsan Razaq** - PEG-based fluid gels for cellular microenvironments: tailoring chemistry and gelation mechanics via temperature and mixing	Room 211/212

	O11 - Dan Baiocco - Biocompatible electrophoretic ink microcapsules for on-skin interactive displays and sustainable healthcare applications **O12 - Shyam Rana** - Sustainable Terpene-Derived Polymers for Biofilm Prevention in Neonatal Intensive Care Session Chair - Richard Moakes	
11:45 - 13:45	**Lunch**	**Atrium**
11:45 - 12:45	**EPSRC Network Plus SUM4Products** Session Chair - Rosemary Dyson	Room 202
11:45 - 13:45	**HCE (iChemE) - Private Event** Session Chair - Liam Grover	Room 211/212
11:45 - 12:45	**Poster Presentations - Themes** • AI & Data Driven Studies • Formulation Engineering, Sustainable Manufacture & Materials • Healthcare Technologies *Odd poster numbers to be presented in this session	Rooms 118/119

11:45 - 12:45	**Poster Presentations - Themes** • Chemical Recycling of Polymers • Energy & Net Zero & LCA • Process Modelling, Reactions & Simulation • Education • Bioprocessing & Biotechnology *Odd poster numbers to be presented in this session	Rooms M208/M209
12:45 - 13:45	**Poster Presentations - Themes** • AI & Data Driven Studies • Formulation Engineering, Sustainable Manufacture & Materials • Healthcare Technologies *Even poster numbers to be presented in this session	Rooms 118/119
12:45 - 13:45	**Poster Presentations - Themes** • Chemical Recycling of Polymers • Energy & Net Zero & LCA • Process Modelling, Reactions & Simulation • Education	Rooms M208/M209

	- Bioprocessing & Biotechnology *Even poster numbers presented in this session	
12:45 - 13:45	**Publishing with Impact: Journals, Peer Review, and Editorial Pathways for Early Career Researchers Workshop**	Room 202
13:45 - 14:45	**Special Session: Chemical Engineering of Public Policy (IChemE)** Panel: **Ollie Folayan -** Institution of Chemical Engineers **Joan Cordiner -** Institution of Chemical Engineers **Peter Styring -** Great Britain Chemicals Centre **Parimala Shivaprasad -** GO Science Session Chair - Jonathan Radcliffe	Room 202
13:45 - 15:15	**Bioprocessing and Biotechnology** (15 minutes each) **O13 - You Cheng** - Scalable Production of Virus-Mimicking Polymer-Enveloped Lipid Nanoparticles for RNA Formulations with Enhanced Efficacy and Thermostability **O14 - Vinay Patel** - Studying The Viability of Termite Hydrogen Production for Renewable Energy **O15 - Angeliki Xyderou Malefaki** - Optimising Fig Peel Waste Phenolic Extraction through a Life Cycle and Cost-Analysis **O16 - Abraham Chacko** - From Microstructure to Bioeconomy: SEM–EDX	Lecture Theatre 1 (LG18)

	Characterisation of Nettle Leaves for Value-Added Applications **O17 - Sharon Velasquez Orta** - Second Generation Bioethanol and Bioelectricity Production- An Empirical and Economic Analysis **O18 - Parimala Shivaprasad** - Valorising UK’s horticulture waste: bio-based ingredients for the consumer goods sector Session Chair - Owen Thomas	
13:45 - 15:00	**Process Modelling, Reactions & Simulation** (15 minutes each) **O19 - Blessings Malimusi** - Numerical modelling of chlorine-mediated selectivity in direct seawater electrolysis **O20 - Sylvanus Lilonfe** - Integrated techno-economic, life cycle, and surrogate modelling for scaling production of bioplastic precursors **O21 - Jack Grogan** - Discrete element method study of the impact of vessel wall friction on the mixing dynamics of a resonant acoustic mixer **O22 - Luisa Attfield** - Assessing the Feasibility of a Drag Force Flow Sensor for the Inline Monitoring of High Shear Wet Granulation Using the Discrete Element Method (DEM) **O23 - Thabang Selalame** - Process modelling for bottom-up estimation of emissions from ethylene production in Europe Session Chair - Thomas Abadie	Lecture Theatre 2 (102)

13:45 - 15:15	**Special Session: EDI and Athena Swan** (20 minutes each) **Prof. Pangiota Angeli** - How to Get Athena Swan Gold **Dr Claudia Favero** - EDI Belonging Project & Toolkit **Dr. Holly Foss** - 100 Years of Women in Engineering Followed by a 30-minute panel discussion Session Chairs - Taghi Miri & Joe Wood	Room 211/212
15:00 - 15:15	**Sponsor Talk: Henry Heckmann,** GUNT Technology	Lecture Theatre 2 (102)
15:15 - 15:45	**Refreshments**	**Atrium**
15:45 - 16:45	**Bioprocessing and Biotechnology** (15 minutes each) **O24 - Sylvanus Lilonfe** - Sustainable production of rose oil terpene esters for fragrance applications: economic and environmental insights **O25 - Peace John-Banjo** - Green Extraction of Phenolic Compounds from Sea buckthorn (Hippophae rhamnoides) leaves **O26 - Yuting Han** - Valorisation of Brewers' Spent Yeast for Biodegradable and Active Food Packaging Films	Lecture Theatre 1 (LG18)

	O27 - Darlington Nnabodo - Activated Carbon Synthesis from Microalgae (Chlorella sp.) Session Chair - Yin Hoon Chew	
15:45 - 16:45	**Process Modelling, Reactions & Simulation** (15 minutes each) **O28 - Fawaz Alwarthan** - Co-processing of Bio-Based Fischer Tropsch Wax in an Industrial Hydrocracking Unit: A Pathway Toward Lower-Carbon Fuel Production **O29 - Charlie Brayson** - Multiphase CFD Modelling of a Calcination System Using OpenFOAM **O30 - Ali Rabeeah** - Boosting Chemical Looping Hydrogen Generation and CO2 Removal by Integrating with the Charcoal Gasification Process **O31 - Aran Klair** - Numerical Simulation and AI-Driven Geometry Optimisation of Cohesive Material Feeders Session Chair - Amin Rahmat	Lecture Theatre 2 (102)
15:45 - 16:45	**Education** (10 minutes each) **O32 - Luis Roman** - AI Developed MATLAB Apps for Enhanced Learning of Thermodynamics in Chemical Engineering **O33 - Mauryn Chika Nweke** - Exploring the feasibility of integrating personalised AI in project work and its impact on student learning and staff load in Biochemical Engineering	Room 211/212

	O34 - Eleni Routoula - Bridging the Digital Gap: Mapping Digitalisation Skills in Undergraduate Chemical Engineering Curricula **O35 - Abdul Wadood Sharif** - Smoke and Mirrors: A Grounded Theory of Chemical Engineering Students' Motivations and Perception of GenAI-Learning Followed by a 20-minute panel discussion Session Chair - Matt Keith	
16:45 - 17:15	**Refreshments**	**Atrium**
17:15 - 18:15	**Special Session: AI in Process industries** **Dominica D'Arcangelo and Alexandra Araujo Alvarez**, BridgeAI **Brian Liu**, Johnson Matthey Session Chair - Kit Windows Yule	Lecture Theatre 1 (LG18)
17:15 - 18:15	**Early careers: Sponsored special session** **Panel Discussion (Freya Barrett, Theodoros Papalas, William Ryden**, **Luisa Attfield)**	Lecture Theatre 2 (102)

17:15 - 18:15	**Education** (10 minutes each) **O36 - Hosam Aleem** - Labs 4.0: Redefining Chemical Engineering Laboratories **O37 - Rana Khalife** - Investigating the Usage of Labster and Its Future Implications for Industry and Academia **O38 - Michaela Pollock** - Embedding safety and sustainability in the capstone design project **O39 - Polina Yaseneva** - Seeing the Connections: Teaching Systems Thinking through SDG Network Visualization Followed by a 20minute panel discussion Session Chairs - Matt Keith and Phil Robbins	Room 211/212
18:15 - 21:00	**Social Event - Drinks Reception with Street Food**	**Atrium**

Friday 17 April 2026

Time	Session	Location
08:30 - 09:00	**Registration and Refreshments**	**Atrium**
09:00 - 09:45	**Plenary Speaker - Peter Styring** Session Chair - Sarah Walker	Lecture Theatre 1 (LG18)
09:45 - 10:15	**Refreshments**	**Atrium**
10:15 - 12:00	**Energy & Net Zero & LCA** (15 minutes each) **O40 - Idris Uthman** - Life Cycle Assessment of Low-Carbon Olefin Production from Waste Biomass via Methanol to Olefins with Carbon Capture and Storage **O41 - Israa Alghurabi** - Experimental Screening of Zeolite Adsorbents for CO_2 Capture Using Temperature Swing Adsorption (TSA) **O42 - Ijudigal Amtagu Birdling** - Enhanced CO_2 mineralisation using a biogenic Ni-HAp composite in a continuous plug flow reactor **O43 - Alexandra Brochoire** - Enhanced catalytic effect of chloride ions for iridium catalysts in proton exchange membrane water electrolysers	Lecture Theatre 1 (LG18)

	O44 - Maria Mourkou - Experimental study of green H2 production via photocatalytic ethanol dehydrogenation by Pt/CGCN in flat-plate reactor **O45 - Fahad Alajmi** - Ball Milling for Mechanical Valorisation of Asphaltene **O46 - Kenechukwu Ugonabo** - Enhancing CaO Based Thermochemical Energy Storage through Metal Oxide Doping Session Chair - Neha Mehta	
10:15 - 12:00	**Formulation Engineering, Sustainable Manufacture & Materials** (15 minutes each) **O47 - Lucie Hlubinková** - Effect of shear, cooling rate and composition on crystallisation of solid fabric enhancer **O48 - Zhentao Wu** - From Membranes to Transport-Integrated Porous Beads: Redesigning Diffusion in Chemical Engineering Materials **O49 - Evelyn Tait** - Plant protein textures through freeze structuring **O50 - Hiya Deshpande** - UK-India consortium for Bio-based chemicals and sustainable innovation: A case study **O51 - Sam Hare** - DEM Simulations of the dry mixing of NMC 622 lithium-ion battery cathodes **O52 - George Truc** - Bespoke High-resolution 3D particle tracking for a 21L Stirred Tank	Lecture Theatre 2 (102)

	O53 - Aled Williams - Power and Flow Analysis of a High Throughput Testing System for the Formulation of Lamellar Gel Networks Session Chair - Richard Greenwood	
10:15 - 12:00	**AI & Data Driven Studies** (15 minutes each) **O54 - Ali Tarik Karagoz** - When Data Augmentation Improves Metrics but Not Design Quality: Insights from AI-assisted Process Design **O55 - Daniel Rhymer** - Optimisation of the Granular Section of a Twin-Screw Extruder for Sustainable Plastic Processing **O56 - Arun Pankajakshan** - Gaussian Processes and Active Learning for Drug Particle Size Characterization in Continuous Flow Antisolvent Crystallization **O57 - Abdullah Al Rammah** - Limitations of Classical Force Fields for CO_2 Adsorption in MOFs: Toward Quantum Accuracy at DAC-Relevant Pressures **O58 - Xianfeng Jian** - Automated Flow Platform for Kinetic Model Identification **O59 - Mehryar Jafari** - From Infrared Spectra to Gas Transport: Group-Aware Machine Learning for Polymer Membranes **O60 - Yihang Fang** - Systematic Data Generation through automated HTE Acrylamide Coupling Synthesis for future ML reaction optimisation Chair - Dan Rhymer	Room 211/212

12:00 – 14:00	**Lunch**	Atrium
12:00 – 13:00	**EPSRC Network Plus 4D Health Tech**	Room 202
12:00 - 13:00	**Poster Presentations** • AI & Data Driven Studies • Formulation Engineering, Sustainable Manufacture & Materials • Healthcare Technologies *Even poster numbers to be presented in this session	Rooms 118/119
12:00 - 13:00	**Poster Presentations** • Chemical Recycling of Polymers • Energy & Net Zero & LCA • Process Modelling, Reactions & Simulation • Education • Bioprocessing & Biotechnology *Even poster numbers to be presented in this session	Rooms M208/M209
13:00 - 14:00	**Poster Presentations** • AI & Data Driven Studies	Rooms 118/119

	- Formulation Engineering, Sustainable Manufacture & Materials - Healthcare Technologies *Odd poster numbers to be presented in this session	
13:00 - 14:00	**Poster Presentations** - Chemical Recycling of Polymers - Energy & Net Zero & LCA - Process Modelling, Reactions & Simulation - Education - Bioprocessing & Biotechnology *Odd poster numbers to be presented in this session	Rooms M208/M209
13:00 - 14:00	**Food & Drink Networking (IChemE)**	Room 202
14:00 - 15:30	**Energy & Net Zero & LCA** (15 minutes each) **O61 - Ashraf Hauwa Nyako** - Hot Microbubble Gas Stripping for In Situ Butanol Recovery from continuous Fermentation **O62 - Liqiu Liu** - Chloride-Induced Morphology Control of Pt Coatings on Titanium Porous Transport Layers for Proton Exchange Membrane Water Electrolysers **O63 - Zhenxi Li** - Do national policies reflect country archetypes in petrochemical	Lecture Theatre 1 (LG18)

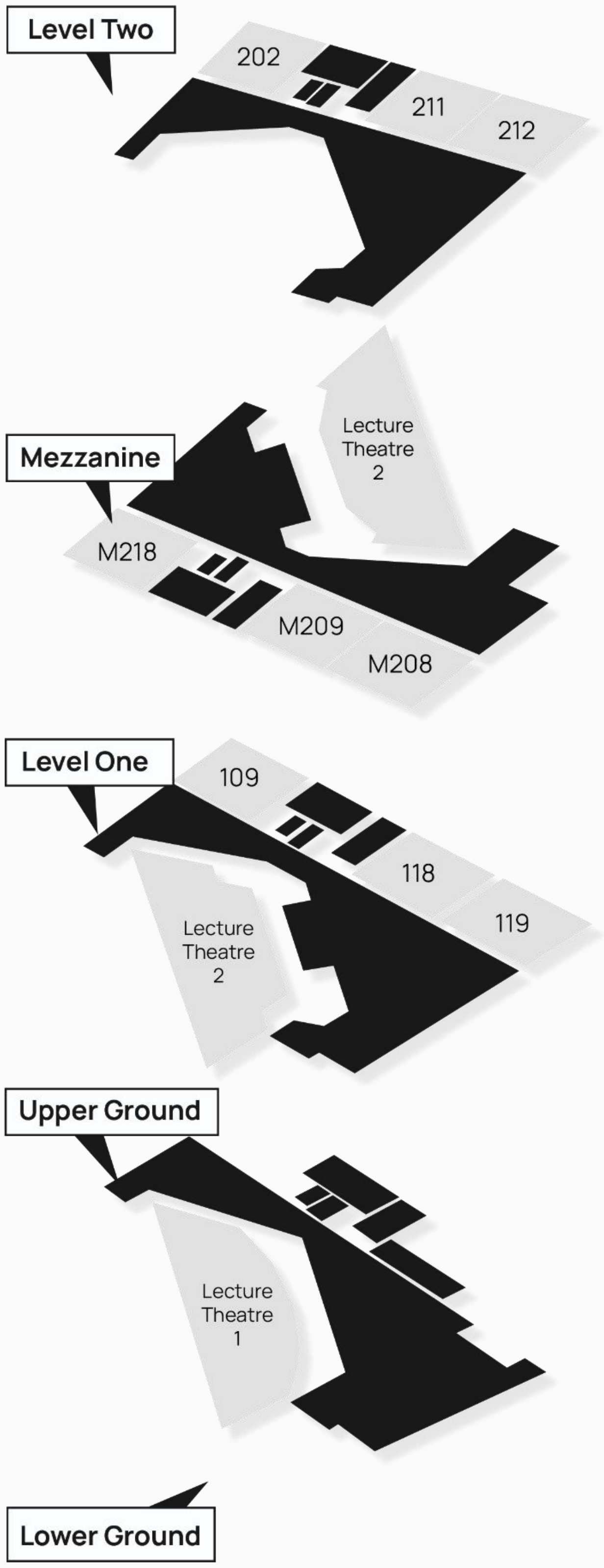
	decarbonization? A cross-country analysis **O64 - Xiaoling Ma** - Highly Dispersed Ru Clusters Supported on CeO2 Nano-islands Enabling Efficient and Stable H2-SCR of NOx **O65 - Niko Hilmi** - ZIF-7/Polyetherimide Mixed Matrix Membranes for Hydrogen Purification **O66- Marwah Shnaiter** - Gas diffusion layers based on recycled carbon fibre for PEM fuel cells and electrolysers Session Chair - Lisa Sun	
14:00 - 15:30	**Formulation Engineering, Sustainable Manufacture & Materials** (15 minutes each) **O67 - Cara Anderton** - Tailoring hydrocolloid-based fluid gels for fat replacement: the role of sucrose in agar systems **O68 - Preshti Ram** - Effect of sour gas on the CO2 capture performance of a prototypical zeolite **O69 - Eleonora De Giorgi** - Optimising PAT for Continuous Powder Formulation Quality Monitoring Using the Feed Frame Simulator **O70 - Jiayan Zhou** - The preparation of novel aerogels with paper pulp and calcium phosphate **O71 - Khizra Abdul Wadood** - Utilising Powder Characterisation and Data-Driven Models to Predict Dispersion and Dissolution in Drug Product Development	Lecture Theatre 2 (102)

	O72 - Dan Baiocco - Sustainable dual-shell chitosan-silica microcapsules for potential personal care applications Session Chair - Mark Simmons	
14:00 - 15:30	**Special Session: Chemical Recycling of Polymers** (15 minutes each) **O73 - Stefano Iannello** - Experimental investigation of a cold multistage fluidized bed system for waste chemical recycling **O74 - Kyle Batchelor** - Thermo-responsive Catalysts for PET Glycolysis: High-Throughput Design Towards Circular Recycling. **O75 - Xing Liu** - An integrated process modelling and sustainability assessment framework for chemical recycling towards a circular economy **O76 - Yuya Watanabe** - Dual Acid-Base Catalysis toward Chemical Sorting of Mixed Poly(ethylene terephthalate) and Poly(vinyl chloride) **O77 - Dingchang Yang** - Electrochemical Membrane Processes for Closed-Loop Recycling and Upcycling of polyethylene terephthalate (PET) **O78 - River Gowans** - Evaluating Zinc Catalysts for Resin-Fibre Dual Recovery in Solvolytic Recycling of CFRP Session Chair - Joe Wood	Room 211/212

15:30 - 15:45	**Closing Ceremony**	Lecture Theatre 1 (LG18)

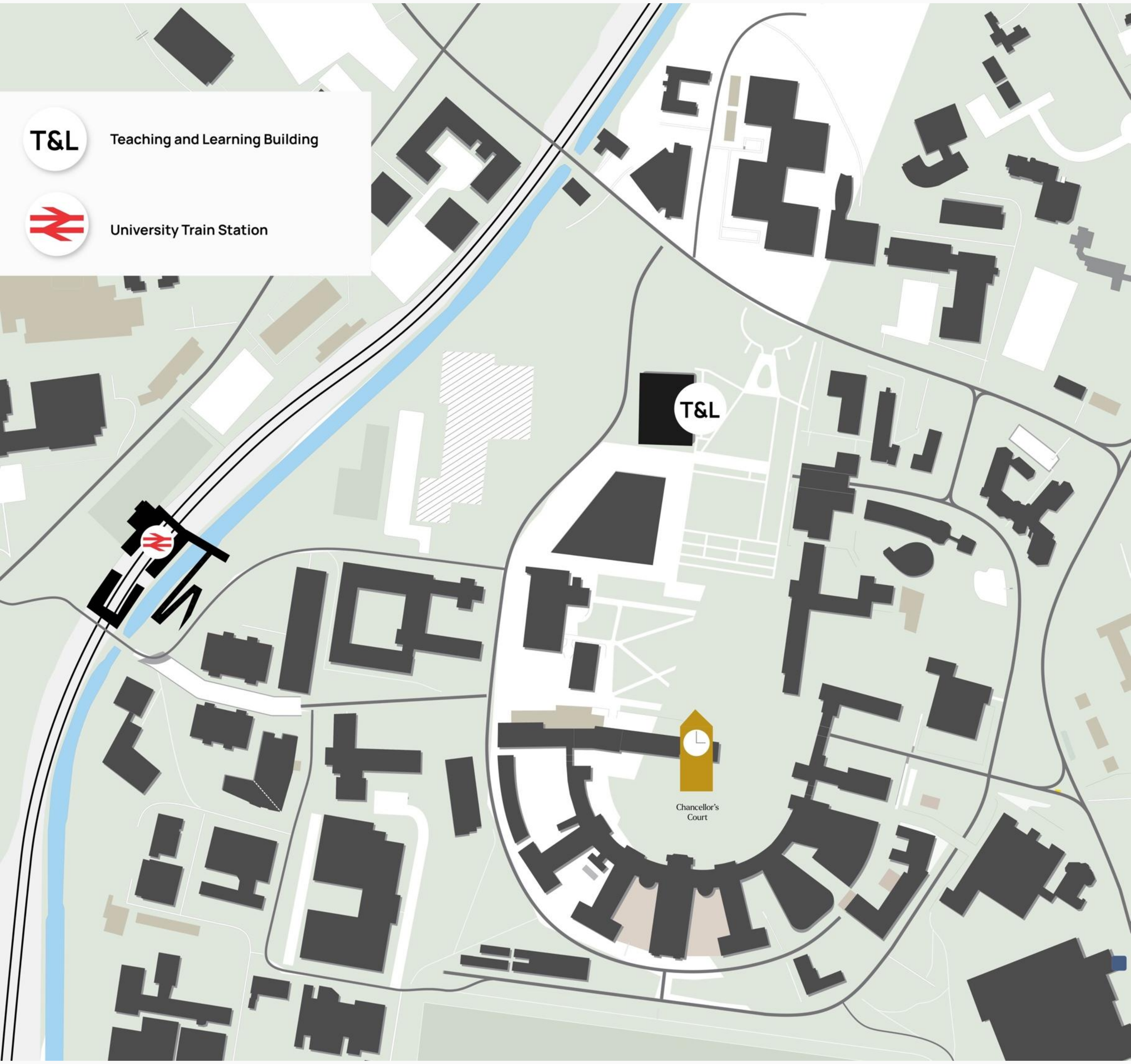
Teaching and Learning Building

Floor plan



Campus Map

University of Birmingham



Plenary speakers

Professor Marianne Ellis

Chemical Engineering, University of Bath

Abstract:

Towards Circularity in Cellular Agriculture Bioprocess Design for Sustainable Food Systems

The global imperative for sustainable food systems necessitates innovative approaches to food production. Cellular agriculture (Cell Ag), encompassing precision fermentation and tissue engineering, offers a transformative pathway to diversify food sources and mitigate the environmental impact of traditional livestock agriculture. This presentation addresses the critical role of circularity in Cell Ag bioprocess design, presenting insights from the Cellular Agriculture Manufacturing Hub (CARMA).

CARMA's transdisciplinary mission is to integrate responsible tools and technologies into current food systems, aiming for a just transition to environmentally, economically, and socially sustainable food production. This is achieved through interdisciplinary and transdisciplinary responsible research, fostering collaboration between physical, biological, and social sciences, and engaging diverse stakeholders. A core focus is the development of circular bioprocesses, emphasizing high-purity, low-loss downstream processes coupled with water recycling and resource recovery, and designing sustainable, scalable, and secure Cell Ag supply chains, leveraging life-cycle assessment to create net-zero manufacturing roadmaps.

This presentation will explore how CARMA's research contributes to overcoming manufacturing bottlenecks through novel cell culture media, scaffold innovations, and bioreactor advancements, all while embedding principles of circularity. Crucially, this includes iterative engagement with social science research and stakeholder platforms like the Citizens Forum, ensuring that technological development is aligned with societal needs and concerns. By focusing on resource efficiency, waste reduction, and the valorisation of by-products, CARMA's work aims to deliver robust, ethical, and acceptable supply chains. The discussion will highlight the potential of these integrated approaches to enhance food security, address climate change, and foster resilient, localized food production systems globally.

Professor Peter Styring
Chemical, Materials and Biological Engineering, University of Sheffield

Abstract:

Great British Chemicals: A Journey in Progress

As we move towards defossilising the chemical using industries and decarbonising the planet in general we need to move towards being custodians of carbon as opposed to simply consumers. Great British Chemicals was created in 2025 through a large investment by EPSRC-NERC to create a virtual centre for acceleration to scale to create the foundations of a Sustainable Industrial Future. Led by the University of Sheffield with nine other Founder universities, GBC will develop novel chemical manufacturing processes to a point they can be demonstrated at a scale and in an industrial setting that will provide evidence for further investment towards commercial deployment.

We will look at the whole supply chain from carbon capture through to end-of-life product use, considering the technical, economic, environmental, societal and political interconnectivities in a whole system thinking approach. We will consider how this impacts People, Planet and Prosperity and will support technician development and the entrepreneurship required to make societal impact.

Technically, we seek to optimise and intensify processes looking at direct emissions and embedded carbon while considering the requirements of energy use, co-reactants and land-use. While hydrogen will be required in many of the processes, we will consider non-molecular hydrogen approaches using an array of intensified processes such as photo-, electro- and plasma chemistries as well as hybrid approaches.

The research undertaken will be underpinned through many years of research and development expertise and gives us an opportunity to celebrate the advances made through support from UKRI legacy investments. Real life examples of how the field of carbon capture and utilisation has developed over 2 decades of research and will demonstrate how microreactor technologies have formed the basis for demonstration at scale with industrial partners. This is testimony of how chemical engineers and chemists can work together to make rapid advances.

Oral abstracts

O1: Process intensification through design: digitally manufacturing biocatalytic reaction systems

Theme: Bioprocessing & Biotechnology

Mr Ricky Wildman, Dr Anca Pordea, Professor Derek Irvine, Dr Simon Attwood, Dr Bruno Vuillod, Dr Jordan Hill, Dr Valentina Crucitti, Dr Eduards Krumins

[1]University of Nottingham, United Kingdom

Process intensification for biocatalysis demands reactor environments that can sustain high enzyme activity while overcoming the mass transport limitations that restrict productivity in conventional batch and packed bed reactors. We present a digital design and manufacturing framework that enables the creation of distributed, small scale biocatalytic reactors whose architectures are engineered specifically to enhance transport, control microenvironments, and improve overall process performance.

In this approach, enzymes are immobilised within 3D printed hydrogel structures that can be fabricated in a wide range of geometries and internal configurations. These hydrogels provide precisely defined microenvironments that alleviate diffusion constraints and enable improved catalytic efficiency. The reactor architectures are generated using a digital platform that integrates computational fluid dynamics (CFD) modelling of flow and scalar transport with design optimisation tools. This allows users to specify performance objectives, such as productivity, yield, or economic return, and obtain bespoke geometries optimised for those criteria.

The digital outputs transition seamlessly to additive manufacturing, enabling rapid, penalty free fabrication of complex reactor structures. This tight coupling between digital design and physical realisation not only accelerates development cycles but also permits exploration of geometries that are impractical or impossible to produce with conventional manufacturing methods.

We demonstrate how this framework enhances mechanistic understanding of enzyme laden flow reactors and provides an ability to “dial up” performance through informed geometric design. When combined with 3D printing, the approach offers substantial improvements in process efficiency and represents a viable route towards agile, decentralised manufacturing of high value chemicals and pharmaceutical intermediates.

O2: Identifying biofilm-forming conditions in probiotic bacteria

Theme: Bioprocessing & Biotechnology

Mr Alexander Brooks[1], Mrs. Michelle Christison[2], Mr. Leyton Gapper[2], Dr. Ashling Ellis[2], Dr. Alan Welman[2], Prof. Eddie Pelan[1], Dr. Tim Overton[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Fonterra Research and Development Centre, Palmerston North, New Zealand

Probiotics are defined as “bacteria which, when administered in an effective dose, confer a benefit on the health of the patient”. Probiotics have been proven to assist with the treatment of conditions such as ulcerative colitis, inflammatory bowel disease, hypercholesterolaemia, antibiotic-associated diarrhoea, and various allergenic diseases. Whilst there are many examples of probiotic products available on the market, some of the most popular with consumers are yoghurt drinks. The probiotics market is worth an estimated $15 billion per year and is growing by 7% per year.

For greatest effectiveness of the resultant product, it is crucial that maximal bacterial survival is achieved; this is important both during extended shelf storage, and also to maximise the concentration of bacteria that are able to survive and proliferate in the human gut. Multiple novel approaches have been explored for the development of systems to enhance the survival of probiotic bacteria in formulated products.

Previous studies have suggested that biofilm formation may enhance probiotic survival. As such, in this project, we are investigating culture conditions that lead to increased probiotic biofilm production and utilising this information to inform the development of a novel system for probiotic bacteria formulation in the dairy industry.

O3: Virus-Mimicking pH-Responsive Polymer-Functionalised Lipid Nanoparticles for Effective RNA Delivery and Enhanced Thermostability

Theme: Bioprocessing & Biotechnology

Ms Zichen Fan[1], Dr. Karnyart Samnuan[1], Dr. Apanpreet Kaur[1], Prof. Rongjun Chen[1]

[1]Department of Chemical Engineering, Imperial College London, London, United Kingdom

RNA-based vaccines and therapeutics are increasingly important for disease prevention and treatment. Lipid nanoparticles (LNPs) are widely used for RNA delivery, but efficient endosomal escape remains a key barrier to intracellular delivery. In addition, the reliance of mRNA/LNP on ultra-cold storage or lyophilisation introduces significant challenges to storage, distribution and cost. In this study, we develop a virus-mimicking, pH-responsive polymer-functionalised LNP (PF-LNP) for effective RNA delivery and stable storage at ambient temperatures.

PF-LNP encapsulating self-amplifying RNA (saRNA) were prepared using a microfluidic device. Particle size, zeta potential and RNA encapsulation efficiency were characterised. PF-LNP demonstrated significantly enhanced RNA delivery compared to commercial LNP. Freshly prepared PF-LNP exhibited luciferase expression two orders of magnitude higher than LNP in HEK293 cells. Enhanced expression was also observed in ex vivo skin models and in vivo mice studies of PF-LNPs. The formulations were then stored under different temperature conditions to assess their thermostability. It was demonstrated in vitro and in vivo that PF-LNP/saRNA remained stable after long-term storage in liquid at 4 °C and room temperature. These findings highlight the potential of PF-LNP to serve as a versatile and effective RNA delivery platform and to eliminate the need for cold-chain storage, potentially reducing costs and improving accessibility across diverse RNA applications.

O4: Real-time Determination of Monoclonal Antibody Structure During Chromatography

Theme: Bioprocessing & Biotechnology

Dr Charles Moore-Kelly[1], Dr Maria Bruque[2], Dr Jean Aucamp[3], Prof Tim Dafforn[4], **Professor Owen Thomas**[4]

[1]Oxford Biomedica, Oxford, United Kingdom, [2]UCB Pharma, Slough, United Kingdom, [3]Lonza Biologics, Slough, United Kingdom, [4]University of Birmingham, Birmingham, United Kingdom

Continuous manufacturing platforms offer new opportunities for the biopharma industry; however, their adoption is hindered by a lack of process analytical technologies capable of directly and autonomously measuring product critical quality attributes from process streams in real-time.

Here, we convert a high-throughput capillary-based circular dichroism/fluorescence (CD/F) system designed for bioprocess development tasks into a tandem in-line detector for use in chromatography and use CD/F measurements to reveal changes in the folding state of monoclonal antibodies (mAbs) during elution from various chromatography columns under different conditions.

Specifically, we show:

- (i) the measures taken to employ CD/F for in-line analysis of chromatographic streams containing high mAb and buffer concentrations;
- (ii) how and why tandem readouts of CD240 nm g-factor (a dimensionless measure of mAb folding state independent of concentration and path length) and fluorescence wavelength maximum (λmax) were selected as high frequency 'on-the-fly' reporters of mAb structure;
- (iii) how characteristic pairings of CD240 nm g-factor and λmax define different structural states and reveal striking transitions in conformation across elution peaks issuing from conventional Protein A and G affinity columns;
- (iv) that in some cases, the extent of unfolding in late eluting molecules is greater than expected from exposure to acidic buffer alone;
- (v) the impact of elution additives can be tracked and assessed; and finally
- (vi) that native mAb structure is preserved during thermal elution from a commercial thermoresponsive Protein A matrix.

The structural dimension that in-line CD/F provides allied with the speed with which data can be collected and interpreted lends it considerable potential for real-time release testing within continuous manufacturing, as real-time data can be collected, readily interpreted, and recognized as falling outside predetermined acceptable limits.

O5: Process Compatible Modelling of Bubbling Fluidised Bed Gasifiers for Steam Oxygen Gasification of Waste to Fuel Systems

Theme: Process Modelling, Reactions & Simulation

Bara Anaya[1], Dr Massimiliano Materazzi[1], Dr Stefano Iannello[1], Dr Alex Sebastiani[1]

[1]University College London, London, United Kingdom

A major barrier to credible system-level decision-making for waste-to-fuel pathways is the limited fidelity of bubbling fluidised-bed gasifier (BFBG) models embedded within end-to-end process flowsheets. Most process-level assessments rely on black-box equilibrium or pseudo-equilibrium gasifier models, which systematically neglect the hydrodynamic and kinetic constraints governing real reactor performance. These simplifications, typically adopted to preserve computational tractability, propagate uncertainty through system-level analyses, distorting optimisation outcomes, hydrogen-yield predictions, utility requirements, and CO2-capture performance.

In contrast, current applications of two-phase theory-based models, which incorporate reactor hydrodynamics through semi-empirical closures, are predominantly implemented within specialist computational frameworks with limited accessibility for system-level users, while CFD gas-solid models solve the momentum equations with closure relations on fluid-dynamic platforms. Although both provide more reactor-relevant representations of BFBGs, their reliance on specialised computational environments limits their engineering relevance at the system level due to restricted deployability within integrated process flowsheets and high computational expense.

To address this longstanding trade-off between mechanistic fidelity and process-level deployability, this work develops a process-compatible reactor-network model for large bubbling fluidised-bed gasifiers that explicitly incorporates fluidisation hydrodynamics and detailed reaction kinetics while remaining fully deployable within Aspen Plus and, for the first time, without external coding or embedded subroutines. The model is demonstrated for waste-derived feeds, including refuse-derived fuel, and validated against pilot-scale steam-oxygen gasification data. The model shows high predictive accuracy, with average deviations of 3% for reactor temperature and 8.5% for major syngas species mole fractions, whereas equilibrium-based gasifier models exhibit substantial reactor-level inaccuracies, with outlet syngas composition deviations exceeding 70%. Overall, the proposed reactor-network model enables physically credible, fully deployable system-level analysis of waste-to-fuel pathways.

O6: A Novel Dimensionless Number for the Characterisation of Densification and Segregation in a Vibrationally Excited Granular System

Theme: Process Modelling, Reactions & Simulation

Mr Freddie Barter[1], Mr Aaron Wiggin[1], Mr Jack Grogan[1], Prof Nick Bazin[2], Dr Peter Bolton[2], Mr James Mainwaring[2], Dr Oliver Phillips[2], Prof Christopher Windows-Yule[1]

[1]University of Birmingham, United Kingdom, [2]AWE plc, United Kingdom

Reliable production of densely packed, homogeneous powders is of significant interest to a range of industrial applications. Vibration-based excitation is frequently employed to increase the density of granular packings. However, this same vibration can lead to segregation - especially pronounced in systems of wide size distribution - which is generally undesirable. Existing research primarily focuses on densification and segregation individually, but the simultaneous optimisation of both phenomena remains underexplored. Discrete Element Method (DEM) simulations were conducted in LIGGGHTS to investigate the densification and segregation in a bidisperse-by-size granular system over a broad range of vibration frequencies and amplitudes, comparing continuous and tap-settle excitation in both vertical and horizontal directions. To test the generality of the proposed tap characterisation, additional horizontal tapping datasets were also generated for two further binary size ratios and for a polydisperse continuous PSD (Weibull) system. It was found that discrete, horizontal 'taps' provide the best packing density for the principal binary system explored, and the optimal conditions for the densest and most homogeneous steady-state packing do not correspond to the most rapid packing. There is therefore a small trade-off between steady-state packing density and the speed at which it is achieved. Two distinct densification behaviours were identified, reflecting stable densification and slow segregation-driven density loss. A novel dimensionless number, the 'dimensionless action,' is proposed and shown to outperform the commonly used control parameters tested here in collapsing packing-density and segregation-intensity data for three bidisperse systems and a polydisperse continuous-PSD system.

O7: Toward offshore wind to green hydrogen: Multiphysics insights into rotation and magnetic-field induced electrolysis

Theme: Process Modelling, Reactions & Simulation

Mr Mostafa Delpisheh[1], Dr Mohamed Mamlouk[1]

[1]School of Engineering, Newcastle University, Newcastle upon Tyne, United Kingdom

The UK is expected to deliver 10 GW of low-carbon hydrogen by 2030, yet the technology pathway to achieve this at scale remains under active discussion. Today, around 95% of global hydrogen is produced via steam methane reforming, which is associated with substantial CO_2 emissions and requires extensive carbon capture to approach carbon-neutral operation. Renewable-powered water electrolysis offers a route to truly green hydrogen, but it is not yet widely cost-competitive due to high capital and operating costs. With abundant offshore wind resources, the UK is well positioned to integrate wind power with hydrogen production.

In this work, we investigate a concept that leverages offshore wind turbine mechanical power directly via rotation, alongside magnetic-field-induced transport effects, to enhance water electrolysis performance. We consolidate the governing physics relevant to magnetically influenced electrolysis, including electrochemistry, electromagnetics, turbulent fluid flow, ionic species transport (diffusion, migration, and convection), and magnetohydrodynamic (MHD) coupling. A fully coupled COMSOL Multiphysics framework is developed to serve as a digital twin of the system, enabling interpretation of interacting phenomena and providing a foundation for model validation and subsequent design optimization.

O8: Molecular Insights into Enzyme Selectivity for Terpene Alcohol Esterification in Flower Essential Oils

Theme: Process Modelling, Reactions & Simulation

Dr Aiden Cranney[1], Miss Federica Biancot[2], Assistant professor Simone Morra[1], Professor Jonathan Hirst[1], Assistant Professor Parimala Shivaprasad[1]

[1]University of Nottingham, Nottingham, United Kingdom, [2]University of Turin, Turin, Italy

The floriculture industry generates large amounts of flower waste that are often underutilised. Two of the most important of these compounds, geraniol and citronellol, are widely used in the flavour and fragrance industries but are difficult to separate because of their very similar physicochemical properties.[1] Converting terpene alcohols into their corresponding esters increases their commercial value and facilitates separation; however, achieving selective conversion within mixtures such as essential oils remains challenging.[2] Selective biocatalysis offers a promising solution to this problem, enabling selective conversion that can simplify downstream separation.[3]

In this work, molecular dynamics simulations were employed to investigate the selectivity of Pseudomonas fluorescens lipase toward geraniol and citronellol during transesterification reactions. In the absence of a crystal structure for this enzyme, a set of proxy structures was considered, including homology models, AlphaFold-predicted structures, and the homologous lipase Candida antarctica lipase B. These structures were used to construct acetylated enzyme models representative of the catalytic intermediate. Productive binding was assessed using geometric criteria associated with near-attack conformations (NACs), enabling a quantitative comparison of how frequently each substrate adopts catalytically competent poses.

The simulations reveal a higher population of productive conformations for geraniol compared to citronellol, providing a molecular-level explanation for experimentally observed selectivity. Further to this, issues regarding predicted enzyme structures highlight the potential risks of integrating them into such computational models. This work highlights how molecular modelling can complement experiments by providing mechanistic insight into enzyme selectivity.

[1] M. Fan, S. Yuan, L. Li, J. Zheng, D. Zhao, C. Wang, H. Wang, X. Liu and J. Liu, Fermentation, 2023, 9, 119.

[2] Dianqi Yang, Xuxu Li, Chenyu Zhang, Hong Liang, and Xiaoqiang Ma, J. Agric. Food Chem. 2024, 72 (44), 24677-24686

[2] Michelle S. S. Amaral, Milton T. W. Hearn & Philip J. Marriott, Anal. Bioanal. Chem., 2023, 415, 3189–3199

O9: Development of biomimetic extracellular matrix coatings to improve tissue integration of arteriovenous grafts

Theme: Healthcare Technologies

Mr Ben Cassidy[1], Dr Inmaculada de Dios Perez[1], Professor Liam Grover[1,2], Professor Thomas Emil Andersen[3], Dr Tobias Hedberg[4], Mr Martin Alm[5], Dr Patricia Perez Esteban[1,2]

[1]Healthcare Technologies Institute, University of Birmingham, Birmingham, United Kingdom, [2]Department of Chemical Engineering, University of Birmingham, Birmingham, United Kingdom, [3]Department of Clinical Research, University of Southern Denmark, Odense, Denmark, [4]VERIGRAFT AB, Gothenburg, Sweden, [5]Biomodics APS, Rodovre, Denmark

Arteriovenous grafts (AVGs) offer the vascular access required for haemodialysis (HD) treatment of chronic kidney disease. Currently, up to 70% of AVGs fail within the first year following implantation and integrate poorly with the surrounding tissue, resulting in infections, leaks and recurrent thrombosis (1,2). With 3.5 million patients worldwide regularly undergoing this treatment, there is a remarkable requirement to improve the biocompatibility, anti-infection and anti-thrombosis qualities of existing AVGs (3).

This project involves the development of a thermosensitive decellularised extracellular matrix (dECM) biomimetic coating and its ability to reduce adverse host responses and improve tissue integration of a new, enhanced AVG for HD was investigated using a combination of in vitro cytotoxicity and morphological assays, interrogation of the inflammatory reaction and in-vivo measures of host response.

Addition of Pluronic F-127 contributed a thermoreversible property to the dECM hydrogel which improved its rheological and adhesive properties at physiologically relevant temperatures. dECM coatings developed here showed superior results for maintaining cell viability and regular morphological features of primary smooth muscle and fibroblasts compared to commercially available biocompatibility coatings. Macrophage polarisation displayed an M2 phenotype bias, reflecting that the dECM hydrogel provided a pro-regenerative, anti-inflammatory immune environment which can facilitate tissue remodelling whilst minimising chronic inflammation and fibrosis. In-vivo assessment of the immediate immune response demonstrated an unaltered inflammatory reaction when implanting hydrogel coated AVG material under the skin in a murine model.

Collectively, the improved cellular compatibility, mechanical suitability and immune tolerance is expected to considerably improve tissue integration and minimise inflammation and fibrotic capsule formation, reducing the risk of thrombosis and subsequently extending the long-term patency of AVGs in a clinical setting. dECM hydrogel coated AVGs are now being investigated in a larger animal study, involving the monitoring and repeated cannulation of these grafts in an ovine model.

O10: PEG-based fluid gels for cellular microenvironments: tailoring chemistry and gelation mechanics via temperature and mixing

Theme: Healthcare Technologies

Mr Ahsan Razaq[1], Dr Richard Moakes[1]

[1]Healthcare technologies institute, School of Chemical Engineering, University of Birmingham, UK, Birmingham, United Kingdom

Fluid gels are emerging as versatile scaffolds in biomaterials, exhibiting solid like behaviour at rest yet flowing under small strains—useful property for minimally invasive tissue engineering. Through formation as microgel suspensions through shear during the sol–gel transition. Synthetic Fluid Gels (SyMGels) based on poly (ethylene glycol) diacrylate (PEGDA) are especially promising, as their chemical functionality can be tailored with relative ease to influence cellular behaviour.[1] However, achieving control over local particle stiffness while maintaining bulk mechanics remains a key challenge.

SyMGel gelation kinetics are concentration dependent which are usually offset by mixing speed, enabling particle formation within shear flow. However, radical based processes undergo rapid gelation due to the Tromsdorff effect, necessitating high shear to suppress gelation. Yet such shear simultaneously inhibits initiation, resulting in no gel formation.

To address this, two strategies were employed to modulate reaction and transport kinetics: a two step mixing regime (low speed initiation followed by high speed propagation) and temperature control during mixing. SyMGels formed by two-step mixing yielded gels at 3–5% (v/v), while heating (50 °C) yielded 4–5% (v/v) gels, both at 1000 rpm. Comparisons between these at 5% concentration revealed that: heated gels produced smaller particles ($D_{4,3}$ 363 µm vs. 663 µm), lower elastic moduli (86 Pa vs. 217 Pa), and greater strain dependent behaviour. Elevated temperatures facilitated faster initiation and termination through increased mass transport and limiting particle growth. In contrast, auto acceleration during two step mixing drove rapid particle growth and subsequent breakdown under high shear. These findings expand SyMGels potential as next generation cellular scaffolds, offering mechanical cues to guide cell fate.

1. Foster, N. C., Allen, P., El Haj, A. J., Grover, L. M., & Moakes, R. J. A. (2021). Tailoring Therapeutic Responses via Engineering Microenvironments with a Novel Synthetic Fluid Gel. Advanced Healthcare Materials, 10(16). Doi: https://doi.org/10.1002/adhm.202100622

O11: Biocompatible electrophoretic ink microcapsules for on-skin interactive displays and sustainable healthcare applications

Theme: Healthcare Technologies

Dr Dan Baiocco[1], Professor Zhibing Zhang[1], Wenda Zhao[2], Professor Anne Roudaut[2]

[1]University of Birmingham, Birmingham, United Kingdom, [2]University of Bristol, Bristol, United Kingdom

Electrophoretic ink (e-ink) technology offers exceptional promise for ultra-low-power, rewritable displays. Yet, its adaptation to flexible, biocompatible formats suitable for direct skin application has remained elusive [1]. This study presents a new generation of biopolymer-based electronic ink microcapsules (EIMCs) engineered for safe, conformable, and energy-efficient wearable interfaces.
Complex coacervation at pH 4.1 with gum acacia and gelatine was employed to yield spherical core-shell EIMCs (22.4 ± 0.4 μm) encapsulating a hexylsalicylate-tetrachloroethylene electrophoretic medium, which was primed with negatively charged TiO_2 nanoparticles (30 nm) and gentian violet dye for enhanced contrast.

The microcapsules exhibited negligible leakage and exceptional mechanical strength (nominal rupture stress = 3.9±0.9 MPa; elastic modulus = 0.17±0.03 GPa), which are pivotal for on-skin applications. Rapid electrophoretic switching (~0.5 s at 20 V, 2 Hz refresh rate) was demonstrated, enabling reversible e-ink writing, stencil pattern toggling, and matrix-based data visualization. Comprehensive biocompatibility assessments revealed low cytotoxicity and negligible sensitisation response (cell viability ~65%, CD54 expression ~1.7%), confirming the potential suitability of the proposed materials for skin-integrated healthcare systems. These may include real-time physiological monitoring, biomedical data displays, responsive wound-dressing interfaces, and treatments for chronic conditions, such as topical melanocyte deficiency (vitiligo). The synergistic combination of renewable biopolymers, robust mechanical and barrier properties, and stable electrophoretic activity promotes this technology as a compelling route toward next-generation, sustainable, on-skin digital displays that bridge material science, human-computer interaction (HCI), and healthcare innovation. The details of the work will be presented.

O12: Sustainable Terpene-Derived Polymers for Biofilm Prevention in Neonatal Intensive Care

Theme: Healthcare Technologies

Mr Shyam Rana[1]

[1]University of Nottingham, United Kingdom

Healthcare-Associated Infections (HAIs) in Neonatal Intensive Care Units (NICUs) present a critical challenge, often stemming from bacterial biofilms on medical devices. These infections significantly contribute to morbidity in vulnerable neonates. [1] Conventional "active" antimicrobial coatings (e.g., silver) raise toxicity concerns and contribute to Antimicrobial Resistance (AMR). This research develops a sustainable, circular economy solution using passive, anti-biofilm polymers derived from waste terpene alcohols (Geraniol, Citronellol) found in waste plant biomass.

A significant hurdle in utilising terpenes is their inherent reactivity, which typically results in uncontrolled cross-linking. This study optimised free-radical polymerisation conditions and purification protocols to synthesise soluble polymers. The synthesised materials are characterised via 1H NMR and Gel Permeation Chromatography (GPC). These polymers are subsequently applied to medical substrates via dip-coating, with coating uniformity and chemical composition targeted for assessment via SEM and ToF-SIMS.

The optimisation protocols effectively suppressed cross-linking, successfully yielding soluble polymers suitable for post-polymerisation processing, a key milestone for this class of bio-derived materials. 1H NMR analysis confirmed the structural incorporation of the terpene monomers, while GPC data indicated controlled molecular weight distributions. Current work focuses on the translation of these polymers into stable coatings, evaluating their mechanical durability and surface topography against clinical requirements.

This work demonstrates the feasibility of transforming waste biomass into processable medical materials. By preventing bacterial attachment through surface chemistry, these coatings offer a scalable strategy to reduce NICU infections. The study highlights the role of sustainable chemical engineering in addressing critical healthcare challenges.

References:
[1] Sass L, Karlowicz MG. Healthcare-Associated Infections in the Neonate. Principles and Practice of Pediatric Infectious Diseases, Elsevier; 2018, p. 560-566.e3. https://doi.org/10.1016/B978-0-323-40181-4.00094-3.

O13: Scalable Production of Virus-Mimicking Polymer-Enveloped Lipid Nanoparticles for RNA Formulations with Enhanced Efficacy and Thermostability

Theme: Bioprocessing & Biotechnology

Mr You Cheng[1], Dr Karnyart Samnuan[1,2], Dr Yifan Liu[1], Dr Xuhan Liu[1], Dr Robin J. Shattock[2], Dr Rongjun Chen[1]

[1]Department of Chemical Engineering, Imperial College London, London, United Kingdom
[2]Department of Infectious Disease, Imperial College London, London, United Kingdom

While RNA technology holds great promise in therapeutics and vaccine development, its application is limited by delivery challenges, high instability, and scalable production. Current approved mRNA COVID-19 vaccines formulated by lipid nanoparticles (LNPs) have poor thermostability, thus requiring storage and distribution in very challenging ultra-cold chains at -70 or -20°C. Conventional LNPs consist of four lipid components, which adds the manufacturing complexity. To provide a next-generation RNA delivery system, we have developed a novel structure of Polymer-Enveloped Lipid Nanoparticle (PE-LNP). This system mimics viral structure to not only enhance delivery efficacy but also improves stability at ambient temperatures.

In this work, novel PE-LNPs were synthesized using reduced lipid components via a simple, one-pot production method. Process enhancement enabled the use of a safer and greener solvent in synthesizing PE-LNP and the facile solvent evaporation ensured the complete solvent removal. The novel nanostructures displayed high encapsulation efficiency and efficient intracellular delivery of RNA. In addition, PE-LNPs were optimised for long-term thermostability to eliminate the need for ultra-cold storage. This new PE-LNP technology represents a promising platform for the development of thermostable RNA-based vaccines and therapeutics.

O14: Studying The Viability of Termite Hydrogen Production for Renewable Energy

Theme: Bioprocessing & Biotechnology

Vinay Vinay Patel[1]

[1]University of Birmingham, United Kingdom

Termites are naturally able to digest cellulosic biomass and produce/emit hydrogen via microbial fermentation of cellulose in their hindguts, yet their potential for renewable energy production remains virtually unexplored. This research investigates the feasibility of termite-assisted hydrogen generation by quantifying all of their rates of chemical consumption and production under controlled lab conditions, followed by a simulation of a termite hydrogen plant in Aspen Plus using the model built, to produce a functional unit for LCA.

The model built will also include their respiration rate, nitrogen consumption and reproduction rate, amongst other relevant biochemical reactions. The aim is to quantitatively integrate termites into engineering and assess the viability and scalability of termite-derived hydrogen as a decentralized, low-energy route for circular bioeconomy applications.

Global hydrogen production is dominated by steam reformation of methane, contributing heavily to carbon emissions, whilst electrolysis is hindered by its high electricity requirement. Biological routes, such as dark fermentation, suffer from biological limitations stemming from poor adaptation of key organisms to non-natural settings. Termite hydrogen presents a novel yet natural biogenic pathway for energy production and creates a circular economy for cellulosic waste such as wood, paper, organic fibers and inedible crop husks.

Termites also create valuable side-products in the form of nutrient-rich soil and eggs (which can replace soymeal as poultry and fish feed). Although methane is also produced, infusion of certain antibiotics into their diet can increase hydrogen production by up to 7 times and strongly inhibit methane production. Based on the findings of a recent study, a 14m3 enclosure containing Psammotermes hybostoma termites, produces enough hydrogen to generate 30kWh of energy daily. However, the chemical stoichiometry and kinetic parameters have not been studied and are essential for optimization and scale up. This study aims to do so whilst creating an easily replicable methodology.

O15: Optimising Fig Peel Waste Phenolic Extraction through a Life Cycle and Cost-Analysis

Theme: Bioprocessing & Biotechnology

Ms Angeliki Xyderou Malefaki[1], Dr Athanasios Angelid-Dimakis[1], Dr Maria Dimopoulou[2]

[1]University of Huddersfield, Huddersfield, United Kingdom, [2]Teesside University, Middlesbrough, United Kingdom

Fig (Ficus carica L.) is an important Mediterranean fruit crop valued for its nutritional and health-promoting properties. Fig production generates substantial by-products, particularly peels, which are rich in phenolic compounds, such as flavonoids, phenolic acids, and anthocyanins. These bioactives exhibit antioxidant, anti-inflammatory, and cardioprotective effects, with Black Mission dark-skinned cultivars showing especially high levels. Life Cycle Assessment (LCA) and Life Cycle Cost (LCC) Analysis offer a holistic valorisation supporting decision making in complicated systems depending on the compound of interest.

Fig peel waste was dried, milled, and subjected to solid-liquid extraction under varying time, temperature, and pH conditions. Extracts were evaluated for yield, total phenolics, antioxidant activity, and phenolic profile, with process optimisation via Response Surface Methodology (RSM) and sustainability assessed using LCA/LCC. The RSM successfully optimised the aqueous extraction of phenolics from fig peel, identifying pH as the most influential parameter, followed by extraction time and temperature. Maximum total phenolic content (12.28 mgGAE/gDW) was predicted at 37.5 °C, 38 min, and pH 7, with antioxidant capacity generally increasing alongside TPC.

However, extraction yield did not consistently correlate with phenolic enrichment or bioactivity. HPLC analysis revealed compound-specific behaviour. Chlorogenic acid was favoured at pH 5, lower temperature, and longer time; quercetin benefited from mildly acidic conditions and rutin was abundant at neutral pH but less directly linked to antioxidant activity. Integrating RSM with LCA-LCC demonstrated that high-yield conditions are not necessarily sustainable. Medium extraction time at pH 7 and room temperature minimised environmental impact and cost per mgGAE while maintaining acceptable bioactivity, representing the best compromise between performance and sustainability for fig peel valorisation.

O16: From Microstructure to Bioeconomy: SEM–EDX Characterisation of Nettle Leaves for Value-Added Applications

Theme: Bioprocessing & Biotechnology

Mr Abraham Chacko[1]

[1]Bioinspired Engineering Research Group, SPACES, Canterbury Christ Church University, Canterbury, United Kingdom

Stinging nettles and their Urticaceae relatives are promising biorefinery feedstock for the circular bioeconomy, offering marginal-land cultivation, high-value fibres, pharmaceutical precursors and bioenergy products. European stinging nettles offer a carbon capture potential of 10 to 18 t CO_2 ha^{-1} yr^{-1}. The global stinging-nettle fibre market, currently valued at approximately 11 to 13 million USD, is projected to exceed 30 million USD over the next decade. This growth suggests nettle-based biomass could meaningfully contribute to net-zero chemical manufacturing. However, process design faces a critical knowledge gap: the spatial distribution of elements across plant tissues directly influences extraction efficiency, reactor performance and downstream separations, yet comprehensive characterisation remains costly, labour-intensive and time-consuming.

This study aims to overcome this challenge by employing Scanning Electron Microscopy with Energy-Dispersive X-ray Spectroscopy (SEM-EDX) to map, in minutes, the elements across nettle leaf structures to inform valorisation strategies. Understanding where elements concentrate within the biomass enables targeted pretreatment design, selective extraction protocols and feedstock preparation tailored to specific conversion pathways.

Morphological analysis revealed distinct processing considerations: lamina regions showed structural uniformity with scattered trichomes, suggesting suitability for mechanical extraction, whereas veins displayed complex topography indicating challenges for homogeneous chemical treatment. Elemental mapping confirmed operational implications. Calcium showed consistent distribution across lamina areas, supporting predictable conversion stoichiometry. Surprisingly, this study found considerable amounts of biogenic silicon, a material of emerging interest in energy storage, biomedicine and electronics. Silicon varied approximately four fold across leaf regions (0.77–3.54 wt% Si), with structure dependent accumulation that motivates targeted processing strategies for catalyst protection, hydrothermal optimisation and silica recovery.

Heterogeneous elemental distribution in nettles enables fractionation-based processing with optimised conversion routes for different anatomical regions. By linking composition to processability, this work could support techno-economic assessment of nettle value chains aligned with UN SDGs.

O17: Second Generation Bioethanol and Bioelectricity Production- An Empirical and Economic Analysis

Theme: Bioprocessing & Biotechnology

Dr. Sharon Velasquez Orta, Miss Ashley Craig, Miss Phoebe Mullet, Mr James Black, Dr Leonardo Rios Solis

[1]Newcastle University, Newcastle upon Tyne, United Kingdom

This study explores the pretreatment of synthetic food waste and its dual application for bioethanol and bioelectricity production using batch fermentation and microbial fuel cells (MFCs), respectively. Food waste was pretreated using acid or hydrothermal hydrolysis methods. Acid hydrolysis resulted in a lower pH of 1.24 (±0.01) when compared to hydrothermal treatment with a pH of 5.91 (±0.01). Characterisation revealed no significant difference in the carbohydrates (391 mg/L ±51.5) or glucose (234 mg/L ±16.4) in hydrolysed waste, when compared with hydrothermal pre-treated waste (283 mg/L ±68.5 and 222 mg/L ±11.1,respectively). Fermentation using Saccharomyces cerevisiae or Candida utilis under aerobic and anaerobic conditions revealed higher yields with S. cerevisiae. Anaerobic conditions consistently produced more ethanol throughout fermentation with a peak production of 0.0164 g/g of food waste (FW) at 24 hours, whereas aerobic fermentation peaked at 24 hours (0.0121 ±0.0007 g/g of FW) before declining to zero. Microbial fuel cells (MFCs) were fed post-fermentation digestate and inoculated with S. Cerevisiae or anaerobic digestate. Current outputs for MFCs using yeast were 0.7± 1.7μA (n=3), whilst MFCs inoculated with anaerobic sludge produced 22± 0.6μA (n=4) . MFC using S. cerevisiae achieved a peak power density of 0.33 ± 0.16 mW/m^2 (n=2) versus 17.80 ± 2.62 mW/m^2 (n=4) in MFCs inoculated with sludge. Cyclic voltammetry revealed the electrochemical activity of S. cerevisiae and anaerobic sludge. Results suggested the need for improvement when using yeast in MFCs, for example, via using electron transfer mediators or anode surface modifications. The capital budget estimate for a capacity of 1000 tonnes of ethanol per year was £4,859,175. Annual operating costs would constitute 9.92% of the capital costs. Economic investigations will need continuation to fully assess economic viability. These findings pave the way for future studies to improve microbial performance and yields, reinforcing the potential of circular waste-to-energy systems.

O18: Valorising UK’s horticulture waste: bio-based ingredients for the consumer goods sector

Theme: Bioprocessing & Biotechnology

Dr Parimala Shivaprasad[1], Miss Alisa Wikaputri[1], Miss Sarah Jennings[1], Miss Monika Dabrowska[1]

[1]University of Nottingham, Nottingham, United Kingdom

Did you know the UK produces over half a million tons of horticultural waste each year and yet most of it ends up discarded or composted? Imagine treating this waste as a feedstock for a new, circular chemical supply chain!

Flowers are an underutilised biomass stream: they contain high concentrations of terpenoids and low lignin, making them easier to process than conventional agricultural residues. My group is developing the UK’s first flower-waste biorefinery to convert unsold and spent flowers into fragrance ingredients, bioactive compounds and hydrophilic polymers for home and personal care applications.

We extract crude flower oils using portable, low-energy ultrasound systems and convert the terpenoid fraction into fragrance esters through enzyme catalysis. A central challenge working with flower biomass is the feedstock complexity: multi-substrate mixtures inhibit or compete within conventional enzymatic and catalytic systems. We have addressed this by integrating multi-substrate kinetic modelling with biocatalysis and reaction engineering to enable selective transformations directly from crude flower extracts. Using these tools, we have demonstrated continuous enzymatic production of terpene esters in intensified reactor systems that operate at the point of waste generation. This reduces transport costs for low density biomass and shifts production from large centralised assets to flexible, local units integrated with horticultural operations. We then valorise the spent flower biomass through microbial fermentation to produce bioactive compounds. In parallel, we are expanding the biorefinery platform to produce hydrophilic polymers from flower-derived substrates using enzymatic oxidation and polymerisation. These polymers offer a circular alternative to petrochemical-based water-soluble polymers widely used in detergents and personal care formulations.

This work on a circular, flower waste biorefinery demonstrates the potential of flower biomass to support a low-carbon, resilient chemical supply chain. Our goal is to deliver scalable, easy-to-operate technologies that turn regional horticulture waste into consistent, high-value chemicals and materials.

O19: Numerical modelling of chlorine-mediated selectivity in direct seawater electrolysis

Theme: Process Modelling, Reactions & Simulation

Mr Blessings Malimusi[1], Mr Abdullah Alyahya[1], Prof Daniel Friedrich[1], Dr Ignacio Tudela[1]

[1]The University of Edinburgh, Edinburgh, United Kingdom

Electrochemical water splitting is widely recognised as a key technology for low-carbon hydrogen production; however, industrial electrolyser systems typically rely on highly purified freshwater to avoid catalyst degradation, membrane fouling, and parasitic side reactions. The desalination and polishing steps required to achieve this water quality impose significant energetic and economic penalties, motivating increasing interest in direct seawater electrolysis (DSWE) as a means of utilising abundant saline water resources without extensive pretreatment. Despite its promise, DSWE is fundamentally limited by poor anodic selectivity due to competition between the oxygen evolution reaction (OER) and the chlorine evolution reaction (CER), leading to efficiency losses and the formation of reactive chlorine species.

In this work, a continuum-scale modelling framework implemented in Python is presented to investigate the coupled hydrodynamic, electrochemical, and chemical mechanisms governing anodic selectivity in DSWE under laminar flow conditions. The model integrates laminar flow transport with tertiary current distribution, multicomponent ionic transport described by the Nernst–Planck equations, Butler–Volmer electrode kinetics, and pH-dependent chlorine speciation involving chlorine, hypochlorous acid, and hypochlorite. Anion-exchange membrane behaviour is incorporated through a simplified but physically consistent representation of hydroxide transport. Spatially resolved simulations reveal the formation of steep pH gradients and chemically distinct microenvironments near the anode–membrane interface, highlighting the influence of chlorine hydrolysis and hypochlorite formation on local reaction thermodynamics and kinetics. The model reproduces experimentally observed trends, including chlorine-dominated behaviour at low current densities and a progressive transition towards oxygen-selective operation at higher applied currents (approximately 200–300 mA cm^{-2}). Sensitivity analysis demonstrates that anodic selectivity is primarily controlled by coupled mass-transport limitations and local pH regulation, underscoring the critical roles of convective flow and membrane-mediated hydroxide flux in enabling oxygen-favoured DSWE operation.

20: Integrated techno-economic, life cycle, and surrogate modelling for scaling production of bioplastic precursors

Theme: Process Modelling, Reactions & Simulation

Dr Sylvanus Lilonfe[1], Dr Michael Pritchard[2], Dr Pierre Reitzer[1], Dr Edward Spence[1], Dr Samantha Bryan[1], Professor Jon McKechnie[1], Dr Harry Goldingay[2], Dr Ioanna Dimitriou[1]

[1]Faculty of Engineering, University of Nottingham, Nottingham, United Kingdom, [2]Aston Centre for Artificial Intelligence Research and Application, Aston University, Birmingham, United Kingdom

Green chemistry can assist industries in decarbonising their use of fossil chemicals and fuels, helping economies achieve decarbonisation targets. 2,5-Furandicarboxylic acid (FDCA), a bioplastic precursor, is listed among the 12 priority chemicals essential for green and circular economies, however, its scale-up and economic viability are crucial for successful operations. This work aims to identify pathways for commercialising FDCA produced from bio-based resources by evaluating and scaling bench-scale designs and operations using Aspen Plus process modelling, techno-economic assessment (TEA), life cycle analysis (LCA), and machine learning surrogate modelling. The novel approach of this work is based on linking techno-economic and life cycle assessment results with surrogate modelling, which enables fast prediction of cost and environmental performance outcomes, minimising computational burden and reliance on conventional process simulation software and TEA/LCA tools. Early results indicate that FDCA production costs range from USD 1,300 to 25,000 per tonne, with associated water use between 0.03 and 5 tonnes of H_2O per tonne of FDCA, across biomass processing capacities from small-scale (24 tonnes per day) to large-scale (2,400 tonnes per day) operation. The main factors influencing cost and water use are economies of scale, capital investment and operating costs. Predictions from the surrogate model show strong agreement with techno-economic and life cycle assessment results, with correlation coefficients (R) ranging from 0.88 to 0.97. These insights provide a robust foundation for guiding future scale-up decisions and accelerating the sustainable commercial deployment of bioplastic precursors like FDCA.

O21: Discrete element method study of the impact of vessel wall friction on the mixing dynamics of a resonant acoustic mixer

Theme: Process Modelling, Reactions & Simulation

Mr Jack Grogan[1], Prof Tomislav Friščić[2], Prof Nicholas Bazin[3], Dr Peter Bolton[3], Prof Christopher Windows-Yule[1]

[1]School of Chemical Engineering, the University of Birmingham, Birmingham, United Kingdom, [2]School of Chemistry, the University of Birmingham, Birmingham, United Kingdom, [3]AWE, Aldermaston, United Kingdom

Resonant acoustic mixing (RAM) has shown promise processing materials within the pharmaceutical and energetics industries. One of RAM's strengths is the freedom to attach a wide variety of mixing vessels to the vibrating plate to induce mixing. This flexibility introduces the vessel material properties as a tuneable parameter for optimising mixing performance within RAM. In addition to material changes, understanding the impact of vessel wear, polishing, or adding a liner to the RAM vessel is key to ensuring optimal RAM operation. Assessing the impact of vessel material changes on RAM performance therefore requires insight into how container frictional properties influence mixing behaviour and internal flow patterns. The effect of particle-wall sliding friction on mixing performance was analysed using the discrete element method (DEM), for powder fill levels ranging from 10 % to 90 % and RAM operating accelerations between 20 and 100 times the acceleration due to gravity. Wall friction was found to significantly impact RAM's performance. Transverse mixing performance was consistently poorer than the vertical and radial mixing performance, highlighting the sensitivity of RAM to the initial loading configuration. Furthermore, the frictional properties of the RAM vessel for optimal transverse mixing differed from those that optimised radial and vertical mixing performance.

O22: Assessing the Feasibility of a Drag Force Flow Sensor for the Inline Monitoring of High Shear Wet Granulation Using the Discrete Element Method (DEM)

Theme: Process Modelling, Reactions & Simulation

Ms Luisa Attfield[1,2], Andy Ingram[1], Kit Windows-Yule[1], Mahmood Mustafa[2], Jason Crooks[2]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Drug Product Development, GSK, Ware, United Kingdom

High shear wet granulation (HSWG) is a widely used method in pharmaceutical tablet manufacturing to improve powder flowability, content uniformity, and processing efficiency. HSWG is a complex, multivariate process. Equipment, formulation and process parameters all impact granulation and the resultant granule properties which in turn influence downstream unit operations and properties of the resultant tablets. This presents challenges for process development and scale-up, which typically rely on traditional empirical approaches and trial-and-error methods.

In-line and at-line process analytical technology (PAT) provide real-time information of the granulation process, and offer opportunities for process development, control and scale-up.

One novel technology being explored is the Drag Force Flow (DFF) sensor as an in-line PAT tool to provide real-time monitoring of granulation dynamics. A DFF sensor is inserted into the granulation bowl. During granulation, particles collide with the probe, and the forces of these collisions are measured. Previous work has shown that force recordings from a DFF probe correlate with offline granule measurements taken from the FT4 powder rheometer, and that the force recordings can be used to predict tablet tensile strength.

However, current studies do not establish how DFF signals relate to particle properties. This work uses Discrete Element Method (DEM) simulations to develop machine learning models of particle size and density using forces recorded by the DFF probe. DEM allows for the exploration of a wide parameter space, which would be time-consuming and challenging to achieve experimentally. In this work DEM was used to create a computational model of a DFF probe in particulate flow. This allows assessment of how particle properties such as size, density and friction affect the forces experienced by the probe, and support development of models predicting particle properties.

O23: Process modelling for bottom-up estimation of emissions from ethylene production in Europe

Theme: Process Modelling, Reactions & Simulation

Dr Thabang Selalame[1], Dr Fanran Meng[1], Dr Jiacheng Sun[1], Dr Alfred Hill[2], Professor Anthony Ryan[1], Dr Nixon Sunny[3], Dr Marwan Sendi[3], Dr Amir F.N. Abdul-Manan[3]

[1]University of Sheffield, Sheffield, United Kingdom, [2]University of Bath, Bath, United Kingdom, [3]Life Cycle Assessment (LCA) Group, Technology Strategy & Planning Department, Saudi Aramco, Dhahran, Saudi Arabia

Ethylene is a foundational building block of the petrochemical industry, with global demand approaching 200 million tonnes per year and projected to grow at approximately 3.4% annually this decade. In Europe, it is predominantly manufactured from the steam cracking of ethane and naphtha. The process involves high-temperature pyrolysis followed by energy-intensive compression and cryogenic separation, resulting in substantial greenhouse gas (GHG) emissions and posing a significant challenge to the region's decarbonisation efforts. Effective and coordinated mitigation strategies require robust, plant-level emissions data, which are currently limited due to commercial confidentiality.

In this study, we quantify GHG emissions from ethylene production across Europe using a bottom-up, plant-level modelling approach. Ethylene production volumes are obtained from country-level trading data sourced from GlobalData Database, and allocated to individual active ethylene plants. Detailed Aspen Plus process models for different ethylene production routes, accounting for feedstock type, production capacity, and technology configuration, are developed in this work. The process models are used to simulate all the active ethylene-producing plants in Europe. The results of the simulations are used to estimate plant-level raw material usage, energy use and material outputs (such as ethylene, propylene, etc.), together with associated GHG emissions. The GHG emissions are then aggregated to obtain national and regional emissions and identify hotspots.

Our results indicate substantial heterogeneity in emissions intensity across plants, with GHG footprints ranging from approximately 0.5 to 3 kg CO2e per kg of ethylene. Most of this variation is driven by feedstock choice and process configuration. Germany and the Netherlands emerge as the largest absolute emitters in Europe, reflecting their production scale and feedstock mix. This work provides the most detailed open-literature inventory of plant-level GHG emissions for European ethylene production to date, offering critical insights for industrial decarbonisation strategies, comparative footprinting, and future policy design in the petrochemical sector.

O24: Sustainable production of rose oil terpene esters for fragrance applications: economic and environmental insights

Theme: Bioprocessing & Biotechnology

Dr Sylvanus Lilonfe[1], Vipada Sansen[1], Dr Akos Cseke[1], Dr Parimala Shivaprasad[1], Dr Ioanna Dimitriou[1]

[1]Faculty of Engineering, University of Nottingham, Nottingham, United Kingdom

Leveraging flower-derived products, such as terpene esters, for fragrances, cosmetics, and insect repellents can advance green chemistry, circular economies, and decarbonisation initiatives. However, deploying these products requires experimentation and technical analysis to establish the feasibility and viability of innovations, especially for scaling up and viable economic operations. This work evaluated the techno-economic performance and life cycle environmental impacts of terpene esters derived from rose oil, including citronellyl acetate and geranyl acetate. The transesterification process was modelled in Aspen Plus to calculate mass and energy balances, while environmental impacts were quantified using SimaPro. An economic analysis was also carried out to assess economic performance, including capital, operating and production costs. The production costs of citronellyl acetate and mixed terpenes were approximately £14 per kg and £7 per kg, respectively, with the main cost drivers being enzyme and solvent costs. The life cycle greenhouse gas emissions ranged from 350 to 2100 kg CO_2e per kg rose oil, with at least 80% of emissions resulting from the rose oil production stage, mainly due to the high consumption of natural gas to generate steam for flower distillation. The production costs and greenhouse gas emissions of rose oil-derived terpene esters were 74% and 20–85% lower, respectively, than those produced by fossil-based processes, demonstrating their economic competitiveness and environmental benefits.

O25: Green Extraction of Phenolic Compounds from Sea buckthorn (Hippophae rhamnoides) leaves

Theme: Bioprocessing & Biotechnology

Mrs Peace John-Banjo[1], Dr Athanasios Angelis-Dimakis[1]

[1]University of Huddersfield, Huddersfield, United Kingdom

This study aimed at evaluating the impact of green solvents on the Total Phenolic Content (TPC) yield and on the Antioxidant Capacity (AC) of extracts from Sea Buckthorn (SBT) leaves via maceration. Using 1g dried SBT leaf powder and 20ml solvent, the effect of three different solvent combinations (water, acetone and 1:1 water/acetone mixture) was investigated, under different temperatures (25, 35 and 50ºC) and extraction durations (1, 30, 60 and 90 mins). The Response Surface Methodology (RSM) was consequently applied to investigate the impact of substrate–solvent ratios (1:15, 1:20 and 1:25) for the best performing solvent. HPLC-DAD was used to identify and quantify phenolic compounds.

For TPC and AC respectively, the results showed that the optimal solvent is the 1:1 water/acetone mixture (with values 293±1.48 mg GAE/g, 243 ± 0.19 mg TEAC/g, respectively), while pure water and pure acetone had lower values (for water 252 ± 0.12 mg GAE/g, 254 ± 3.45 mg TEAC/g and for acetone 225 ± 0.99 mg GAE/g, 194 ± 1.43 mg TEAC/g, respectively).

Both TPC and AC differed significantly among the three solvents (one-way ANOVA, $p < 0.001$), with higher phenolic content corresponding to higher antioxidant capacity, particularly the 1:1 water/acetone mixture.

The RSM showed that the optimal feed-solvent ratio was 1:20. Solvent ratio and temperature showed significant effects at $p \leq 0.05$ on TPC yield and AC of the extracts. The RSM also showed a relationship between TPC and AC, generating a linear regression equation with best fit $R^2 = 99.24\%$, model's p-value $p < 0.05$ to predict TPC yield. Finally, HPLC-DAD showed that all extracts consisted of 20 phenolic compounds including 2-Hydroxybenzoic acid, Catechin, Gallic acid, with Rutin and Quercetin being dominant.

O26: Valorisation of Brewers' Spent Yeast for Biodegradable and Active Food Packaging Films

Theme: Bioprocessing & Biotechnology

Ms Yuting Han[1]

[1]University of Birmingham, Birmingham, United Kingdom

Large volumes of plastic packaging are used in short-lived food applications, contributing significantly to environmental pollution while offering limited functionality beyond physical containment. At the same time, the food and beverage industry generates substantial quantities of organic by-products that remain underutilised. Brewers' spent yeast (BSY), a major by-product of beer production, is rich in polysaccharides, proteins and bioactive compounds, yet is commonly disposed of or used in low-value applications. This PhD research explores the valorisation of BSY as a sustainable feedstock for the development of biodegradable and functional food packaging films.

Yeast cell wall (YCW) materials were obtained through mechanical disruption strategies, including high-pressure homogenisation, with the objective of recovering film-forming yeast-derived components rather than high-purity fractions. This approach avoids energy-intensive purification steps and supports scalable, sustainability-oriented processing. The resulting YCW-based films provide a renewable alternative to conventional plastics while exhibiting inherent antioxidant and light-barrier properties.

To introduce active food protection, the natural antimicrobial peptide nisin was incorporated into the film system. Early-stage results indicated that while direct incorporation of nisin enabled rapid initial antimicrobial activity, its effectiveness typically declined within approximately one week, highlighting the importance of delivery strategy for antimicrobial durability. To address this challenge, a combined approach was adopted, integrating free nisin for immediate antimicrobial action with chitosan–alginate–calcium chloride encapsulated nisin to enable sustained release.

Overall, this work demonstrates how bioprocessing strategies can be integrated with formulation engineering to convert food-system by-products into functional packaging materials. The research highlights the potential of yeast-derived biopolymers for sustainable packaging applications while contributing to circular economy principles and food waste reduction. Future work will explore the feasibility of using yeast cells as natural carriers for nisin encapsulation.

O27: Activated Carbon Synthesis from Microalgae (Chlorella sp.)

Theme: Bioprocessing & Biotechnology

Mr Darlington Nnabodo[1], Dr Taghi Miri[1], Dr Matthew Keith[1], Professor Jude Onwudili[2]

[1]University of Birmingham, United Kingdom, [2]Aston University, United Kingdom

The aviation sector faces increasing pressure to meet growing mobility demands while significantly reducing greenhouse gas emissions. Sustainable aviation fuel (SAF) offers a promising pathway toward decarbonization; however, high production costs, particularly those associated with catalytic processes, remain a major barrier to large-scale deployment. Developing low-cost, sustainable catalyst supports from renewable waste materials could substantially improve the economic viability of SAF production.

In this study, low-lipid Chlorella sp. microalgae biomass, representative of residues remaining after lipid extraction for biofuel production, was investigated as a feedstock for activated carbon (AC) synthesis. Two preparation routes were evaluated: (i) hydrothermal carbonization (HTC) followed by chemical activation and (ii) direct chemical activation without HTC. The resulting activated carbons were characterized using proximate analysis, CHNS-O elemental analysis, thermogravimetric analysis (TGA), and porosimetry, and their properties were benchmarked against commercial activated carbon.

Proximate analysis revealed that the microalgae biomass contained approximately 22 wt.% fixed carbon, indicating sufficient carbon content for char formation. Elemental analysis confirmed significant carbon enrichment following HTC and activation. Thermal stability assessments showed that AC produced via the HTC-assisted method exhibited comparable stability to commercial AC. Porosimetry results demonstrated that the synthesized AC possessed a higher surface area, lower pore volume, and comparable pore diameter relative to commercial material.

These findings demonstrate that microalgae residues can serve as a viable, low-cost source of activated carbon with properties suitable for use as catalyst supports. This approach offers a pathway to valorise microalgal waste streams while contributing to reduced catalyst and overall SAF production costs. Future work will focus on incorporating the synthesized AC as a metal catalyst support in SAF production processes.

O28: Co-processing of Bio-Based Fischer Tropsch Wax in an Industrial Hydrocracking Unit: A Pathway Toward Lower-Carbon Fuel Production

Theme: Process Modelling, Reactions & Simulation

Mr. Fawaz Alwarthan[1], Dr. Massimiliano Materazzi

[1]UCL, London, United Kingdom

Co-processing renewable feedstocks with conventional fossil-based streams in existing refineries has emerged as a promising decarbonization pathway, offering a practical route to producing lower-carbon products. Biobased Fischer Tropsch (FT) crude is considered one of the promising and suitable routes for integration with existing refinery infrastructure. This study evaluates the impact of co-processing bio-derived FT wax in an industrial-scale hydrocracking scheme using Aspen HYSYS. The model was developed and calibrated using real plant data to ensure accurate representation of the results. A series of blending scenarios were investigated to assess the effect of FT wax on product yields, reactor behaviour, and fuel properties. Results show that increasing the FT wax ratio led to reduced feed impurity levels and a significant decrease in hydrogen consumption and reactors exotherms. Minor variations were observed in product yields and properties, all of which remained within specification limits. Overall, the study demonstrates the technical feasibility of integrating renewable FT wax into conventional hydrocracking operations and supports its potential as a scalable pathway for producing lower-carbon fuels.

O29: Multiphase CFD Modelling of a Calcination System Using Open FOAM

Theme: Process Modelling, Reactions & Simulation

Mr Charlie Brayson[1,2], Christoper Windows-Yule[1], Thomas Abadie[1], Christine Bertrand[2], James Kelly[2]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Origen Carbon, Bristol, United Kingdom

There is an urgent requirement for global decarbonisation efforts to be developed and deployed as rapidly as possible to avoid irreversible environmental damage. This is especially true for the lime and cement industries which produce significant amounts of CO2. In this talk I describe the improvement of a calcination technology developed by Origen Carbon, which is used to produce zero-carbon lime for use in lime production and carbon-capture applications, using open-source CFD software OpenFOAM to model the calcination of the limestone material within the system.

Multiple turbulence models are tested and evaluated in a high-efficiency cyclone geometry, with particle modelling implemented using the multi-phase particle-in-cell (MPPIC) method. A modified version of the Lagrangian OpenFOAM solver coalChemistryFoam is developed and utilised to build a turbulent, multi-phase model of a pilot-scale flash calciner. This work will provide results on the output of the system to allow for the refinement of various system parameters.

O30: Boosting Chemical Looping Hydrogen Generation and CO2 Removal by Integrating with the Charcoal Gasification Process

Theme: Process Modelling, Reactions & Simulation

Mr. Ali Rabeeah[1], Dr. Jun Li

[1]University of Strathclyde, Glasgow, United Kingdom

Boosting hydrogen gas production is the most suitable solution to global energy challenges, serving as a carbon-free, sustainable fuel for the future. This project investigates theoretical and experimental approaches to boost hydrogen production by advancing the chemical looping hydrogen generation (CLHG) process and removing CO_2. It converts the high-waste heat of the CLHG's exhaust gases into low-carbon products by integrating a water-gas shift reactor that utilizes the oxygen carrier (Fe2O3) in the CLHG as a catalyst, along with a Mono-Ethanol Amine (MEA) solvent, using sustainable feedstock. In the lab, the CO2 gasification of charcoal to produce CO gas is combined with the modified CLHG as feedstock to reduce the oxygen carrier (O.C.) and recycle the emission CO2, which MEA captures.

The experimental work concludes that the optimal conditions for charcoal gasification were a CO2 flow rate of 51 ml/min and a high-temperature range of 750-935°C for CO gas production. Additionally, the modeling results demonstrate that H2 gas yield was 0.92 Kmol H2/Kmol Fe2O3 at a molar ratio of 1.40 (CO/Fe2O3) and 10 bar pressure, showing a significant increase of 0.64 Kmol H2/Kmol Fe2O3 compared to the conventional CLHG. The CO2 gas was 0.67 Kmol CO2/Kmol Fe2O3 emitted in the CLHG at a molar ratio of 1.14 (CO/Fe2O3), which the MEA would capture, resulting in a total CO2 capture of 100%. Process modeling was conducted to assess the performance and scalability potential of the modified CLHG using Aspen Plus.

O31: Numerical Simulation and AI-Driven Geometry Optimisation of Cohesive Material Feeders

Theme: Process Modelling, Reactions & Simulation

Mr Aran Klair, Kit Windows-Yule, Matt Keith, Yunfei Li Song, Richard Elkes

[1]University of Birmingham, Birmingham, United Kingdom, [2]GSK, Ware, United Kingdom

Transport of cohesive materials remains a significant bottleneck in continuous manufacturing, driven by the formation of stable structures blocking flow within hoppers and the flow instabilities from the erratic discharge in the conveying process.

A numerical simulation of a twin screw loss-in-weight feeder was developed using the discrete element method (DEM). Central to this approach is a custom geometry kernel capable of generating screw configurations given multiple free parameters; this allows the replication of industry-standard designs in addition to a near-infinite design space of novel geometries. By coupling the DEM simulation and geometry kernel with an evolutionary algorithm, this study aims to find optimal parameter sets to minimise flow inconsistencies while maintaining the same mass flow rates as the industry standard geometries.

O32: AI Developed MATLAB Apps for Enhanced Learning of Thermodynamics in Chemical Engineering

Theme: Education

Dr Luis Roman, Dr Matt Keith

[1]London South Bank University, United Kingdom

Thermodynamics is a challenging subject for chemical engineering students at all levels, as it requires both a solid understanding of theoretical concepts and the ability to apply them through rigorous calculations. One of the main difficulties in teaching thermodynamics lies in its extent: the subject encompasses a wide range of topics, and the emphasis placed on each can vary significantly between institutions depending on curricular priorities. Core topics typically covered in chemical engineering programmes include the thermophysical properties of pure substances and mixtures, phase equilibria, heat transfer, combustion, and thermodynamic cycles.

Although a variety of learning resources are available to support the teaching of thermodynamics, such as Wolfram demonstrations, online interactive textbooks, and educational websites, variations in student cohorts, curriculum updates, and topic-specific learning needs may require targeted tools that are not always readily available.
In this work, we present a series of MATLAB apps developed with the assistance of artificial intelligence (ChatGPT) to enhance student learning in selected thermodynamics topics. The apps focus on the use of steam tables, the calculation of molar volumes using equations of state, and the determination of overall heat transfer coefficients for fluid flow in pipes. The applications were implemented and evaluated with student cohorts at London South Bank University and the University of Birmingham, demonstrating the adaptability of the approach across different institutional contexts.

Preliminary results indicate an improvement in student understanding of the selected topics, as reflected in the assessment outcomes of the corresponding modules.

O33: Exploring the feasibility of integrating personalised AI in project work and its impact on student learning and staff load in Biochemical Engineering

Theme: Education

Dr Mauryn Chika Nweke[1], Dr Rana Khalife[1], Mr Tamas Laufer[1]

[1]University College London, London, United Kingdom

Collaborative project-based learning can require increased staff support compared to other learning techniques but where there are limitations in staffing and staff capacity, tailored AI tools may become a solution. The aim of this work is to assess whether the emergence of more personalised AI tools could both reduce staff load and enhance student learning and experience in project work, as a means of assessing whether these tools could be more permanently integrated into the curriculum. Student learning was assessed via the use of surveys to students enrolled on the Regenerative Medicine module who partook in a team-based Design Project and impact on staff load was assessed via interviews with module staff. 100% of the students on this module partook in this study (17 students -10 male, 7 female). These students evaluated the personalised tool ‘Vitafluence AI’, with findings indicating its positive impact on learning. Over half (53%) reported increased academic confidence, and more than half recommended its integration into formal academic support. While 47% believed it could partially substitute an educator’s assistance, none viewed it as a full replacement. The data also showed that 70% of the students felt encouraged to ask more questions but this had an impact on staff workload as 88% of students still needed to ask further questions to the module leader. Whilst there was no significant difference between male and female responses, one thing of note was that female participants felt less confident in the AI tool’s impact on their academic performance.

O34: Bridging the Digital Gap: Mapping Digitalisation Skills in Undergraduate Chemical Engineering Curricula

Theme: Education

Dr Eleni Routoula[1], Dr Joachim Bestenlehner, **Professor Mohammad Zandi**

[1]University of Sheffield, Sheffield, United Kingdom

Digital skills training within chemical engineering education has advanced considerably, driven by the broader industrial shift toward Industry 4.0 and reinforced by global challenges, which have accelerated the adoption of data-driven process engineering. Although chemical engineers have a longstanding history of using computational and modelling tools, particularly commercial process simulators, such expertise has traditionally been developed post-graduation, during industrial practice. Increasingly, however, employers are requesting clear evidence of digital competence during graduate recruitment. Consequently, digitalisation skills can no longer be considered optional enhancements but must be treated as essential learning outcomes within chemical engineering education.

In response, academic institutions have begun to integrate digitalisation-related content more deliberately within taught curricula. Beyond introductory spreadsheet manipulation and basic programming, many courses are now embedding advanced digital capabilities, including data engineering, scientific programming, process analytics, and optimisation techniques. This shift signals a transition from tool familiarity towards a deeper conceptual and applied understanding of digitalisation as a transformative professional competency. However, there remains significant variation in both the extent and coherence of digital skills provision across undergraduate curricula, potentially attributed to the fast-moving industrial needs and expectations around digitalisation, especially over the last few years.

This study systematically maps undergraduate chemical engineering programmes offered at the University of Sheffield against a digital skills framework (including data analysis/visualisation, process simulation, process automation & control, reproducible workflows, and programming) using a qualitative and quantitative approach. Results reveal a scaffolded exposure of students to digital tools, with digital skills being embedded into the curriculum both in taught/core content but also in applied formats that ask students to apply and practise what they are being taught. This study offers a mapping methodology that can be adopted by other chemical engineering departments seeking measurable uplift in Industry 4.0 readiness and demonstrable impact on graduate outcomes.

O35: Smoke and Mirrors: A Grounded Theory of Chemical Engineering Students' Motivations and Perception of GenAI-Learning

Theme: Education

Dr Abdul Wadood Sharif[1], Mr James MacLenan[1]

[1]University of Strathclyde, Glasgow, United Kingdom

Much like many other fields and disciplines, engineering education in higher education attempts to orientate itself from the impact of of the advent of Generative AI (GenAI). Concerns continue to be raised around assessment and academic integrity, however, there remains mixed views as to whether GenAI use results in positive impacts in student learning. While greatly debated, evidence has emerged suggesting that over-reliance of such tools can negatively impact critical-thinking, and indeed, exam grades. Nevertheless, there is limited understanding of how students themselves perceive and navigate their learning in light of such possibilities.

This presentation will report on updates from an on-going qualitative study of undergraduate students studying chemical engineering at the University of Strathclyde, Glasgow. The study aims to explore the two questions: What factors impact students motivations to use GenAI for their learning and, importantly, how do they perceive such learning?

To explore these questions, an MEng student in their final year of study acts as a co-investigator. The study will make use of novel Grounded Theory methods to explore the research questions, which focusses on iterative data collection and analysis, culminating in an emergent understanding of this complex phenomenon. Data collection has included a brief focused-autoethnography conducted by the student as co-investigator, to explore major influences for using Generative AI and self-reflections on confidence in their learning. Semi-structured, qualitative interviews with chemical engineering students at various stages of their study will be used to further explore the research questions in breadth and will be reported on.

O36: Labs 4.0: Redefining Chemical Engineering Laboratories

Theme: Education

Dr Hosam Aleem[1], Mr William Gunshon

[1]University of Manchester, United Kingdom

In this project we explore how teaching labs for chemical engineering programmes can be improved and adapted to modern academic and industry requirements.

The motivation for this work is the consistent low student satisfaction with the chemical engineering labs at the University of Manchester.

The methodology for this research comprised a two-stage process. First qualitative secondary data from unit evaluation questionnaires spanning five past academic years was analysed which identified the main problem being inconsistency in demonstrating and marking. Additional primary data was then generated using a survey exploring the issues in greater depth, designed and validated through a student focus group. The survey was distributed across year groups using targeted methods including presentations in lectures and placing QR codes in relevant places. Thematic classification of qualitative data was performed by the authors with the aid of AI. Quantitative data was analysed using a collection of statistical methods including Spearmen’s correlation test, Matt-Whitny test and two-way ANOVA, employing the statistical packages Qualtrics, SPSS and NVivo.

Findings suggested several problems with the majority relating to inconsistencies across a number of areas including marking, quality of feedback, lab instructions and time demand across experiments. Sentiments on these problem areas were similar across year groups suggesting a widespread need for improvement. Several potential interventions are suggested such as better integration of pre-lab material, reconsidering the role of graduate teaching assistants (GTAs) by providing better training and aligning a GTA with a group of students rather than with an experiment, the use of AI tutors, and their feasibility. Further research is needed to incorporate the perspectives of GTAs and academic staff.

O37: Investigating the Usage of Labster and Its Future Implications for Industry and Academia

Theme: Education

Dr Rana Khalife[1], Pierre Springer, Dr Mauryn Chika Nweke

[1]Ucl, United Kingdom

The unprecedented impact of COVID-19 on engineering education has resulted in lasting changes in the way educators teach as well as the way students learn. One of the most impacted areas was the inability of students to undertake laboratory training, which is crucial for engineering employability. In 2020-21, UCL Biochemical Engineering implemented the use of Labster – a virtual lab simulator that allows students to complete laboratory experiments online, whilst simultaneously exploring complex theories. This project aimed to investigate the impact of using Labster as a lab training tool to evaluate how well it prepared students for industry, and furthermore to understand any implications this may have for academic practice across other departmental programmes. The method for data collection comprised of interviews and survey dissemination to two MSc cohorts and steering committee members who comprise of key industry players. Analysis of the results shows that over 60% of graduates on the MSc reported back that the use of Labster effectively prepared them for the engineering working environment. Similarly, communications with industry suggested that although many companies use in-house virtual software packages, Labster served as a useful tool in helping to bridge the skills gap. The consensus from all students that partook in the study was that the lab simulator was considered to be very useful for practical theory learning which made it easier for them to carry out practical. Based on this, the use of Labster will be rolled out to lab and non-lab-based modules across a range of programmes

O38: Embedding safety and sustainability in the capstone design project

Theme: Education

Dr Alex Sebastiani[1], Dr Dina Kamel Fathalla[1], Dr Sakiru Badmos[1], Dr Aikaterini Tsatse[1], Dr Ademola Odunsi[1], **Dr Michaela Pollock**[1]

[1]University College London, London, United Kingdom

Safety and sustainability are widely acknowledged as key themes of chemical engineering. In this work we examine how these themes are embedded in the capstone chemical engineering design project at University College London. We will outline how consideration of sustainability is embedded in the project scenario, giving students the opportunity to investigate non-traditional process routes, raw materials and energy resources. The importance of safety and sustainability are then embedded throughout all stages of the project lifecycle through a variety of tasks relevant to each project stage. From a safety perspective, students initially perform a preliminary hazard analysis during the conceptual design stage, identifying key hazards and safety challenges, before moving on to perform a hazard and operability study at the end of preliminary design stage. Safety is implicitly considered during detailed design of a major process unit in a variety of ways before culminating in the completion of a Safety Integrity Level (SIL) Analysis examining the reliability of the process unit. Sustainability is initially considered through stakeholder and PESTLE analyses focusing on the social, environmental and economic impacts relevant to the geographic location of the proposed project. Students then move on to perform a life cycle assessment from qualitative and quantitative perspectives considering different system boundaries before again considering sustainability of a major process unit during detailed design. A series of student surveys have been conducted to examine students' perceptions of how sustainability and safety are embedded in the capstone design project. In this work overarching student perceptions are presented, examining where further updates and signposting is required and how this approach has prepared students for their future roles.

O39: Seeing the Connections: Teaching Systems Thinking through SDG Network Visualization

Theme: Education

Dr Polina Yaseneva[1]

[1]UCL, United Kingdom

Teaching systems thinking is increasingly recognised as essential for sustainability education, particularly in chemical engineering, where technical decisions can have wide-ranging environmental, social, and economic consequences. Sustainable Development Goals (SDGs) provide an accessible and well-established framework through which students can explore sustainability as a complex, interconnected system. For this we developed a workshop (as pedagogical approach to attain specific learning objectives) that explores systems through developing and visualising a network of interactions between SDG targets.

The learning activity guides students through a structured process of analysing selected SDG targets and identifying logical, thematic, and causal relationships between them. These relationships are then translated into a network representation, with nodes and edges constructed through student-led reasoning. Network visualisation is used not as an end in itself, but as a cognitive tool to externalise and interrogate students' mental models of sustainability systems. Visual patterns such as clusters, central targets, and highly connected nodes provide entry points for discussion on systemic interactions, trade-offs, and leverage points.

To connect systems thinking with professional practice, the workshop extends the network analysis to real-world chemical engineering contexts. Students are encouraged to explore how specific technological interventions - such as the development of bio-based polymers - may influence multiple sustainability targets simultaneously. By mapping these interventions onto the SDG network, learners examine potential co-benefits, unintended consequences, and system-wide impacts, reinforcing the relevance of systems thinking for decision-making in engineering practice.

The approach emphasises participatory modelling, critical reflection, and interdisciplinary reasoning, positioning students as active agents in constructing and evaluating sustainability knowledge. This contribution demonstrates how network visualisation can support the teaching of systems thinking through concrete sustainability examples, offering educators a transferable method for embedding complexity-aware reasoning into chemical engineering and sustainability curricula.

O40: Life Cycle Assessment of Low-Carbon Olefin Production from Waste Biomass via Methanol to Olefins with Carbon Capture and Storage

Theme: Energy & Net Zero & LCA

Mr Idris Uthman, Dr Massimiliano Materazzi, Dr Andrea Paulillo

[1]University College London, London, United Kingdom

This study presents a cradle-to-grave life cycle assessment (LCA) of low-carbon light olefin production from UK waste biomass via gasification-to-methanol-to-olefins (BGTO) pathway with carbon capture and storage (CCS). The proposed system is a bioenergy with carbon capture and storage (BECCS) configuration aligned with the UK Biomass Strategy and has the potential to achieve net-negative greenhouse gas (GHG) emissions by permanently storing biogenic CO_2.

The chemical sector is difficult to decarbonise because it relies on carbon as both an energy source and a feedstock. In the UK, the chemical industry accounts for approximately 19% of industrial GHG emissions, with light olefin production accounting for around 17% of this total. Ethylene and propylene are essential feedstocks for domestic manufacturing, with production of 2.98 Mt yr^{-1} and associated emissions exceeding 3.1 $MtCO_2e$ in 2023. With demand projected to increase by 60% by 2050, decarbonising light olefin production is critical for meeting future UK carbon budgets.

An industrial-scale BGTO facility is modelled, integrating waste biomass gasification, CCS, methanol synthesis, and methanol-to-olefins (MTO) conversion. The assessment focuses on waste wood and the biogenic fraction of municipal solid waste. The modelled plant processes approximately 110 kt yr^{-1} of biomass and produces around 13 kt yr^{-1} of light olefins. Environmental performance is benchmarked against a conventional fossil-based steam cracking route.

A key element of the analysis is the evaluation of carbon capture solvent choice. Monoethanolamine (MEA) is used as the baseline solvent and compared with potassium carbonate (K_2CO_3) to assess solvent-specific life cycle impacts. Inventory data are generated using a detailed Aspen Plus process model, and impacts are assessed using the EF 3.0 midpoint method in accordance with ISO 14040 and ISO 14044 standards. Results are expected to demonstrate substantial reductions in climate change impacts and identify key process hotspots.

O41: Experimental Screening of Zeolite Adsorbents for CO_2 Capture Using Temperature Swing Adsorption (TSA)

Theme: Energy & Net Zero & LCA

Mrs Israa Alghurabi[1], Dr Helena Navarro, Dr Tongtong Zhang, Professor Yulong Ding

[1]The University of Birmingham, United Kingdom

Carbon dioxide capture using solid adsorbents is a promising approach for reducing emissions from industrial gas streams, particularly when coupled with temperature swing adsorption (TSA) processes operating at moderate regeneration temperatures. However, the performance of TSA systems is strongly dependent on the selection of an appropriate adsorbent, which must exhibit high adsorption capacity, good reversibility, and stable cyclic behaviour.

Carbon capture is also known to be energy-intensive; reducing energy consumption has become a key research hot spot. Our selection of TSA based method aims to address such a challenge through subsequent thermal integration of thermal energy storage. In this study, a systematic experimental screening of commercially available zeolite adsorbents was conducted to identify a suitable candidate for CO_2 capture under TSA conditions. Zeolites with different pore structures and particle forms were initially evaluated. The effect of particle shape on adsorption performance is considered, as it plays a key role in heat and mass transfer for the scale-up at the device/reactor and system levels. Surface, structural and phase properties were characterised using Brunauer–Emmett–Teller (BET) surface area analysis, X-ray diffraction (XRD), and scanning electron microscopy (SEM). Cyclic CO_2 adsorption–desorption behaviour was investigated using simultaneous thermal analysis (STA), enabling direct measurement of mass change and thermal response during repeated adsorption and regeneration cycles.

Clear differences in CO_2 uptake, reversibility, and baseline stability were observed among the tested materials. Zeolite 13X showed CO_2 mass gains of ~18 wt.% across repeated adsorption cycles at 200 °C, indicating high capacity and good reproducibility. Corresponding desorption losses closely matched these values, confirming predominantly reversible adsorption, low mass drift, and good thermal stability under TSA conditions. The work was done at different temperatures, leading to temperature dependence of the sorption capacity.

The work supports adsorbent screening for TSA-based CO_2 capture, with scope for future thermal integration.

O42: Enhanced CO_2 mineralisation using a biogenic Ni-HAp composite in a continuous plug flow reactor

Theme: Energy & Net Zero & LCA

Mr Ijudigal Amtagu Birdling[1], Professor Lidija Siller[1]

[1]Newcastle University, Newcastle Upon Tyne, United Kingdom

Carbon dioxide (CO_2) mineralisation is a promising approach for permanent carbon sequestration through the formation of thermodynamically stable carbonate minerals. In this study, hydroxyapatite (HAp) synthesised from cow bone was milled to a particle size below 75 µm and impregnated with nickel via a wet chemical precipitation method using nickel(II) chloride, yielding a novel Ni-HAp composite with a nickel loading of 19.8 wt%. The composite was evaluated as a mineralisation enhancer for CO_2 capture in a continuous plug flow reactor operated at ambient temperature (25°C) and moderate pressure (1.5 bar).

CO_2 mineralisation experiments were conducted at gas flow rates of 17 and 34 ml/min using a CaCl solution volume of 1.5 L to assess the influence of gas–liquid residence time on carbonation efficiency. At the lower flow rate of 17 ml/min, the Ni-HAp composite achieved the highest $CaCO_3$ conversion (66%), outperforming pure Ni nanoparticles (52%), pristine HAp (46%), and a $CaCl_2$ control (35%). Increasing the CO_2 flow rate to 34 ml/min led to a substantial decrease in conversion efficiency across all systems, although Ni-HAp maintained superior performance (29%). X-ray diffraction and Fourier transform infrared spectroscopy confirmed calcite as the dominant carbonate polymorph, while scanning electron microscopy revealed minor vaterite formation in selected samples.

The results demonstrate that Ni-HAp significantly enhances CO_2 mineralisation by promoting carbonate nucleation and crystal growth, while also highlighting the critical role of gas–liquid residence time in kinetically controlled mineralisation processes by nickel nanoparticles. Overall, this study establishes biogenic Ni-HAp as an effective and low-cost mineralisation enhancer for CO_2 mitigation under mild operating conditions.

O43: Enhanced catalytic effect of chloride ions for iridium catalysts in proton exchange membrane water electrolysers

Theme: Energy & Net Zero & LCA

Miss Alexandra Brochoire[1], Pr Shangfeng Du[1]

[1]University of Birmingham, United Kingdom

Proton Exchange Membrane Water Electrolysis (PEMWE) allows for sustainable hydrogen production from renewable electricity, whilst benefiting from compact design and easy start up. One of its limitations resides in its dependence on expensive iridium catalysts, necessary for the sluggish Oxygen Evolution Reaction. Optimising catalytic performance via improvement of the catalyst structure is a common method to reduce iridium loading, and thus PEMWE costs, whilst conserving efficiency.

Here, we demonstrate a novel process for the synthesis of Ir nanostructures. K2IrCl6 and H2IrCl6 are investigated as precursors to obtain high performing nanostructured iridium catalysts via a hydrothermal method, with formic acid acting as the reducing agent and no surfactants. These catalysts are then tested by using both electrochemical measurement in liquid electrolyte and as catalyst coated membrane in the single PEMWE cell. The optimal synthesis conditions are determined at 6 hours, 140°C and a pH of 1.75. It is found that using K2IrCl6 yielded better performing catalysts than using H2IrCl6, as Cl- residues help the nanostructure dispersion and reduce the double capacity layer formed to reduce the charge transport performance. The single cell test demonstrates better performance of the catalyst produced under these conditions, outperforming commercial iridium black.

O44: Experimental study of green H2 production via photocatalytic ethanol dehydrogenation by Pt/CGCN in flat-plate reactor

Theme: Energy & Net Zero & LCA

Ms Maria Mourkou[1], Dr Dionysia Koufou[1], Dr Xinjie Luo[1], Dr Xiyi Li[1], Dr Yang Lan[1], Professor Asterios Gavriilidis[1]

[1]Department of Chemical Engineering, University College London, London, United Kingdom

Green hydrogen production through solar-driven catalysis is an attractive method towards decarbonization using earth’s abundant solar energy. Photocatalytic ethanol dehydrogenation offers the advantage of co-production of green hydrogen and a value-added organic. Here, photo-dehydrogenation of ethanol was studied in liquid phase at a laboratory-scale flat-plate reactor under solar light simulator with online GC analysis. The photocatalytic activity of Platinum/Crystalline Graphitic Carbon Nitride (Pt/CGCN), a UV-Vis catalyst with an apparent quantum yield of 73 % at 410 nm [1], was evaluated in settled suspension and coated forms. The stability and reusability of the catalysts in coated forms were assessed for consecutive days of light irradiation. Optimization was performed in terms of catalyst form or type of support (specifically glass fiber filter and sponge cloth), catalyst mass, platinum loading, and ethanol/water ratio. The highest hydrogen production rate of 1.66 mLh-1cm-2 was achieved with 0.5 wt.% Pt/CGCN deposited on glass fiber filter, which was comparable to that for 0.5 wt.% Pt/CGCN in settled suspension form. An excellent solar-to-hydrogen efficiency (STH) of 0.9 % was observed for 0.5 % Pt/CGCN (ΔGr,dehydr = + 53 kJmol-1), slightly surpassing the STH of most important photocatalytic overall water splitting technologies (ΔGr,split = + 237 kJmol-1) [2]. The main organic product was acetaldehyde with a production rate of ~ 0.2 mmolh-1 with a solar-to-chemical efficiency (STC) of 0.15% and selectivity of 50 – 60 % depending on the coated substrate, while acetal was also detected as by-product. In addition, molybdenum disulfide was examined as a non-noble metal cocatalyst (MoS2/CGCN), albeit its lower observed hydrogen production, to eliminate platinum, which was highlighted as a significant environmental hotspot in life cycle assessment.

References:

[1] Shvalagin, V., Tarakina, N. et al. (2024). ACS Catalysis, 14(19), 14836–14854. https://doi.org/10.1021/acscatal.4c04180
[2] Nishiyama, H., Yamada, T. et al. (2021). Nature, 598(7880), 304–307. https://doi.org/10.1038/s41586-021-03907-3

O45: Ball Milling for Mechanical Valorisation of Asphaltene

Theme: Energy & Net Zero & LCA

Eng Fahad Alajmi[1]

[1]University of Strathclyde, Glasgow, United Kingdom

Asphaltenes, the heaviest fraction of crude oil, present significant challenges for efficient conversion due to their complex nature (1,2). A deeper understanding of their molecular behaviour under mechanical stress can build a strategy to enhance their reactivity is of significant industrial interest (3). This study aims investigates the impact of 24-hour of ball milling treatment on asphaltene thermophysical properties including molecular transformation. Various analytical protocol including Raman spectroscopy were implemented to capture the full picture of mechanical effect. The results show that asphaltene underwent mechanochemical oxidation with ~3.7% higher oxygen content while preserving the overall elemental composition of other atoms. The average molecular assemblies became more uniform, as indicated by a reduced dispersion value via GPC, and Raman spectroscopy revealed an increase in both D and G band integrals (from 44.6 and 16.3 to 67.8 and 22.9, respectively), signifying greater aromatisation accompanied by structural disorder. The average aromatic sheet length decreased from 16 to 14.86 Å, evidencing edge defects in the aromatic core. The kinetic analysis further demonstrated that ball milling reduced energy activation at early stages, to facilitate an earlier onset of decomposition. Meanwhile, in the refractory zone, molecular modifications sustained higher conversion and lowered kinetic barriers relative to the asphaltene sample. Overall, ball milling emerges as a green and scalable strategy for asphaltene oxidation and molecular modification, offering potential benefits for both chemical processing and oil industry optimisation for the producing of low carbon fuels.

1- AlHumaidan, F.S., Rana, M.S., Vinoba, M., Ali, D., AlArbeed, B., AlMujaibel, M., AlSheeha, H.M. and Rajasekaran, N., 2025. Asphaltene-derived nanoporous carbon materials for CO2 capture and supercapacitors.

2- Groenzin, H. and Mullins, O.C., 1999. Asphaltene molecular size and structure.

3- Al-Ajmi, F. and Li, J., 2024. Crystal structure of asphaltene under mechanical stress of ball
milling.

O46: Enhancing CaO Based Thermochemical Energy Storage through Metal Oxide Doping

Theme: Energy & Net Zero & LCA

Mr Kenechukwu Ugonabo[2]

[1]Teesside University, Middlesbrough, United Kingdom, [2]Airhive LTD, Middlesbrough, United Kingdom

Thermochemical energy storage based on the reversible hydration and dehydration of calcium hydroxide to calcium oxide remains a promising pathway for high density and long duration heat storage. However, high regeneration temperatures, slow hydration kinetics, and significant energy penalties continue to limit its integration with renewable heat sources and low carbon industrial processes. Improving material performance is therefore essential for unlocking the full potential of calcium oxide based thermochemical storage.

This research introduces a novel material modification strategy in which magnesium based salts, specifically magnesium oxide, are incorporated into calcium oxide to shift the operating window of the CaO system and overcome kinetic and energy barriers. A series of carefully controlled bench scale experiments were conducted to evaluate the influence of magnesium oxide on dehydration behaviour, hydration kinetics, and overall cycle efficiency. Samples containing varying magnesium oxide concentrations were synthesised and subjected to repeated hydration and dehydration cycles, with their performance characterised using thermogravimetric analysis, calorimetry, and kinetic modelling.

The newly developed materials, represented as $Ca(1-x)Mg(x)O$ prior to hydration, demonstrate a substantial improvement in thermal and kinetic behaviour. The temperature required to initiate the $Ca(OH)_2$ decomposition reaction decreased from approximately 515 degrees Celsius in the undoped system to around 350 degrees Celsius in the magnesium doped samples. A sample containing 30 weight percent magnesium oxide delivered a 22 percent improvement in overall system efficiency and significantly reduced regeneration heat requirements due to a measurable decrease in activation energy. Hydration times, which typically range from 140 to 160 minutes in conventional calcium oxide thermochemical energy storage systems, were reduced to 50 to 90 minutes in the doped materials, indicating a marked enhancement in reaction kinetics and improved cycle stability.
These findings highlight magnesium based doping as a promising route for advancing calcium oxide thermochemical energy storage systems.

O47: Effect of shear, cooling rate and composition on crystallisation of solid fabric enhancer

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Lucie Hlubinková[1], Fang Liu, Michael Fontaine, Peter J. Fryer, Zhenyu J. Zhang

[1]University of Birmingham, United Kingdom

The possibility of tuning product properties by changing crystallinity via process conditions has been used in many different formulated products (e.g. chocolate). This work investigates the effect of shear, cooling rate and composition on the crystallinity of solid fabric enhancer (SFE). The aim is to determine if tuning of product performance via process conditions (shear, cooling rate) or formulation changes (ratios, clay addition) was possible. Rheometry and differential scanning calorimetry (DSC) were used to study the effect of slow (1s-1) and fast (1000s-1) shear on SFE crystallinity. Both traditional and flash DSC were used to study the effect of slow (1°C/min), fast (10°C/min) and super fast (15, 30, 50 °C/s) cooling on SFE crystallinity. In addition, the effect of formulation composition on crystallinity was investigated as well. The obtained results showed no significant influence of shear and cooling rate on final SFE crystallinity, suggesting tuning of SFE properties via changing process conditions to not be viable. Changes made to SFE formulations (ratio of quaternary ammonium ester:fatty acid (EQ:FA), addition of clay) showed influence on the resulting crystallinity with crystallinity decreasing as EQ content was increased; evidenced by ΔH decreasing with more EQ present in the mixture. Additionally, a second Tm peak which increased in size and separation from the main Tm peak, was observed as EQ content increased. This suggests formation of EQ-rich and FA-rich phases which produce these separate Tm peaks, as we increase the EQ content. Addition of clay caused the formation of another crystalline phase as evidenced by additional peak on the melting DSC curve. This additional phase is believed to be caused by changes in the molecular orientation within the coating caused by the EQ positively charged head groups orienting around the negatively charged clay particle in a micelle-like orientation.

O48: From Membranes to Transport-Integrated Porous Beads: Redesigning Diffusion in Chemical Engineering Materials

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Dr Zhentao Wu[1], Dr Jiaojiao Zheng[1]

[1]Aston University, United Kingdom

Diffusion and mass transport limitations have long governed the performance of chemical engineering processes, from heterogeneous catalysis and separations to electrochemical and environmental technologies. While intrinsic reaction kinetics are often fast, overall efficiency at realistic length scales is frequently constrained by tortuous transport pathways within porous materials. Over the past two decades, ceramic hollow fibre membranes have provided powerful platforms for intensifying transport–reaction coupling, yet their applicability remains intrinsically linked to membrane-based geometries.

Here, we present a conceptual and structural transition from ceramic hollow fibre membranes to a new class of transport-integrated porous beads, representing a platform-level rethinking of how diffusion constraints can be addressed in functional materials. Building on long-term expertise in microstructural control of ceramic membranes, this work identifies diffusion as a unifying limitation across reaction and separation systems and reframes it as a designable property rather than an unavoidable penalty.

The proposed architecture consists of millimetre-scale porous beads constructed entirely from mesoporous matter, incorporating radially aligned macroporous channels that extend from the core to the external surface. These directional pathways dramatically reduce diffusion length scales and tortuosity while preserving high internal surface area, effectively reconciling accessibility with reactivity under realistic operating conditions. Unlike conventional hierarchical or coated systems, mass transport is intrinsically integrated into the material geometry itself.

This structural concept has been extended beyond ceramics to include organic–inorganic hybrids and metallic systems, enabling applications spanning catalysis, advanced oxidation processes, separations, and multifunctional materials. Supported by patented designs and advanced characterisation techniques, this work establishes a versatile porous-materials platform that generalises principles originally developed for membranes into a broader materials framework.

By bridging membrane science and porous materials engineering, this contribution offers a unified strategy for overcoming diffusion-limited performance in chemical engineering, opening new opportunities for the design of next-generation catalytic, separation, and energy materials.

O49: Plant protein textures through freeze structuring

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Evelyn Tait[1], Professor Bettina Wolf[1], Professor Mark Simmons[1], Dr Isabel Fernández[2]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Heura Foods, Barcelona, Spain

The aim of this research is to enhance the textural properties and consumer acceptance of plant-based meat analogues. The poorer texture and mouthfeel compared to animal meat, in particular whole cuts, discourages consumers from switching to a more-sustainable, healthier, plant-based diet. The unsatisfactory texture of plant-based meats is attributed to a fibrous texture that does not resemble the hierarchical fibrous texture of animal muscle. Structure is linked to water holding capacity and water release which drives succulency. Both attributes are compromised for meat analogues. The commercial technology of choice, extrusion, fails to create desirable, aligned structures.

Freeze structuring presents an alternative approach. Although this technology is not novel, it needs to be further developed to overcome challenges of scale-up and ingredient functionality. In brief, ice crystals are grown unidirectionally through a protein slurry and structures form between the ice crystals. Melted structures require kinetic trapping such as via melting in salt solution for protein cross-linking and gelation of polysaccharides for firmness. To offset the need for polysaccharides, protein functionality should be optimised. Here, the hypothesis that the functionality of the protein in aqueous dispersion relates to the final texture of freeze-structured samples was tested. Commercial pea protein isolates were characterised and functional properties adjusted through alkalisation. Following unidirectional freezing, anisotropy was assessed by texture analysis and imaging using X-ray tomography.

Alkalisation of protein increased solubility, water holding capacity, and cysteine availability of the isolates, as internal bonds were broken. Unidirectionally frozen samples were texturally and visibly anisotropic. Higher alkaline pH resulted in firmer textures and smaller protein structures, which better replicated meat. In contrast, nondirectionally frozen untreated dispersions were disordered and not self-supporting structures; structure is not only dependent on freezing conditions. The results demonstrate that it is possible to enhance freeze-structured plant protein textures by modulating initial protein functionality.

O50: UK-India consortium for Bio-based chemicals and sustainable innovation: A case study

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Hiya Deshpande[1], Dr. Rahul Nabar[2], Dr Parimala Shivaprasad[1]

[1]University of Nottingham, United Kingdom, [2]IIT Bombay, Mumbai, India

The transition from fossil-derived chemicals to sustainable, bio-based alternatives is central to achieving global net-zero targets. Although many bio-based chemical processes are technically viable, large-scale deployment is limited by scale-up, economic, and policy barriers rather than technology readiness. The UK-India Workshops on Bio-based Chemicals and Sustainable Innovation were convened to explore how bilateral collaboration could address these challenges and accelerate low-carbon chemical production.

This initiative builds on the complementary strengths of the two countries. The UK has a strong research and innovation base in industrial biotechnology, synthetic biology, and chemical engineering, supported by translational programmes such as the Networks in Industrial Biotechnology and Bioenergy (NIBB), which have successfully derisked emerging bio-based technologies. India, by contrast, is a major global chemical producer with established manufacturing capacity, access to diverse biomass feedstocks, and significant scale-up potential. Leveraging these strengths presents an opportunity to develop a UK-India consortium for bio-based chemicals that supports industrial decarbonisation, economic growth, and supply-chain resilience.

Two workshops with distinct formats and stakeholders were held to gather insights. A UK-based workshop at the University of Nottingham focused on early-stage innovation, academic research, and policy perspectives, while a second workshop at IIT-Bombay engaged industry, funding bodies, and policymakers. This structure enabled comparative analysis across geographies, technology readiness levels, and shared bottlenecks.

Discussions highlighted differences between speciality and commodity chemicals: speciality products offer nearer-term commercialisation due to higher margins, whereas commodity chemicals promise greater long-term impact but face substantial economic challenges. While the academics emphasised barriers in transitioning from pilot to real-world deployment, alongside limited funding and infrastructure. Across both workshops, participants stressed the need for stable regulation, carbon incentives, and long-term policy certainty. Outcomes are being consolidated into a policy-focused white paper to guide governments and funders on UK–India collaboration, coordinated investment, and policy support for bio-based chemicals and net-zero.

O51: DEM Simulations of the dry mixing of NMC 622 lithium-ion battery cathodes

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Dr Sam Hare[1], Dr Alok Tiwari[2], Prof Emma Kendrick[1], Prof Rachel Smith[2], Prof Mark Simmons[1]

[1]University of Birmingham, United Kingdom, [2]University of Sheffield, United Kingdom

Understanding of dry mixing in the manufacturing of lithium-ion battery electrodes has the potential to improve process sustainability by either reduction or elimination of organic solvents and consequent energy costs of slurry drying. The dry mixing dynamics of NMC 622, a cathode electrode material used in lithium-ion batteries, were simulated using the Discrete Element Method (DEM), with the simulation calibrated from the material properties of NMC 622. These simulations were then validated using experimental Positron Emission Particle Tracking (PEPT) data across a range of rotor tip-speeds at a fixed co-rotating pan speed and fill height. Both methods captured a previously unobserved disengagement of the free surface of the electrode material from the rotor at higher tip-speeds, and diminishing mixing performance, confirmed by estimating the transient mixing time using the Lacey mixing index.

The DEM simulations were used further to explore the granular dynamics of NMC 622 at different fill heights within the mixer. Fill height was adjusted by adding more particles into the system up to 2.5 times the initial number of particles. It was found that this increased the volume of the granular fluid around the rotor and lowered the number of particles in the granular gas above, as less are thrown clear of the main material flow by the rotor. Particle velocities, changes in vessel circulation time, dispersion and Péclet number were calculated. These gave an understanding of the dominant mixing mechanism and vessel turnover; the Lacey mixing index was calculated to compare transient mixing times and particle dynamics in the granular fluid.

O52: Bespoke High-resolution 3D particle tracking for a 21L Stirred Tank

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr George Truc[1], Professor Mark Simmons[1], Professor Kit Windows-Yule[1], Dr Li Liu[2], Dr Carl Tipton[2]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Johnson Matthey, Sonning Common, United Kingdom

Traditional flow visualisation techniques such as Particle Image Velocimetry (PIV) and Positron Emission Particle Tracking (PEPT) are expensive and are essentially limited to specialist University Laboratories.

Particle Tracking Velocimetry (PTV) is a 3D Lagrangian tracking technique for visualising fluid flow. Parallax setups limit the field of view in PTV systems. This study has addressed these issues by developing a low-cost optical PTV alternative based on a single-frequency light source and orthogonal mirrors to increase the field of view, which can be deployed in any open laboratory.

The new PTV rig is presently optimised for a 21 L standard stirred tank. The development phase was primarily based on finite element modelling of the system, including the optical properties of the materials, thereby enabling design and optimisation based on first principles.

This work discusses the development of the reconstruction model from first principles, handling high data throughput to obtain a more representative mixing study across a wide range of fluid mixing dynamics, and using optical mechanics to achieve lower signal-to-noise ratios.

The conventional PTV setup methodology relies on a narrow camera offset, which minimises stereographic depth due to obscuration constraints. As PTV does not have the same seed-particle number density as PIV, the camera angle offset does not need to be minimised. This work found that an orthogonal arrangement maximises the spatial field while maintaining high spatial resolution.

The benefits of combining the PTV digital twin with experimental PTV results in a stirred tank will be discussed, with example results presented.

Acknowledgements:

George Truc is funded by a studentship from the EPSRC Centre for Doctoral Training in Formulation Engineering: Sustainable Structured Products (EP/S023070/1) at the University of Birmingham and Johnson Matthey.

The authors would like to acknowledge Ben Watson for their contribution to this project and Hugh Stitt for their helpful comments.

O53: Power and Flow Analysis of a High Throughput Testing System for the Formulation of Lamellar Gel Networks

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Aled Williams[1,2], Dr Thomas Abadie[1], Dr David Bell[2], Professor Mark Simmons[1]

[1]School of Chemical Engineering, University of Birmingham, West Midlands, United Kingdom, [2]Unilever Research and Development, Port Sunlight, United Kingdom

Lamellar gel networks (LGN) are multiphase structures found in a range of personal care products including hair conditioners. Changing fill height and an evolving fluid rheology during manufacture present significant mixing challenges in production and in scale-down for discovery of new formulations. This work explores the potential of a high throughput testing device for the investigation of new formulations, employing a helical ribbon in a 34 mm diameter cup filled to a height of 36 mm (100%), attached to a rheometer. Since flow characteristics at this scale are not normally representative of those at pilot and production scale, this work aims at linking the scales through characterisation of the fluid dynamics and mixing.

Dynamic torque measurements employing Newtonian and shear-thinning model fluids have shown that power draw in the laminar regime is generally linear with respect to rotational speed at fill levels of 25, 62.5 and 100%. In the laminar regime, inverse proportionality of the power number to the Reynolds number is found ($3 < Re < 24$), as expected. Comparison with OpenFOAM CFD simulations using the SIMPLE algorithm at low rotational speeds, where the free surface is modelled as flat, are in good agreement. However, as the rotational speed increases, significant deformation of the free surface occurs in the experiments, leading to an overprediction of torque, and consequently power draw in the SIMPLE simulations. Volume of fluid (VOF) simulations allowing for free surface deformation give improved predictions, further validated by 2-D Particle Image Velocimetry (PIV) data obtained in both horizontal and vertical planes.

O54: When Data Augmentation Improves Metrics but Not Design Quality: Insights from AI-assisted Process Design

Theme: AI & Data Driven Studies

Mr Ali Tarik Karagoz[1], Mr Zhang Wan[1], Dr Jie Li[1]

[1]University of Manchester, Manchester, United Kingdom

Machine learning (ML) and artificial intelligence (AI) methods are increasingly used in chemical engineering, particularly for conceptual process design and synthesis, where the limited availability of high-quality flowsheet data remains a major bottleneck. Synthetic data generation and data augmentation offer practical routes to address this limitation, yet most prior work evaluates their effects primarily through syntactic metrics without assessing how they influence the operational performance or quality of generated flowsheets. In this work, we study data augmentation in a generative process synthesis framework where candidate flowsheets are screened based on optimization results rather than syntactic validity alone. A cyclic augmentation scheme is introduced, expanding the dataset through rotational permutations of linear text representations of supercritical CO_2 power-cycle layouts. Three regimes are considered: no augmentation (NA), training-only augmentation (A), and fully augmented training and validation (FA), evaluated using two generator models (LSTM and a decoder-only transformer). The LSTM benefits consistently from augmentation, with the fraction of high-performance designs increasing from 24% (NA) to 35% (FA). In contrast, the corresponding fraction decreases from 33% to 11% for the transformer, and the best design quality degrades when augmentation is applied during pretraining. These results indicate that learning from process structure alone, even when combined with performance-based filtering, does not reliably guide generative models toward high-quality designs, since performance is not an explicit part of the learning signal. As a result, established ML tools such as data augmentation may improve model-level metrics while potentially degrading the usefulness of generated designs under these limitations.

O55: Optimisation of the Granular Section of a Twin-Screw Extruder for Sustainable Plastic Processing

Theme: AI & Data Driven Studies

Dr Daniel Rhymer[1], Oluwatobiloba Henry[1], Joe Wood[1], Deborah Crawford[2], Matthew Seabrook[3], John Williams[3], Kit Windows-Yule[1]

[1]School of Chemical Engineering, University of Birmingham, Birmingham, United Kingdom, [2]School of Chemistry, University of Birmingham, Birmingham, United Kingdom, [3]Aquapak Polymers Limited, Birmingham, United Kingdom

Plastics are responsible for 3.3% of global emissions, or more than the entire aviation industry [1]. Solutions are required to reduce this, and Aquapak Polymers has developed Hydropol [2], a sustainable polymer that dissolves at the end of its life, leaving no harmful trace to the environment. However, the underpinning polyvinyl alcohol (PVOH) compound is challenging to manufacture due to its narrow operating window. PVOH is often synthesised in a twin-screw extruder. A pair of parallel screws transports the process material along their length, and a carefully ordered sequence of conveying and kneading elements mix and synthesise these to form the desired product. The extrusion process is highly complex, and simulating the full process is too difficult as several process phenomena are involved. Therefore, this submission focuses on optimising the granular conveying region at the start of the process using the Discrete Element Method.

For granular conveying, a special SK element is used that has better powder scraping capability than other conveying elements. By mathematically describing this element and applying an evolutionary optimiser, the geometry of the screws could be modified to enhance overall performance. Six features of the screw design were optimised. The radius, clearance and pitch of the screws had the greatest effect on the observed throughput, while adjusting three curvature parameters on the screw cross-section had a greater effect on the average particle force. The best design improved the simulated throughput by 31.2%, while reducing the average force on each particle by 57%. A selection of the optimised screws were 3-D printed to validate the throughput results. The experimental results were qualitatively identical to the simulations, and showed a throughput improvement of 20%, indicating that the optimiser has found a valid design.

References:
[1] H. Ritchie (2023), https://ourworldindata.org/ghg-emissions-plastics/
[2] Aquapak Polymers (2025), https://www.aquapakpolymers.com/hydropol/

O56: Gaussian Processes and Active Learning for Drug Particle Size Characterization in Continuous Flow Antisolvent Crystallization

Theme: AI & Data Driven Studies

Mr Arun Pankajakshan[1], Ms Ishaa Mane[1], Dr Maximilian O. Besenhard[1], Prof Asterios Gavriilidis[1], Prof Luca Mazzei[1], Prof Federico Galvanin[1]

[1]Department of Chemical Engineering, University College London, Torrington Place, WC1E 7JE, London, United Kingdom

Driven by advances in computing power and algorithmic development, machine learning methods have recently demonstrated impressive capabilities in data-rich domains and have created a wave in computational research. Yet their applicability remains limited in many engineering and industrial problems where data are scarce, expensive or difficult to obtain. This limitation is particularly relevant in chemical engineering and pharmaceutical applications, where experiments are costly and time consuming with strict operational bounds.

Gaussian process (GP) models, a form of generative artificial intelligence operating in a latent function space, are inherently well suited for low-dimensional, small data settings, as they provide probabilistic predictions, uncertainty quantification and sample efficient learning. When combined with active learning, an algorithm similar to optimal experimental design, GP-based approaches offer a principled and practical framework for developing accurate models to be used as digital twins under data-scarce conditions.

In this work, we discuss and demonstrate the closed loop development of a GP model via constraint-adaptive active learning, applied to pharmaceutical drug particle size characterization. Our approach proved effective in developing a predictive model for drug nanoparticle size during automated continuous flow antisolvent crystallization. Constraint learning and its adaptation within the active learning framework ensured that the GP model development was carried out in a region of operating conditions that never caused fouling in the antisolvent crystallization process. Overall, our approach provides an autonomous (fast and efficient with no human intervention) way of creating a digital twin model for predicting drug particle size that can accelerate the continuous flow drug synthesis processes with improved quality control.

O57: Limitations of Classical Force Fields for CO_2 Adsorption in MOFs: Toward Quantum Accuracy at DAC-Relevant Pressures

Theme: AI & Data Driven Studies

Mr Abdullah Al Rammah[1], Dr. Ashwin Rajagopalan[1], Prof. Lev Sarkisov[1], Dr. Miguel Jorge[2], Prof. Flor Siperstein[1]

[1]University of Manchester, United Kingdom, [2]University of Strathclyde, United Kingdom

Molecular simulations offer a fast route to screening experimental and hypothetical MOFs, but their reliability hinges on the quality of the force field, and experimental validation is challenging due to framework defects and subtle errors in low-pressure measurements [1]. Our calculations show that isotherms calculated with generic classical force fields for anion-pillared MOFs (relevant for direct air capture (DAC)) generally overpredict uptake at low pressures, and no single parameter set accurately describes adsorption across this family. Framework flexibility can also alter uptake at low pressures. We therefore perform simulations informed by quantum-mechanical calculations of MOF–CO_2 interaction energies, thereby establishing benchmarks that are independent of experimental uncertainty and generic force fields. We evaluate universal machine-learning (ML) interatomic potentials trained on quantum data, which offer reduced cost relative to density functional theory (DFT), and identify significant errors in short-range interaction energies that can induce unphysical adsorption. Consequently, we are working to parameterise classical force fields directly from DFT energies for representative MOFs. Overall, we assess uncertainties associated with force field selection, framework flexibility, experimental artefacts, and ML potentials, and highlight pitfalls in screening MOFs for DAC.

References:

[1] A. F. Al Rammah, A. K. Rajagopalan, L. Sarkisov, F. Siperstein, Adsorption 31, 94 (2025).

O58: Automated Flow Platform for Kinetic Model Identification

Theme: AI & Data Driven Studies

Mr Xianfeng Jian[1], Dr Maximilian Besenhard[1]

[1]University College London (UCL), London, United Kingdom

Flow chemistry is becoming increasingly utilized in synthesis and process optimization. However, most continuous production still relies on tubular reactors, which can be limited by more complex transformations involving multiphase flow. Cascades of continuously stirred tank reactors (CSTRs) are emerging as a powerful option, which allow for controlled residence time distributions and sampling at intermediate stages to construct a comprehensive concentration-time profiles of reacting systems.

Amide coupling is a key transformation in pharmaceutical manufacturing, while its kinetics under continuous-flow conditions remain poorly characterized. To address this gap, we developed an automated multi-CSTR cascade platform equipped with inline infrared spectroscopy and online HPLC for intermediate sampling. This design enables systematic kinetic data acquisition under varied residence times, stoichiometries, and operating conditions, providing comprehensive and structured datasets for kinetic analysis.

Based on the experimental datasets obtained from the CSTR cascade, we propose an automated kinetic modelling framework to discover interpretable rate laws. The procedure begins by smoothing concentration–time trajectories to obtain reliable estimates of reaction rates. These rates, together with the smoothed concentration profiles, are then used as inputs to generate candidate kinetic expressions constrained by mechanistic priors. Each candidate is calibrated through nonlinear regressio and ranked according to information criteria, with non-significant terms removed to simplify the models while maintaining predictive accuracy. Model-based design of experiments (MBDoE) can also be used to guide the next set of experiments to best discriminate among remaining candidates. This iterative cycle of kinetic data generation and model discovery yields compact and interpretable kinetic models.

By combining an automated CSTR cascade platform with kinetic model discovery, this framework establishes an integrated route to kinetic characterization of amide couplings under flow. Additionally, the methodology illustrates how hybrid experimental-computational strategies can advance reaction engineering, enabling kinetic models that support process optimization and digital twins for pharmaceutical manufacturing.

O59: From Infrared Spectra to Gas Transport: Group-aware Machine Learning for Polymer Membranes

Theme: AI & Data Driven Studies

Mr Mehryar Jafari[1], Dr Bernardo Castro-Dominguez[1]

[1]University of Bath, Bath, United Kingdom

Accurate prediction of gas permeability in polymer membranes is challenging due to its strong dependence on chemical structure, morphology, and thermophysical properties. Conventional structure–property models typically rely on curated molecular descriptors or extensive experimental data, limiting scalability and transferability to new polymers. Building on prior work demonstrating that Fourier Transform Infrared (FTIR) spectra can encode chemically meaningful information for predicting polymer thermophysical properties, this study extends FTIR-driven machine learning to polymer gas permeability prediction.

A curated dataset of over 850 FTIR spectra linked to experimentally measured permeabilities for He, H_2, CO_2, N_2, O_2, and CH_4 was assembled and pre-processed using interpolation, smoothing, and normalisation. To address heterogeneity in polymer transport behaviour, polymers were classified into four transport-relevant groups—rubbery, glassy-polar, semicrystalline, and styrenic—based on crystallinity and chemical characteristics. Separate group-specific regression models were trained using CatBoost, with log-transformed permeability as the target variable to capture its multi-order-of-magnitude variability. Minimal physicochemical descriptors were included, avoiding explicit molecular structure encoding.

The group-aware modelling strategy substantially outperformed a single global model. For CO_2 permeability, group-specific models achieved out-of-fold R^2 values exceeding 0.90 for semicrystalline and rubbery polymers, with median multiplicative errors close to unity across all groups. Incorporation of glass transition temperature (Tg) further improved predictive stability. While pooled performance metrics were dominated by larger transport classes, smaller groups contributed minimally to overall error, underscoring the importance of reporting both class-wise and pooled evaluations.

Model interpretability was achieved through aggregated feature importance analysis. FTIR-derived features dominated predictive performance, with chemically meaningful spectral regions consistently identified. When PCA was applied, component importances were back-projected to wavenumber space, enabling direct physical interpretation.

Overall, this work demonstrates that FTIR-driven, group-aware machine learning provides an accurate, interpretable, and scalable framework for predicting polymer gas permeability, offering a practical alternative for rapid membrane material screening.

O60: Systematic Data Generation through automated HTE Acrylamide Coupling Synthesis for future ML reaction optimization

Theme: AI & Data Driven Studies

Mr. Yihang Fang[1], Professor Alan Armstrong[2], Professor Claire Adjiman[2], Dr. Lauren Ye Seol Lee[1]

[1]University College London, London, United Kingdom, [2]Imperial College London, London, United Kingdom

Amide bond formation has long been regarded as a cornerstone in organic synthesis, integral to applications across medicinal chemistry, material science, chemical manufacturing[1]. In particular, acrylamide functionality has gained renewed attention due to their importance as monomer for large-scale polymer production and as covalent drugs[2]. One of the simplest ways of introducing the acrylamide functionality is via amide coupling reactions. However, liquid-phase synthesis of acrylamides via amide coupling reaction often unreliable because the α,β-unsaturated carbonyl group is prone to competing side reactions, including premature polymerisation[3]. This sensitivity makes condition optimisation difficult and limits the transferability of reported procedures across substrates[4].

Machine learning (ML) has emerged as a promising tool to accelerate reaction condition optimisation for such complex systems, but model reliability depends heavily on the quality and completeness of reaction data. Existing literature-derived datasets often lack essential experimental parameters, such as precursor solubility and mode of addition, and are biased toward successful reaction outcomes, that can strongly influence acrylamide formation versus side reactions[5].

In this study, we present an automated high-throughput experimentation (HTE) framework designed to generate well-curated, unbiased datasets for acrylamide coupling synthesis that integrates rapid solubility screening as a crucial step to define a feasible concentration window prior to reaction execution, ensuring each substrate pair is tested under practically achievable conditions. We then use automated protocol control to standardise and record reaction-critical variables such as concentration and pre-activation that are frequently missing from the literature. Through automated HTE, we build a high-quality acrylamide library synthesis dataset that includes 432 novel reaction combinations with accurate repetition and cross validation, demonstrating the capacity of HTE to improve reaction accuracy and reproducibility. This comprehensive dataset provides an initial foundation for mechanistic interpretation and for subsequent ML guided condition optimisation of acrylamide synthesis.

O61: Hot Microbubble Gas Stripping for In Situ Butanol Recovery from continuous Fermentation

Theme: Energy & Net Zero & LCA

Ms Ashraf Hauwa Nyako[1], Dr Ahsan Islam[1], Dr H. C. Hemaka Bandulasena[1]

[1]Loughborough University, United Kingdom

Meeting net-zero targets requires expansion in the production and utilisation of bio-based fuels from lignocellulosic biomass. However, fermentation routes remain limited by product inhibition and high separation costs. While hot microbubble gas stripping has been shown to improve performance in thermophilic ethanol systems by intensifying gas-liquid mass transfer and mitigating inhibition, it has not been evaluated for butanol fermentation under mesophilic conditions. This work therefore assesses hot microbubble stripping of butanol from dilute butanol-water solutions prior to fermentation integration.

An external-loop microbubble stripping unit (MSU), developed by Calverley et al. (2024), was coupled to a jacketed dummy fermenter operated at 37 °C. Monodispersed microbubbles were generated using a porous nickel membrane and a fluidic oscillator. Inlet air flowrate was varied between 5 and 15 SLPM and heated to 41 °C. n-Butanol-water solutions initially containing 2 % v/v butanol were stripped in batch and continuous modes. In continuous operation, butanol was added externally to simulate productivities up to 5 $g\ L^{-1}\ h^{-1}$. Spent broth containing non-viable cells was also evaluated, and a dynamic model implemented.

Butanol concentrations decreased from the initial 2 % v/v, achieving a maximum stripping rate of 8.62 $g\ L^{-1}\ h^{-1}$. At the highest simulated productivity, stripping removal closely matched the addition rate, producing condensate concentrations of approximately 18 % v/v and recoveries approaching 95-100 %. Higher flowrates increased stripping capacity but reduced enrichment and led to systematic model overprediction above 10 SLPM. Turnover-based normalisation indicated consistent performance across increasing working volumes, while spent broth imposed only minor penalties. The dynamic model reproduced trends at moderate flowrates but deviated at higher throughputs.

The MSU demonstrates feasible butanol recovery under mesophilic-compatible conditions with scalable performance and a clear trade-off between stripping capacity and product concentration. Numerical modelling provides reliable prediction within practical operating ranges relevant to process design.

O62: Chloride-Induced Morphology Control of Pt Coatings on Titanium Porous Transport Layers for Proton Exchange Membrane Water Electrolysers

Theme: Energy & Net Zero & LCA

Miss Liqiu Liu[1], Dr. Yichang Yan[1], Prof. Yu-Lung Chiu[2], Prof. Shangfeng Du[1]

[1]School of Chemical Engineering, University of Birmingham, United Kingdom, [2]School of Metallurgy and Materials, University of Birmingham, United Kingdom

Low-temperature water electrolysis, particularly proton exchange membrane water electrolysis (PEMWEs), has emerged as a promising technology for green hydrogen production. The Porous Transport Layer (PTL), located between the catalyst layer and the bipolar plate in electrolysers, plays a crucial role in ensuring water delivery to the electrode, facilitating gas removal, and providing efficient electronic conduction. Titanium is commonly employed as the base material for PTLs due to its favourable balance of corrosion resistance, electrical conductivity, and mechanical robustness to meet the requirements under harsh anodic conditions in PEMWEs of an oxidative environment with high temperature (> 60 °C) and working voltage (> 1.6 V). Yet, the challenges remain - the surface passivation of titanium in the water-oxygen environment and the rapid formation of TiO_x layers. Platinum coatings are widely applied on titanium porous transport layers (PTLs) to mitigate passivation and reduce interfacial resistance. However, with the commonly used electrodeposition process, it is still a challenge to form a uniform coating structure. In this work, we introduce chloride ions during the electrodeposition process to control the morphology of Pt coating on Ti felt. Distinct nanostructures of platinum are obtained by the addition of KCl, ranging from rose structure in chloride-free electrolyte to cauliflower-like clusters at low concentration, dense nanoflakes at moderate concentration, and stacked agglomerates at high concentration. The Pt nanoflakes coating exhibits higher surface coverage, significantly reduced interfacial contact resistance, and enhanced corrosion resistance, delivering a superior voltage efficiency of 1.813 V at 2 A/cm^2 in the PEMWE single cell test compared to the commercial Pt-coated PTL. Mechanistic insights are also explored to provide practical guidelines for the design of durable, high-performance PTLs in water electrolysis.

O63: Do national policies reflect country archetypes in petrochemical decarbonization? A cross-country analysis

Theme: Energy & Net Zero & LCA

Dr Zhenxi Li[1], Penny Hamlin[2], Chris Hamlin[2], Professor Anthony Ryan[1], Dr Nixon Sunny[3], Dr Marwan Sendi[3], Dr Amir Abdul-Manan[3], Professor Fanran Meng[1]

[1]School of Chemical, Material and Biological Engineering, University of Sheffield, Sheffield, United Kingdom, [2]HancockHamlin Ltd, Hexham, United Kingdom, [3]Life Cycle Assessment (LCA) Group, Technology Strategy & Planning Department, Saudi Aramco, Dhahran, Saudi Arabia

Emissions from the petrochemical industry are often regarded as hard-to-abate, requiring decarbonization policies to overcome technological, economic, and institutional barriers. Substantial cross-country differences in involvement along the petrochemical value chain further complicate the design of effective decarbonization strategies. In previous work, we classified 152 countries into eight petrochemical archetypes based on their positions and integration in the global value chain [1]. This framework suggests that countries with similar demand, supply, and market characteristics typically face comparable decarbonization challenges, respond similarly to technological options, and require archetype-specific policy support. However, this earlier work remains largely conceptual and offers limited guidance on concrete policy instruments needed to translate these strategies into practice.
Building on this foundation, the present study develops an expanded, policy-oriented framework that links petrochemical archetypes to differentiated decarbonization policy mixes. The framework is empirically examined through a comparative policy analysis of 16 countries representing different archetypes. We first test the explanatory validity of the archetype framework by examining whether countries across archetypes exhibit systematic differences in decarbonization-related policy priorities and instruments in the petrochemical sectors. We then compare policy landscapes within the same archetype to assess structural similarities and differences. Finally, we evaluate the extent to which existing national policies align with archetype-specific decarbonization strategies proposed in earlier work and with the policy framework developed in this study.

The results indicate that countries associated with different petrochemical archetypes display substantial and systematic variation in both policy emphasis and instrument choice, providing empirical support for the archetype model. In addition, policy formulation and implementation are embedded in broader socio-political and economic contexts, including levels of economic development and regulatory environments, which can lead to partial alignment, delayed adoption, or divergence from theoretically predicted policy pathways.
Reference:[1] Jennings, E.T., et al. Connected, complexand carbonized:The country archetypes of the petrochemicals sector. EnergyResearch&SocialScience

O64: Highly Dispersed Ru Clusters Supported on CeO2 Nano-islands Enabling Efficient and Stable H2-SCR of Nox

Theme: Energy & Net Zero & LCA

Dr Xiaoling Ma[1], Dr Chao Xue[2], Dr Evangelos Papaioannou[3], Professor Qiong Cai[1]

[1]University of Surrey, Guildford, United Kingdom, [2]Zhengzhou University, Zhengzhou, China, [3]Newcastle University, Newcastle upon Tyne, United Kingdom

Accelerating the achievement of net-zero emission targets requires effective control of NOx emissions from both stationary sources and mobile exhaust engines. Conventional NH_3-selective catalytic reduction (NH_3-SCR) technologies are often associated with ammonia slip, poor low-temperature activity (<200 °C) under cold-start conditions, and long-term stability of catalyst compromised by thermal deactivation and poisoning. In contrast, hydrogen-assisted SCR (H_2-SCR) exhibits stronger reducing property than NH_3 or hydrocarbons SCR systems and offers the potential for high deNOx efficiency at low temperatures. Therefore, H_2-SCR represents a promising alternative for overcoming several bottlenecks of SCR systems.

Herein, a series of Ru/CeO_2-SiO_2 catalysts were synthesized, in which highly dispersed Ru clusters were anchored onto CeO_2 nano-islands supported on monodisperse SiO_2. The unique CeO_2 nano-island architecture provides abundant oxygen vacancies and strong metal-support interactions, enabling effective stabilization of Ru species and enhanced redox properties. Ru-based catalysts were evaluated in a fixed-bed reactor under H_2-SCR conditions. Among the investigated samples, the catalyst containing 4.8 wt% Ru exhibited the highest catalytic performance, achieving a NOx conversion of 97% at 150 °C under oxygen-free condition. Notably, the catalyst maintained high activity and selectivity over 110 h of continuous operation, demonstrating excellent long-term stability. In situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) was employed to probe key surface intermediates and elucidate the reaction pathway. These findings provide insights into the rational design of stable H_2-SCR catalysts and demonstrate the role of nano-island structures for efficient NOx removal.

Acknowledge funding support from UKRI EPSRC through the UK Hub for Research Challenges in Hydrogen and Alternative Liquid Fuels (UK-HyRES) (Grant Number EP/X038963/1).

O65: ZIF-7/Polyetherimide Mixed Matrix Membranes for Hydrogen Purification

Theme: Energy & Net Zero & LCA

Mr Niko Muhammad Hilmi[1], Professor Begum Tokay[1], Professor Ed Lester[1], Dr Andrea Laybourn[2]

[1]University of Nottingham, United Kingdom, [2]University of Leeds, United Kingdom

Hydrogen is one of the fuels of the future due to its high gravimetric energy density and no greenhouse gas emissions during combustion. Membrane-based separation technologies are sustainable processes due to a 50% operational cost reduction.[1] This presentation will discuss the feasibility of using the metal-organic framework (MOF) ZIF-7 and a polyetherimide (PEI) polymer matrix to form MMMs for hydrogen purification.

The porosity of the MMM can be altered by thermal treatment after membrane casting. The membrane left to dry at room temperature creates a porous cross-section, while the membrane dried at 100 °C creates a totally dense cross-section. The alteration of the membrane's morphology due to post-casting thermal treatment has not been discussed before and affects the gas separation performance of the membranes.

ZIF-7 was able to be synthesised rapidly with the aid of microwave heating, cutting down the synthesis time from 48 hours to 10 minutes. Moreover, exceptional compatibility between ZIF-7 and PEI was exhibited, as 50 wt% of ZIF-7 loading was achieved.

The hydrogen purification performance of the prepared membranes is evaluated by single-gas permeabilities and selectivities of hydrogen compared to methane and carbon dioxide. The porous PEI membranes dried at room temperature showed a high hydrogen permeability of 2500 Barrer. Moreover, a H_2/CO_2 selectivity of 4.3 was achieved, surpassing the Robeson Upper Bounds, indicating exceptional gas separation performance for a polymer membrane. The success of this project will open the possibility of using cost-efficient hydrogen purification membranes in future gas networks.

References:
[1] G. Bernardo, T. Araújo, T. da Silva Lopes, J. Sousa, and A. Mendes, “Recent advances in membrane technologies for hydrogen purification,” Int. J. Hydrogen Energy, vol. 45, no. 12, pp. 7313–7338, Mar. 2020, doi: 10.1016/J.IJHYDENE.2019.06.162.

O66: Gas diffusion layers based on recycled carbon fibre for PEM fuel cells and electrolysers

Theme: Energy & Net Zero & LCA

Dr Marwah Shnaiter[1,2], Dr Shangfeng Du[1], Dr Yichang Yan[1], Mr Frazer Barnes[2], Mr Mohammed Riaz[2]

[1]University of Birmingham, United Kingdom, [2]Gen2Carbon Ltd, United Kingdom

Gas diffusion layers (GDLs) are critical for charge/heat conduction, reactant/product transport, water management, and mechanical support in PEM fuel cells (PEMFCs) and PEM water electrolysers (PEMWEs) [1]. Commercial carbon papers rely on energy-intensive virgin carbon fibre supply chains [2]. This work develops GDLs based on recycled carbon fibre (rCF) to enable a lower-cost, lower-impact pathway while meeting key structure-property requirements for PEM devices.

rCF-based GDL substrates are fabricated and tuned via fibre processing and binder/hydrophobisation strategies, with optional microporous-layer (MPL) integration. A structure-property-performance (SPP) workflow is applied: (i) microstructure quantification (thickness, and porosity) using X-ray micro-CT and complementary metrology; (ii) transport/electrical metrics including permeability/ interfacial contact resistance (ICR) under representative compression; and (iii) benchmarking in single-cell PEMFC and PEMWE hardware against commercial reference GDLs.

The study will report how rCF processing variables tune pore morphology and compression-dependent ICR-parameters strongly linked to ohmic and mass-transport losses, and identify design windows that balance permeability, conductivity, and mechanical robustness for both PEMFC and PEMWE operation.
The results demonstrate a strong potential of rCF-based GDLs as circular-economy components for hydrogen technologies. The presented SPP workflow provides a transferable route to qualify rCF media against device-relevant benchmarks and accelerate translation to stack-level evaluation.

References:

[1] T. Zhang et al., ‘Similarities and Differences between Gas Diffusion Layers Used in Proton Exchange Membrane Fuel Cell and Water Electrolysis for Material and Mass Transport’, Adv. Sci., vol. 11, no. 32, p. 2309440, Aug. 2024, doi: 10.1002/advs.202309440.
[2] A. Dér et al., ‘Modelling and analysis of the energy intensity in polyacrylonitrile (PAN) precursor and carbon fibre manufacturing’, J. Clean. Prod., vol. 303, p. 127105, 2021.

O67: Tailoring hydrocolloid-based fluid gels for fat replacement: the role of sucrose in agar systems

Miss Cara Anderton[1], Prof. Bettina Wolf[1], Dr. Lucio Cicerelli[2], Dr. Fotis Spyropoulos[1]

[1]University of Birmingham, BIRMINGHAM, United Kingdom, [2]Pladis Global, High Wycombe, United Kingdom

Dietary fat is an important component of formulated foods as it contributes to both the flavour and mouthfeel that we associate with fattiness. However, the current trend in low-fat reformulation is challenging because removing fat has a significant negative impact on the eating experience. The loss in functionality (provided by the fat) can be balanced through microstructural design.

Fluid gels are proposed by many authors as a promising option for fat replacement. Fluid gels are concentrated dispersions of gelled particles formed when gelation occurs within a shear field. Their characteristic hair-like protrusions and soft particles give rise to rheological properties that are typically associated with "creaminess": high viscosity, yield stress, and shear thinning and lubricating behaviour. However, these inherently “creamy” rheological and tribological properties are strongly influenced by sugars, often present at high concentrations in confectionery fillings. Applying fluid gels as fat replacers in confectionery requires understanding of the effect of sugar on the rheological and tribological properties, from which the influence on mouthfeel can be inferred.

In this research, rheology and tribology were used in conjunction to predict the effect of sucrose on the mouthfeel of agar fluid gels. Sucrose is found to positively contribute to fat-related rheological properties but detrimentally affect the lubricity of the formulation, indicating a trade-off between thickness and slipperiness, both of which are required for “creaminess” perception. Additionally, the interdependency of these variables and range of effects that sucrose has on the system makes it difficult to pin-point individual contributions to the final material properties. By systematically varying fluid gel size, shape and stiffness, the mechanisms underlying fluid gel rheology and tribology are elucidated. Hence, this work provides mechanistic insight essential for tailoring hydrocolloid systems to achieve desirable texture and mouthfeel in low-fat, high-sugar products, directly supporting enhanced product development.

O68: Effect of sour gas on the CO2 capture performance of a prototypical zeolite

Miss Preshti Ram[1], Mr Connor Hewson, Dr Paul Iacomi, Professor Daryl Williams

[1]Imperial College University, London, United Kingdom, [2]Surface Measurement Systems, London, United Kingdom

Complex flue gas mixtures are common feedstocks for industrial carbon capture systems. Even after flue gas desulphurisation (FGD), gas mixtures can contain acidic impurities such as SO_2 and NO_2 at levels of ~10–100 ppm. These gases are highly reactive oxidising species that form strong chemical bonds with basic or nucleophilic sites present on adsorbents. Zeolite 13X, a sorbent used in pilot-scale studies of post-combustion CO_2 capture due to its high adsorption capacity and strong affinity for CO_2, is vulnerable to performance loss in real flue gas environments. This work investigates the impact of low concentration SO_2 and NO_2 on the CO_2 capture performance, adsorption strength, and regenerability of 13X.

13X was activated at 450 °C under nitrogen prior to the experiment. Baseline single-component CO_2 adsorption isotherms were measured at 25, 40, and 60 °C using dynamic vapour sorption gravimetry to establish CO_2 capacity and enthalpies of adsorption. SO_2 adsorption was then studied at 75 ppm, followed by temperature-programmed desorption (TPD) at 1 and 5 $°C\ min^{-1}$. Additional TPD experiments with NO_2 were performed to compare adsorption strength and desorption profiles of the two contaminants. Cyclic adsorption experiments involved repeated 10% CO_2 uptake cycles, exposure to sour gases and subsequent CO_2 cycling to analyse performance degradation.

The results showed that 13X has a CO_2 uptake (≈14–16 wt%) and adsorption enthalpies of 25–40 $kJ\ mol^{-1}$, indicative of strong physisorption. SO_2 exhibited substantial uptake (~17 wt%) and incomplete desorption, with TPD peaks around 90 °C. After regeneration, residual mass was seen – indicating chemisorption. NO_2 displayed a higher TPD peak (~255 °C), highlighting strong, less reversible binding. After SO_2 exposure, the CO_2 capacity of 13X decreased by ~50%, with NO_2, causing a significant ~20% loss. These findings demonstrate competitive sorption effects, irreversible active-site poisoning, and long-term deactivation of zeolite 13X by sour gases.

O69: Optimising PAT for Continuous Powder Formulation Quality Monitoring Using the Feed Frame Simulator

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Eleonora De Giorgi[1], Sean Clifford[2], Kevin Sutcliffe[2], Nathan Cumberbatch[2], Estefania Lopez-Quiroga[1], Christopher Windows-Yule[1]

[1]School of Chemical Engineering, University of Birmingham, Edgbaston, B15 2TT, United Kingdom, [2]Global Product Development, Pharmaceutical Technology & Development, Operations, AstraZeneca, Macclesfield, UK

Monitoring powder formulation quality during the Continuous Direct Compression (CDC) tableting process to maintain product specifications is complex. Achieving the correct Active Pharmaceutical Ingredient (API) content and preventing blend segregation can be controlled by adjusting Critical Process Parameters (CPPs), such as material feed rate, as a key component of the overall control strategy. Determining appropriate CPPs solely through process data is challenging; however, this can be improved via an enhanced control strategy incorporating chemometric modelling through Process Analytical Technology (PAT). PAT sensors enable in-line monitoring of critical quality attributes, reducing time and effort required for sampling and off-line analysis of powder blends and tablets.

This work delves into optimising PAT for CDC, focusing on integrating spectroscopic techniques into the feed frame simulator, a tool for simulating the powder flow dynamics within a tablet press feed frame. By employing Near-Infrared (NIR) spectroscopy, Raman spectroscopy and NIR-spatially resolved spectroscopy, the project aims to enhance the accuracy and efficiency of these technologies and the resulting models for low-dose formulations, ensuring consistent product quality. These emerging products often face challenges near the limit of quantification, for example in low dose API formulations down to 1% w/w, or when compounds of interest are less responsive to specific techniques. Adopting advanced technologies offers compelling benefits for real-time process monitoring and control.

Key components include optimising acquisition parameters such as integration time and number of averages across the technologies. This enables dynamic data collection and model development using partial least squares regression to predict API concentration in the powder blend. A critical aspect of this study is a technology sensitivity comparison to analyse selected drug formulation blends, based on the optimised parameters. By standardising data analysis methodologies and developing an integrated real-time release testing strategy, the project seeks to address current challenges in PAT applications.

O70: The preparation of novel aerogels with paper pulp and calcium phosphate

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Jiayan Zhou[1]

[1]Newcastle University, Newcastle upon Tyne, United Kingdom

Aerogel has been widely used in the world because of its low density, low thermal conductivity and high biocompatibility. In this study, tetraethyl orthosilicate (TEOS) and methyltrimethoxysilane (MTMS) as precursors are used to successfully synthesize composite aerogel material with multi-function performance, which can be used, for example, in drug delivery and medical protective dressing. TEOS and MTMS were introduced as the organic silicon source to realize the cross-linking and construction of silicon oxygen network in wet gel system under the catalysis of acidic materials or ammonium bicarbonate to form organic-inorganic hybrid aerogel. Firstly, wet gel was prepared by the sol-gel method, which after aging and solvent exchange, the final aerogel sample was obtained by the ambient pressure drying method. The results of material characterization by FTIR and SEM showed that the aerogels obtained had multistage pore structure and specific chemical bonds and functional groups. Morphological and mechanical properties will be revealed by contact angle testing, BET, and stress-strain testing.

O71: Utilising Powder Characterisation and Data-Driven Models to Predict Dispersion and Dissolution in Drug Product Development

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Khizra Abdul Wadood[1]

[1]University of Birmingham, Birmingham, United Kingdom

Powder drawdown, dispersion, and dissolution strongly influence drug product performance and manufacturability, yet they are often the least predictable stages during formulation screening and process development. These behaviours arise from a complex interdependence among powder properties, environmental conditions, and process history, creating persistent challenges for process robustness and scale-up. As a result, formulation development continues to rely heavily on experimentation, with limited scope to generalise learning across formulations and operating conditions.

In this study, an experimentally grounded, data-driven framework is developed to support predictive classification of powder dispersion and dissolution behaviour. A diverse set of (N > 30) pharmaceutical powders, covering APIs, fillers, binders, and lubricants with broad particle size distributions, was characterised using dynamic flow measurements obtained with GranuDrum (GranuTools, Belgium) at controlled relative humidity levels of 25%, 55% and 75%. These measurements capture cohesion and flow hysteresis. From the sequence-cycle Cohesive Index trend with drum speed, a shear-response index was derived to quantify whether cohesion increased (shear-thickening) or decreased (shear-thinning). Powders exhibiting shear-thinning were consistently corresponded to swelling or gelling phenomena.

Time-resolved dispersion and dissolution experiments were conducted using an EasyViewer™ 100 imaging system (Mettler Toledo, USA), which provides direct observation of wetting, agglomeration, and dissolution phenomena. A standardised annotation rubric converted qualitative behaviours into objective labels, defining wetting-limited, gelling, or swelling, and fully dispersed regimes. Across 30 powders, 10-12 exhibited persistent gelling or swelling behaviour.

Supervised learning models were trained using the curated dataset to classify dispersion regimes and quantify sensitivity to humidity. The rheological index correlated strongly with agglomerate persistence and outperformed individual GranuDrum parameters considered in isolation.
These findings demonstrate that integrating targeted powder characterisation with data-driven classification provides a mechanistic and generalisable route beyond empirical formulation workflows, with relevance across oral solid dosage, parenteral reconstitution, and inhalation product development.

O72: Sustainable dual-shell chitosan-silica microcapsules for potential personal care applications

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Dr Dan Baiocco[1], Professor Zhibing Zhang[1]

[1]University of Birmingham, Birmingham, United Kingdom

The rising demand for clean beauty products has intensified the search for sustainable alternatives to microplastic-based cosmetic microparticles widely used for exfoliation and fragrance delivery [1]. However, achieving high performance alongside environmental compatibility remains a critical challenge.

Herein, we report a green and facile strategy to fabricate dual-shell fungal chitosan-silica microcapsules for efficient encapsulation and controlled release of cosmetic oils, using hexyl salicylate as a model fragrance oil. Emulsified oil droplets were electrostatically stabilised by sodium dodecyl sulphate and sterically protected by silica nanoparticles, followed by the deposition of a primary fungal chitosan shell at pH 2. A secondary inorganic silica layer was subsequently mineralised via alkaline sodium silicate treatment, yielding robust organic-inorganic hybrid microcapsules.

Morphological analysis revealed uniform spherical capsules with Sauter diameters of 42.3±0.4 µm for single-shell chitosan microcapsules and 51.4±0.4 µm for dual-shell structures featuring a distinct mineralised silica crown. Barrier performance testing demonstrated significantly enhanced fragrance retention for dual-shell capsules, with only ~2.5% oil release after 15 days in neutral pH aqueous media, compared to ~10% for single-shell counterparts. Mechanical micromanipulation confirmed superior structural properties, with the nominal rupture stress increasing from 1.7±0.1 MPa to 3.0±0.2 MPa following silica deposition.

Overall, these results highlight the critical role of inorganic shell integration in improving both durability and encapsulation efficiency. This sustainable dual-shell microcapsule platform offers a green, promising, high-performance alternative to conventional microplastic carriers for skincare, fragrance, and beauty formulations. Future investigations will focus on evaluating their mechanical resilience and fragrance release performance on soft artificial skin.

References:
[1] Baiocco, D., J.A. Preece, and Z. Zhang, Microcapsules with a fungal chitosan-gum arabic-maltodextrin shell to encapsulate health-beneficial peppermint oil. Food Hydrocolloids for Health, 2021: p. 100016.

O73: Experimental investigation of a cold multistage fluidized bed system for waste chemical recycling

Theme: Chemical recycling of polymers

Dr Stefano Iannello[1], Dr Massimiliano Materazzi[1]

[1]University College London, London, United Kingdom

Bubbling fluidized beds (BFB) are one of the best reactor configurations for Advanced Thermochemical Technologies (ATT), including pyrolysis and gasification, due to favorable mixing between gas and solid phases, and good mass and heat transfer properties. However, when BFB are used for chemical recycling of plastic waste, feedstock segregation, melting and bed bypass of the volatile matter, disrupt the fluidization behavior and proper mixing of the waste. During operation, this can lead to reduced process efficiency and product quality.

To mitigate these problems, a new BFB configuration has been developed at UCL. This is based on multiple vertically stacked BFB sections to improve contact between the bed solids, waste, and product gases. An internal system is present to allow the bed solids to circulate between the bed sections, to further enhance mixing and phase contact in a counter current fashion. This work presents an experimental investigation using advanced X-ray imaging to explore hydrodynamic behavior of a cold model, two-stack BFB operating with nitrogen and at different fluidization velocities, ranging from 20 to 40 Nlpm.

Results from X-ray images show that the voidage fraction decreases over time in the bottom section, due to the increase of bed solids coming from the top section. The average voidage in the bottom section ranges from approximately 0.73 to 0.61 and from 0.73 to 0.60 after 100 s from the onset of bed fluidization for experiments conducted at 20 Nlpm and 40 Nlpm, respectively, indicating no significant difference between the two cases.

This work also shows a feasibility study and proof of concept for the new multistage BFB configuration applied to plastic pyrolysis. This technology enables staged and controlled waste conversion with excellent heat and mass transfer, giving high conversion efficiency, flexible process control, and improved tolerance to heterogeneous and contaminated feedstocks.

O74: Thermo-responsive Catalysts for PET Glycolysis: High-Throughput Design Towards Circular Recycling.

Theme: Chemical recycling of polymers

Dr Kyle Batchelor, Dr Steve Street[2], Mr Joseph Sutton[1], Mr Samual Baker[1], Mr Owen Young[1], Prof Andrew Dove[1], Prof Joseph Wood[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]University of Liverpool, Liverpool, United Kingdom

Poly(ethylene terephthalate) (PET) is a widely used thermoplastic in textiles and packaging, but its durability and low recycling rates have made it a major contributor to global plastic waste. Mechanical recycling dominates industrial practice but degrades polymer quality, prompting interest in chemical recycling methods such as glycolysis, which breaks PET into bis(hydroxyethyl) terephthalate (BHET) for closed-loop reuse [1]. Conventional metal-based catalysts for glycolysis raise concerns over toxicity, separation, and recyclability, while organocatalysts offer a metal-free alternative with tuneable activity and thermal stability. However, their high solubility in ethylene glycol complicates recovery and reuse. To address this, heterogenization and thermo-responsive systems have emerged as promising strategies, enabling reversible phase transitions for catalyst recovery without sacrificing activity [2]. This work focuses on designing recyclable, thermo-responsive organocatalysts supported on phenol-functionalized polymers, leveraging hydrogen bonding to achieve Upper Critical Solution Temperature (UCST) behaviour. High-throughput experimentation screening (HTE) was adopted to systematically screen 66 organobase-polymer combinations for catalyst performance, thermo-responsiveness, and sustainability. A 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU) supported polymer system emerged as a lead candidate, exhibiting UCST behaviour under glycolysis conditions. Scaling up under optimised conditions resulted in high BHET yield and enhanced sustainability metrics. Kinetic analysis revealed a shrinking-core mechanism with two distinct regimes, linked to in-situ changes in catalyst speciation driven by acidic by-products. These observations coincide with a gradual loss of thermo-responsiveness as the reaction progresses, ultimately leading to catalyst deactivation. Overall, the study highlights the potential of UCST-active catalysts for sustainable PET recycling while identifying catalyst stability under evolving reaction conditions as the key challenge for future development.

[1] M. Babaei, M. Jalilian, K. Shahbaz, J. Environ. Chem. Eng. 12 (2024) 112507.
[2] V.D. Lechuga-Islas, D.M. Sánchez-Cerrillo, S. Stumpf, R. Guerrero-Santos, U.S. Schubert, C. Guerrero-Sánchez, Polym. Chem. 14 (2023) 1893–1904.

O75: An integrated process modelling and sustainability assessment framework for chemical recycling towards a circular economy

Theme: Chemical recycling of polymers

Mr Xing Liu[1], Dr Oliver Fisher[1], Professor Jon McKechnie[1], Dr Ioanna Dimitriou[1]

[1]Faculty of Engineering, University of Nottingham, Nottingham, United Kingdom

Plastic waste has become a significant environmental concern, demanding the development of energy-efficient and cost-effective management technologies. Among emerging solutions, chemical recycling technologies such as pyrolysis show promise but remain largely at the demonstration stage, facing persistent challenges related to feasibility and sustainability. Consequently, a systematic assessment of these technologies is urgently needed to evaluate their technical, economic, and environmental viability. This study establishes an integrated assessment framework by linking Aspen HYSYS with Python, enabling seamless coupling of process simulation, cost modelling, and life cycle assessment (LCA). Mixed plastic waste (MPW) is used as the target feedstock to compare pyrolysis-based energy recovery pathways in terms of their technical, economic, and environmental performance. The results indicate that using non-condensable gas combustion for internal heat is the most cost-effective option, with a total capital cost of $19.6 million, an annual operating expenditure of $8.1 million, and a net present value (NPV) of $53 million. This scenario also demonstrates the lowest environmental impact, achieving –0.6 kg CO_2 eq. per kg of pyrolysis oil in greenhouse gas (GHG) emissions. Sensitivity analysis indicates that pyrolysis oil price, operating hours, and interest rate are the primary cost drivers. Heat generation is identified as the main contributor to GHG emissions, followed by utility consumption. The economic and environmental sustainability of the optimal scenario was further evaluated under varying plastic waste feedstocks, geographical locations, and plant capacities. Among the tested feedstocks, MPW had the highest economic benefit and slightly lower carbon emissions, primarily due to its composition and treatment costs. Regional analysis indicates that establishing the plant in China provides the greatest economic advantage, followed by India, though both demonstrate relatively higher GHG emissions.

O76: Dual Acid-Base Catalysis toward Chemical Sorting of Mixed Poly(ethylene terephthalate) and Poly(vinyl chloride)

Theme: Chemical recycling of polymers

Dr Yuya Watanabe[1], Dr Arianna Bandolese[1], Prof Andrew Dove[1]

[1]University of Birmingham, United Kingdom

The vast production and usage of plastics, coupled with inadequate end-of-life management, have resulted in significant environmental pollution. Chemical recycling has gained considerable attention as an attractive solution that can convert plastic waste into valuable products. Furthermore, it allows selective depolymerisation leveraging differences in the chemical reactivities of mixed plastics, thus reducing the need for the labour-intensive sorting process.

Our group recently reported the selective depolymerisation of mixed plastics comprising poly(ethylene terephthalate) (PET), bisphenol-A polycarbonate, and poly(lactic acid) using a Lewis acid–base dual catalyst. Control over the catalytic activity by judicious choice of the acid–base pairs, as well as reaction temperatures, enabled the selective reactions. In contrast, chemical recycling of PET mixed with poly(vinyl chloride) (PVC) is more challenging as PVC degrades to release HCl during reactions, causing catalyst poisoning and plant corrosion. However, their comparable densities hamper their separation by conventional sorting techniques.

Hence, we investigated the catalytic activity of a series of metal-containing Lewis acid/organobase pairs for PET glycolysis mixed with PVC. Our catalysts exhibited superior activity to the parent acids and bases and tolerance against HCl generated via PVC dehydrochlorination. Furthermore, some combinations selectively catalysed PET glycolysis in the presence of PVC, affording a terephthalate monomer and unreacted PVC. Control experiments suggested that the formation of insoluble metal/organobase complexes is the key to the selective catalysis.

O77: Electrochemical Membrane Processes for Closed-Loop Recycling and Upcycling of polyethylene terephthalate (PET)

Theme: Chemical recycling of polymers

Ms Dingchang Yang[1], Dr Hui Luo[2], Dr Qilei Song[1], Professor Magda Titirici[1]

[1]Imperial College London, London, United Kingdom, [2]University of Surrey, Guildford, United Kingdom

Recycling and upcycling of plastics, such as polyethylene terephthalate (PET), into value-added chemicals offers a promising pathway toward a circular economy. However, conventional chemical recycling processes often rely on energy-intensive downstream separation steps. For example, alkaline PET depolymerization generates complex mixtures containing charged species (e.g., terephthalate dianions and hydroxide ions) and neutral compounds (e.g., ethylene glycol), which requires multi-step separation processes, including acid neutralization, crystallization, and distillation.
Electro-membrane separation processes offer a compelling alternative to address these challenges, yet their application to PET recycling streams remains largely unexplored. In this work, I will present our patented ElectroPET process for PET recycling and upcycling, which integrates electrochemical separation and conversion. Specifically, we combine selective electrodialysis (ED) and bipolar membrane electrodialysis (BMED) to extract NaOH from the depolymerized solution and recover high-purity terephthalic acid while retaining ethylene glycol. The recovered ethylene glycol can be further converted into the value-added product glycolic acid using an anion exchange membrane electrolyzer.

These electrochemical approaches enable efficient recovery of monomers and production of valuable chemicals without neutralization or energy-intensive thermal separations, supporting closed-loop, low-waste PET recycling. Moreover, this electrochemical separation strategy can be extended to other plastic recycling streams, including polyesters and mixed textiles.

References:

[1] Hui Luo*#, Dingchang Yang#, Helen Tyrrell#, Rukayya Ibrahim Muazu#, Enrico Manfredi-Haylock#, Zhongming Chen, Alain Li, Julian Black, Ifan Stephens, Nilay Shah, Qilei Song*, Maria-Magdalena Titirici*. Closed-loop sustainable chemical processes to transform poly(ethylene terephthalate) waste into high-value chemicals and fuels. Nature Chemical Engineering. Under revision.

O78: Evaluating Zinc Catalysts for Resin-Fibre Dual Recovery in Solvolytic Recycling of CFRP

Theme: Chemical recycling of polymers

Mr River Gowans[1], Dr Reda Felfel[2], Dr Xiaolei Zhang[1]

[1]Department of Chemical & Process Engineering, University of Strathclyde, Glasgow, United Kingdom, [2]Department of Mechanical & Aerospace Engineering, University of Strathclyde, Glasgow, United Kingdom

Carbon fibre reinforced polymer (CFRP) composites present a growing end-of-life challenge as increasing volumes of high-performance materials reach decommissioning age. Conventional recycling routes often follow value-dissipative pathways that are poorly aligned with the transition towards a circular economy. This work investigates a green, catalyst-assisted solvolytic approach to CFRP recycling, aiming to enable dual recovery of high-quality carbon fibres and matrix-derived chemicals from commercial composite waste.

A hydrophobic-switchable natural deep eutectic solvent (NADES), composed of thymol and decanoic acid, is employed as a swelling and solvolytic medium for epoxy-based CFRP. Catalyst-assisted solvolysis is investigated under fixed solvent-to-composite ratios and reaction times, with moderate reaction temperatures evaluated between 140-180°C. A comparative evaluation of zinc-based Lewis acid catalysts (zinc chloride and zinc 2-ethylhexanoate) is used to assess catalyst-solvent compatibility and temperature-dependent solvolysis behaviour, while non-zinc catalysts are benchmarked in subsequent studies.

Solvolysis performance is assessed primarily through resin removal efficiency determined via mass-loss analysis, with recovered fibre quality evaluated using microscopy. Liquid-phase products are separated via pH-induced switching of the NADES to a hydrophilic phase, facilitating separation of hydrophobic, matrix-derived chemicals, which are subsequently characterised using GC–MS. This allows the examination of depolymerisation behaviour and infers differences in reaction pathways associated with polymer-catalyst interactions.

Results demonstrate temperature-dependent differences in epoxy solvolysis efficiency and fibre recovery for zinc-based catalysts, suggesting that catalyst–solvent compatibility, influenced by ligand environment and polarity, affects depolymerisation behaviour within hydrophobic NADES systems. These results contribute to improved understanding of catalyst- solvent–polymer interactions relevant to CFRP recycling and inform the development of low-impact, circular processing routes for high-value composite waste.

Poster abstracts

P1: High Throughput Robotic Experimentation for Automated Nanoparticle Synthesis and Analysis and the Training of Machine Learning Models.

Theme: AI & Data Driven Studies

Mr Jacob Danks[1], Dr Maximillian Besenhard[1]

[1]UCL, London, United Kingdom

To design, optimise and understand complex chemical reactions, comes with a large experimental design space to explore. However, in recent years, many advancements have been made in the automation and robotics field for chemistry to tackle this. High throughput capabilities have existed for decades within the biological industry, especially surrounding liquid handling robotics, but where these are primarily targeted at aqueous sample preparations. For chemical applications, the adoption of increased throughput screening has been slower. As a result, customised, bespoke solutions have been developed by those that are pushing and developing the field, whilst commercially viable, affordable and effective solutions are still not widely available; those that are available come with their own limitations or expense. Many solutions for overcoming advanced chemistry issues (harsher reagents, increase temperature, pressure, analytics and sample storage) are platforms which require the implementation of multiple robots and a dedicated workspace or laboratory. This work presents the development of an all-in-one benchtop automated reaction platform centred around a liquid handling robot. This has been achieved through the integration of various synthetic and analytical modifications to facilitate high throughput active stirring, heated reactions, cleaning operations, and DLS and UV-Vis analysis. These automated protocols are aligned by implementation of a python-based orchestrator for system control and data capture. Leveraging high throughput reaction capabilities enables automated reaction screening, optimisation and particle analysis whilst carrying out design of experiment (DoE) approaches for dataset gathering. This not only facilitates the training of machine learning models, but drives towards the possibility of autonomous, self-driven screening optimisation platforms. This workflow has been successfully demonstrated on both silica and silver nanoparticle systems, showcasing the platform’s ability to take on various synthetic challenges, and in a completely automated protocol, perform synthesis and capture analytical data across a wide experimental space.

P2: Coupling Physics-Informed Neural Networks and X-ray imaging for modelling plastic particles motion during fluidized bed pyrolysis

Theme: AI & Data Driven Studies

Dr Stefano Iannello[1], Mr Andrea Friso[1], Dr Federico Galvanin[1], Dr Massimiliano Materazzi[1]

[1]University College London, London, United Kingdom

Chemical recycling of plastics, including pyrolysis, using fluidized bed reactors represents a promising pathway to tackle the ever-increasing amount of plastic waste produced worldwide, as an alternative to conventional waste management strategies, including incineration and landfilling. However, several challenges remain, particularly concerning the insufficient mixing of gas and solid phases when processing highly volatile solid feedstocks, such as plastic waste.

This work focuses on the fundamental investigation of hydrodynamic interactions between a lab-scale fluidized bed reactor operating under pyrolysis conditions using nitrogen and single polypropylene particles. The fluidized bed was operated at temperatures and fluidization velocities in the range of 500 – 650°C and 1.25 – 2Umf, respectively. Umf is the minimum fluidization velocity, which was obtained via pressure drop measurements. Particle tracking data obtained from advanced X-ray imaging techniques were used to build three different modelling frameworks. The former model is based on the second law of motion. The second one is a Physics-Informed Neural Network (PINN), built by embedding the second law of motion in the loss function. The third model is a modified version of the PINN, built by augmenting the mechanistic model (augPINN) by introducing a new interphase distribution parameter, P, which was obtained directly from X-ray data without priori assumptions.

Results show a clear dependance of the axial segregation profiles of the plastic particle with both fluidization velocity and temperature. From a modelling perspective, augPINN significantly outperforms both mechanistic and standard PINN models in capturing the complex hydrodynamic behaviour of polypropylene particles. Furthermore, parameter P was found to be physically interpretable.

The novelty of this work is to show how different frameworks based on the PINN concept can be successfully applied to complex and real-world hydrodynamic datasets. This work presents a valuable methodology to advance modelling of fluidized bed-plastics interaction during chemical recycling.

P3: Automated Kinetic Model Discovery from TEAS Data Using Sparse Identification

Theme: AI & Data Driven Studies

Miss Wenyao Lyu[1], Dr Rebecca Ingle[2], Dr Tom Oliver[3], Prof Federico Galvanin[1]

[1]Dept of Chemical Engineering, University College London, London, United Kingdom, [2]Dept of Chemistry, University College London, London, United Kingdom, [3]School of Chemistry, University of Bristol, Bristol, United Kingdom

Transient Electronic Absorption Spectroscopy (TEAS) is an ultrafast, time-resolved technique used to study the excited-state dynamics of photophysical and photochemical processes. Traditionally, excited-state dynamics from time-resolved TEAS data are identified through a model-based workflow involving data preprocessing, spectral assignment, wavelength selection and kinetic trace extraction, followed by the proposal, fitting, and validation of predefined kinetic models via global analysis.
The traditional approach requires the a priori proposal of a reaction scheme and prior knowledge of the photoproducts, making kinetic identification highly time-consuming. If the proposed scheme is inconsistent with the experimental data, the workflow must be iteratively reworked, a difficulty that becomes more pronounced when prior knowledge is limited. Moreover, the reliability of the identified kinetic model is highly sensitive to spectral assignments and the choice of probe wavelengths used for kinetic analysis, making it challenging to ensure the consistency and convergence of the identified models.

To accelerate kinetic model identification and mechanism discovery from TEAS data, and to improve model robustness and reliability, this work aims to develop an automated Sparse Identification of Nonlinear Dynamics (SINDy)-based workflow. In this study, the excited-state dynamics of anthocyanin derivatives in aqueous solution, previously analysed using traditional global analysis, are employed as a benchmark to evaluate the proposed approach. At this preliminary stage, the SINDy-based workflow can automatically identify statistically adequate and physically interpretable kinetic models within one minute, without prior specification of reaction schemes or manual trial-and-error global fitting. The results reveal a clear dependence of the identified models on the chosen fitting time window and probe wavelength selection. Consequently, multiple statistically plausible kinetic mechanisms can be recovered, highlighting the need for further validation using additional physical constraints, spectral analyses, model selection strategies, and integrated optimal experimental design approaches such as DoE-SINDy.

P4: Inverse Modelling of Reaction Vessels for Optimal Control

Theme: AI & Data Driven Studies

Mr Zaw Phyo Oo[1]

[1]University of Birmingham, United Kingdom

Most Johnson Matthey (JM) products pass through a stirred tank during manufacture, yet understanding internal flow behaviour in stirred tank reactors, such as mixing times, remains challenging, particularly when fluid rheology evolves during processing. Process control is recipe-driven and relies heavily on offline characterisation, limiting flexibility, online insight and optimisation capabilities.

Over the next four years, this research will develop a physics-informed digital twin capable of leveraging available process measurements to reconstruct internal reactor states, providing operators with real-time visibility into unmeasured process variables. This will increase right-first-time batches and reduce cycle times.

This will encompass: (1) development of reduced-order physics-based models incorporating rheological characterisation, (2) implementation of inverse algorithms blending Machine Learning (ML) and data assimilation methods for state and parameter estimation, and (3) validation and deployment as an advisory tool for operator decision-making.

Model validation will employ a dual approach: computational fluid dynamics (CFD) simulations will provide reference data under various flow conditions, while Particle Tracking Velocimetry (PTV) using orthogonal high-speed cameras will generate “ground-truth” three-dimensional velocity fields under representative mixing conditions. These datasets will support model calibration, validate ROM predictions and train ML components of the digital twin.

This work will bridge traditional process modelling and Industry 4.0 digitalisation, providing real-time insights into reactor behaviour and rheological evolution, ultimately enabling the transition towards advanced process control in formulation manufacture.

P5: Closing the Loop - Enabling More Sustainable Operations With Machine Learning Based Advanced Process Control

Theme: AI & Data Driven Studies

Mr Arjun Singh[1,2], Dr. Estefania Lopez Quiroga[1], Prof. Mark Simmons[1], Mr. Robert Gallen[2], Dr. Joseph Emerson[2], Dr. Carl Tipton[2]

[1]University of Birmingham School of Chemical Engineering, Edgbaston, United Kingdom,
[2]Johnson Matthey (JMTC), Sonning, United Kingdom

This study investigates the development of data-driven closed-loop control strategies for mixing systems, with a particular focus on detecting and preventing bubble and foam formation using machine learning and computer vision are presented. Traditional feedback controllers such as PID provide a useful baseline but are limited when applied to poorly instrumented, nonlinear systems where key process states, such as surface behaviour or incipient gas entrainment, are not directly measured.

Current work centres on the design and construction of a bench-scale experimental mixing rig, integrating low-cost sensors, embedded control hardware, and a camera-based measurement system. This platform is used to generate experimental datasets linking impeller speed, mixing performance, and visual indicators of bubble formation. Computer vision methods will be explored to extract physically meaningful features from image data, providing an additional sensing layer that complements conventional measurements.

Foundational principles from control theory, electronics, and embedded systems guide the implementation of baseline controllers and data acquisition pipelines. Machine-learning models are being developed for system identification and state estimation, with the longer-term objective of embedding these models within a hybrid control framework that combines first-principles understanding with learned representations.

By progressively closing the loop between visual detection, data-driven modelling, and actuation, the research aims to demonstrate how non-intrusive or intrusive sensing and ML-assisted control can improve stability and operating limits in mixing processes. The project will contribute an experimental framework and control methodology suitable for extension to more complex process systems.

P6: Developing Methods for Big Data Capture in Support of the Digital Twin for Investment Casting Shelling Operations

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Rahul Suresh Arath[1]

[1]HTRC, Coventry, United Kingdom

The manufacture of single crystal turbine components via investment casting is critical to the efficiency of the modern jet turbine. One key factor in their production is the shelling operation which creates the ceramic mould for casting. Control of processing variables are essential in making a mould with the correct properties required for a defect free casting.

Recent advances in 3D dimensional characterisation techniques allow the measurement of shell dimensions during the process. This data can be used to develop advanced process models to understand how process variation affects the formation of a casting defect called High Angle Boundaries, which currently reduces the productivity of single crystal casting foundries worldwide.

Methods to infer dimensional variation of each ceramic mould, using data from a Rolls-Royce foundry, have been developed. These methods were applied to a large volume of historic data and significant variation was found, despite the employment of a very advanced and tightly controlled manufacturing process.

These variation metrics, along with data from other process unit operations, were used to train machine learning models to predict defect occurrence. However, model analysis suggests no correlation between these metrics and the defect in question.

Currently, an observational study is in progress to record detailed defect maps not normally measured in the process. This will enable defect type and position on the component to be clearly distinguished, and this is hypothesized to allow better correlation of shell variation data to a wider range of casting defects.

P7: Developing sustainable hair conditioning technologies

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Ms Thanmaya Arunkumar[1], Ms. Jennifer Marsh[2], Peter Fryer[1], Zhenyu Zhang[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Procter and Gamble, Hair Care, Business Innovation Centre, Mason, United States of America

Hair conditioning involves applying conditioning agents to the hair surface to reduce friction and enhance the other perceivable consumer benefits. Silicone oil has been a key ingredient in conventional hair conditioning formulations. Sustainable bio-derived materials could help reduce environmental impact, but non-silicone conditioners often fall short in performance compared to silicone-based ones. The aim of this work is to characterise the spreading and wetting kinetics of silicone oil, which constructs the design framework for bio-derived oils.

Spreading and wetting were analysed on different substrates. The Wilhelmy plate measured surface tension of 20 silicone oils, while a contact angle goniometer tracked spreading on Glass and PET. Samples included PDMS and industrial silicone oils. By studying interfacial tension and spreading, models for bio-derived oils can be developed and validated.

Different models have been explored to describe the maximum spreading parameter βmax = Dmax/D0 as a function of non-dimensional numbers, such as the Reynolds number (Re) and the Weber number (We). Most models in the literature are restricted to Re >100. This raised the need for a new model specifically designed for high-viscosity samples. The scaling laws in the literature suggested that the spreading parameter βmax scaled with Re and We according to a power law. After correlating and fitting the data with a power law, it was observed that βmax scaled with $Re^{0.05}$ and $We^{-0.03}$. It was observed that We played a more dominant role in determining spreading effectiveness compared to Re, which could be attributed to a similar rheology. This emphasised the critical role of surface tension-driven forces in the spreading dynamics of the silicone oils, which needs to be balanced with the lubrication performance requirement.

P8: Characterization of physics of photopolymer curing in development of casting core for Air turbine blades

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Niranjan Kumar Subramanian Ashokkumar[1], Dr Aleksander Cendrowicz[2], Dr Stewart Welch, Dr Andrew Dove

[1]University of Birmingham, Birmingham, United Kingdom, [2]High Temperature Research Centre, Coventry, United Kingdom

Aircraft equipped with gas turbine engines operate under conditions that continuously push turbine blades to their high-temperature limits. The hot, high-pressure gases exiting the combustion chamber of a gas turbine engine impinge on the turbine blades, exposing them to severe thermal and mechanical loads. Hence cooling channels are required to ensure component longevity and the design of the cooling channels needs to have tight geometric control.

Nickel superalloy single crystal castings manufactured using dissolvable ceramic cores are used extensively to produce high-pressure turbine components used for aircraft propulsion. Ceramic cores are sacrificial components in the process as it is used for creating an intricate cooling channel inside the turbine blade which increases the operating temperature, efficiency of Engine and service life of the Blade.

Ceramic cores which are made of silica-based material will have to withstand the high temperature casting process. Producing the cores using additive manufacturing offers an opportunity to enhance the cooling effectiveness through allowing higher operating temperatures.

Additive manufacturing is becoming a viable methodology to design and manufacture ceramic cores which enables a rapid design optimization compared to the traditional tool and die methodology.

To enhance the capability of additive ceramic core technology, the proposed research focuses on the key role that ultraviolet curing of highly filled ceramic slurries plays in achieving fine features and dimensional capability in the production of ceramic components by additive layer manufacturing techniques.

Laboratory procedures to characterize the curing process in combination with modelling techniques will be developed to understand residual stress development during component build, de-bind and sintering. The mechanistic understanding developed will subsequently be used to understand how the formulation affects fine feature formation and dimensional stability.

P9: Numerical Modelling and AI-driven Optimisation of Particulate Systems for Defence Applications

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Daniel Barbet[1], Dr Christopher Windows-Yule[1], Mr Aran Klair[1], Mr Freddie Barter[1], Mr Jack Grogan[1], Mr Aaron Wiggin[1]

[1]University of Birmingham, Birmingham, United Kingdom

Resonant acoustic mixing (RAM), as a relatively new technology, has shown to be significant for the energy-efficient mixing of both particulate and fluid systems. RAM's applications for powder mixing have proven especially relevant for the mixing of sensitive and energetic materials, rendering it of particular interest in the Pharmaceutical and Defence sectors [1]. Partly due to the technology's novelty, RAM has thus far used cylindrical vessels. In this talk, we demonstrate, using numerical simulation and artificial intelligence, how expanding beyond this standard can significantly improve RAM's capabilities.

By systematically describing possible vessel shapes according to 7 variables, this project will investigate the effects of wall and end angles as well as aspect ratio, whilst maintaining consistent vessel volume. Geometries are compared by quantifying the mixing performance as the time to achieve a desired degree of mixing. More than 10,000 distinct vessel geometries have been autonomously created and tested via computer-aided design (CAD) and discrete element modelling (DEM).

An unique evolutionary framework [2] was used for optimisation, minimising the mixing time metric as an objective function. Across all optimisations, total vessel volume was held constant, but separate runs were used to investigate the effects of both mixing intensity and fill height on ideal vessel geometry. The results demonstrated significant performance improvements for all system conditions. Notably, the optimal design was observed to strongly differ for different combinations of fill and excitation, suggesting that there does not exist a single "ideal RAM vessel", but rather different optima should be sought for different materials and conditions.

1. Wright, C.J., et al., Is ResonantAcoustic Mixing®(RAM) a game changer for manufacturing solid composite rocket propellants? Propellants, Explosives, Pyrotechnics, 2022. 47(1): p. e202100146.
2. Nicusan, L., D. Gobby, and K. Windows-Yule, HARPPP: Autonomous Geometric Design Optimisation of Stirred Tank Reactor Impellers and Baffles. ArXiv, 2025.

P10: On the Thermally Induced Cross-Linking of Poly-Vinyl Alcohol: Insights from Time-Resolved Rheometry and Implications for Industrial-Scale Processing

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Ms Chloe Bruno[1]

[1]University of Birmingham, School of Physics and Astronomy, Birmingham, United Kingdom

Poly(vinyl alcohol) (PVA) is a biocompatible polymer with advantageous physical and chemical properties for the synthesis of sustainable and environmentally friendly plastics. However, it is highly susceptible to thermal degradation at industrially relevant processing temperatures, with a melting point close to its degradation temperature. Understanding the degradation processes and mechanisms involved is therefore critical for the design, scale-up, and optimisation of PVA extrusion operations. Dynamic oscillatory rheology provides insight into polymer molecular structure by probing multiple length scales, enabling the detection of subtle changes that are inaccessible using conventional characterisation techniques. When coupled with time-resolved rheology (TRR), the evolution of viscoelastic properties with time can be monitored, allowing key aspects of the degradation mechanism to be resolved. This work applies TRR to PVA to obtain a fully time-resolved assessment of its undegraded and degraded rheological behaviour, thereby elucidating the factors governing degradation. This methodology will allow characterisation of degradation under varying conditions, including temperature to derive Arrhenius-type kinetic expressions; formulation to assess the effects of molecular weight, degree of hydrolysis, and plasticiser content; environmental conditions to distinguish thermo-oxidative from purely thermal degradation; and mechanical shear to evaluate thermo-mechanical effects. The outcomes will also include complete flow curves to improve the accuracy of polymer flow simulations for processing equipment such as extruders. Initial work has focused on developing suitable sample preparation methods that avoid thermal exposure while ensuring representative and reproducible rheological measurements. Preliminary results highlight the significant role of polymer cross-linking during degradation, an effect that is underreported and often overlooked in the literature. The present results thus allow maximum thermal treatment times and initial flow curves to be understood, with direct implications for industrial processing techniques.

P11: Fluid gels as long-acting injectable hydrogel implants

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Alannah Byron[1], Bettina Wolf[1], Thomas Robinson[1], Fotis Spyropoulos[1]

[1]The University of Birmingham, United Kingdom

Hydrogels are commonly used within Regenerative Medicine due to their tuneable mechanical properties, biocompatibility and biodegradability. Hydrogels are excellent extracellular matrix mimetics and are commonly used for the controlled delivery of bioactives/cells. However, hydrogels are structured (gelled) prior to use and thus require surgery for implantation, resulting in tissue damage and increased therapeutic costs. These issues have led to interest in minimally invasive implantation strategies and fluid gels (FGs) have emerged as promising candidates for use as injectable hydrogels. Due to their high viscoelasticity and capacity to self-structure at rest, FGs have gained attention for use as a dynamic hydrogel scaffold; one that is gelled exogenously and then injected into the body, forming robust structures once in place (at rest). Emulsion fluid gels (EFGs) build on the FG microstructure and are characterised by the presence of oil droplets that are embedded with the FG formulation. Their capacity to carry/discharge hydrophilic/lipophilic actives can be utilised to develop unique drug delivery platforms including dual release systems.

The present study focuses on the development of FGs/EFGs as long-acting injectable hydrogel implants. This work reports on FGs/EFGs rheological characteristics and how these influence formulation injectability and drug release performance. Rheological measurements were performed to assess FG viscoelasticity, while microscopy was used to determine particle size and shape. Textural analysis with a universal syringe rig was used to characterise FG injectability for a range of needle sizes and relevant injection flow rates. Release profiles for model hydrophilic/lipophilic actives were obtained by placing FGs/EFGs within a dialysis bag and immersing this in an aqueous acceptor phase. The released active content was measured at predetermined time points using spectrophotometry. Overall, the reported preliminary data offers clear promise in terms of the utility of FGs and EFGs as injectable drug delivery hydrogel constructs.

P12: Computational modelling of drag reduction agents (DRAs) in pipe flow

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr David Cattell, Dr Amin Rahmat, Professor Ian McRobbie, Dr Azhar Prodhan, Dr Philip Maltas, Professor Zhenyu Jason Zhang

[1]University of Birmingham, Birmingham, United Kingdom, [2]Innospec Ltd., Ellesmere Port

The pumping of fluids, especially at high Reynolds numbers, accounts for an estimated 20% of the world's electrical energy demand. DRAs have the potential to reduce the drag in these flows by up to 80%, thus reducing pressure losses and/or increasing throughput. Therefore, they have the potential to play a crucial role in the road towards Net Zero.

By developing a computational model of DRAs in pipe flow, an understanding of how they work and degrade can be built so more effective DRAs can be formulated and injected optimally. There have been a few attempts to simulate DRAs in pipe flow but they have been limited to moderate Reynolds numbers. In industry very high Reynolds numbers are seen, often exceeding 500,000. There have been very few attempts to simulate DRA degradation.

The computational model will use Computational Fluid Dynamics (CFD). Three elements will make up the model, namely the fluid flow itself described by the Navier-Stokes equations, a polymeric model to simulate the DRAs' behaviour and finally a degradation model to represent DRA breakdown.

A Reynolds-Averaged Navier-Stokes, a turbulence modelling technique, CFD simulation has been developed to model a flow with a Reynolds number of around 44,000. The velocity profiles and turbulent kinetic energy distributions show good agreement with literature. The pressure drop shows a close alignment with the Blasius correlation too.

The next stages of the project are to increase the Reynolds number closer to those seen in industry and begin developing a Large Eddy Simulation to investigate the eddy structure of the flow. Further down the line, a polymeric model, likely FENE-P, and a degradation model will be introduced to the simulation.

P13: High Particle Actives as Sustainable Consumer Goods

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Emily Chapman[1], Dr. Dan Xu[2], Dr. Carlos Amador[3], Prof. Zhenyu Zhang[4]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Procter & Gamble, Beijing, China, [3]Procter & Gamble, Newcastle, United Kingdom, [4]University of Birmingham, Birmingham, United Kingdom

Solid unit-dose laundry detergents are emerging as a sustainable alternative to conventional liquid and powdered formulations, contributing to companies' net zero targets through reduced material usage, lower transportation emissions, and decreased water consumption during manufacture. Advances in formulation strategies further enhance these benefits by enabling more compact dose formats and reduced raw material demand. However, the implementation of such approaches has highlighted key challenges related to product performance during use and material handling.

This study aims to establish the relationship between formulation, particle properties, and dissolution through a combined experimental approach that will include dissolution testing under controlled conditions, rheological measurements, small-angle X-ray scattering (SAXS), optical and electron microscopy, spectroscopic analysis, and particle characterisation. These techniques will enable correlations between surfactant phase behaviour, moisture interactions, particle mechanical properties, and overall formulation performance, thereby providing guidance for the design and optimisation of future formulations.

P14: Modulating Oral Biofilms Through Prebiotics

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Jasmin Clark[1], Dr Brinta Chakraborty[2], Dr Lyndsay Schaeffer-Korbylo[2], Dr Tom Mills[1], Prof Anthony Metcalfe, Dr Tim Overton[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Colgate-Palmolvie Company, Piscataway, USA

Introduction: Caries and periodontitis are the two most prevalent noncommunicable diseases worldwide, accounting for over 3.5 billion cases (WHO, 2022), driven by microbial dysbiosis. Pathogenic bacteria, such as Streptococcus mutans, thrive through increased attachment and biofilm formation, overcoming beneficial commensals like Streptococcus sanguinis (Zhu et al., 2018). Interventions that restore a beneficial microbiome and inhibit pathogenic biofilms are key preventative strategies. Prebiotics, defined as substrates selectively utilised by host microorganisms to confer a health benefit, represent a promising therapy.

Aims: This study investigates the potential of oral prebiotics to modulate the oral microbiome and, consequently, prevent caries and periodontitis. Specifically, we aim to quantify the impact of selected prebiotics on the growth and surface-specific biofilm formation of key oral bacteria, typified by the beneficial S. sanguinis and the pathogenic S. mutans.

Methods: We used S. sanguinis and S. mutans as model organisms to assess the effect of various prebiotics on microbial growth kinetics and biofilm formation. We quantified biofilm mass and structure established on physiochemically distinct surfaces, mimicking oral tissues, to address the spatial heterogeneity of the oral cavity.

Results & Conclusion: Our work to date demonstrates that prebiotics significantly impact the growth and, critically, the surface-dependent biofilm formation of key oral bacteria. Understanding the interplay between prebiotics, bacterial species, and surface characteristics is crucial for developing targeted preventative therapies. This work validates the concept of prebiotic modulation as a viable strategy for restoring a beneficial microbial balance and preventing the world's most common oral diseases. We will present work to date demonstrating the impact of prebiotics on biofilm formation on different surfaces by key oral bacteria.

P15: Enhancing the Penetration of Cosmetic Actives into the Skin

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Harshita Dani[1], Mark Johnson[2], Thomas Mills[1], Anthony Metcalfe[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]No7 Beauty Company, The Boots Group, Nottingham, United Kingdom

Many commercial cosmetic skincare products contain active ingredients for the treatment and/or prevention of certain non-clinical skin conditions. However, effective penetration of active ingredients into the skin is not readily achieved due to the protective nature of the outer layer of the skin, particularly the stratum corneum, acting as a barrier. This project aims to develop cosmetic formulations with improved penetration of actives into the skin to achieve effective delivery to the target area.

Efforts to overcome this issue of limited penetration have previously included increasing the quantity of active in formulations, though this may result in reduced skin tolerance, increased costs and lower sustainability. Hence, understanding how actives can be delivered more effectively to the skin, and reach the appropriate target site, is of considerable interest. Additionally, the controlled release of actives may also improve product efficacy while increasing skin tolerance and consumer benefits.

Several formulations have been explored to develop basic gel-cream formulations as a chassis for the loading of an active ingredient. These oil-in-water emulsions include a medium chain-triglyceride (MCT) as the oil phase, Tween 20 as an emulsifier, and incorporate thickeners like xanthan gum and Aristoflex® AVC to improve the texture. Several oil concentrations have been investigated, using techniques such as tribology and rheology to assess the textural attributes and mechanical properties of the formulations upon application. This determined that varying the oil concentration did not significantly affect the rheological properties of the formulations. However, the friction coefficients were noticeably different in the tribological data. Present work involves incorporating niacinamide, as a cosmetic active, into the gel-cream formulations. A skin mimic model will then be used to investigate the quantity of niacinamide able to penetrate and assess the depth of delivery into the model to understand how effectively the niacinamide is able to penetrate.

P16: PIV studies into the effect of fluid rheology and impeller geometry on the flow fields generated by sawtooth impellers

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Shreyasi Deshpande[1,2], Dr Thomas Abadie[1], Prof. Bettina Wolf[1], Dr Cesar Mendoza[2]

[1]School of Chemical Engineering, University of Birmingham, Birmingham, United Kingdom,
[2]Unilever R&D, Port Sunlight, United Kingdom

Paste formulations, exhibiting non-Newtonian rheological characteristics such as a yield stress and shear thinning behaviour, are a common format used to deliver a range of personal care products. In a full formulation high-shear mixing is used to achieve agglomerate break-up and powder dispersion into the continuous phase. It is of interest to improve the understanding of the effects of geometry, operating conditions and fluid properties on the flow field in such processes.

Sawtooth impellers are a common type of high-shear mixing element used in industrial processes. Limited studies exist on their agitation performance, and these are restricted to geometries pre-fabricated by suppliers. In this work, particle image velocimetry (PIV) was used to investigate custom sawtooth impeller geometries. Flow profiles were obtained for 3 impellers [4, 8 and 16 teeth] when agitating fluids with different rheological properties [Newtonian – glycerol and glycerol solutions (50 and 80 wt. %), shear thinning non-Newtonian – Carbopol solution (1.5 wt. %)]. Experiments were carried out at a rheometer scale [D = 15 mm and T = 35 mm] as power draw and computational fluid dynamics (CFD) models have been established at this scale in previous work.

Mean flow patterns in the vertical plane reveal the shape and position of internal flow recirculation loops above and below the impeller position. Deformation of the free surface is also observed as the draw-down towards the impeller intensifies as agitation conditions change. Axial and radial velocity profiles are presented as a function of impeller surface area, viscosity and rotational speed. In the horizontal plane, flow patterns show fluid movement through the gaps between impeller teeth and the change in these patterns as the number of teeth increase. Understanding shear rates near and between impeller teeth will underpin studies into manufacturing industrially relevant formulations and their dependence on agitator geometry.

P17: Preparation, Physicochemical Characterisation, and Antimicrobial Assessment of Cinnamon Essential Oil–Montmorillonite Nano-Hybrid Systems for Food Packaging Applications

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mrs Ghufran Eshaq[1], Dr. Taghi Miri[1], Dr. Helen Onyeaka[1]

[1]University of Birmingham, Birmingham, United Kingdom

The use of natural antimicrobial agents in sustainable food packaging is increasingly attractive; however, their practical application is often limited by poor stability and uncontrolled release. Cinnamon bark essential oil (CEO) is a well-established antimicrobial and antioxidant, but its high volatility and low aqueous stability restrict its direct incorporation into packaging systems. In this study, a cinnamon essential oil–montmorillonite (CEO–MMT) nano-hybrid system was developed and characterised as a stabilised antimicrobial platform for food packaging applications.

Hydrophilic sodium montmorillonite (Na-MMT) nanoclay was dispersed, exfoliated, and purified through controlled magnetic stirring, probe ultrasonication, and low-speed centrifugation to obtain a stable nanoscale suspension. CEO was formulated into a food-grade nanoemulsion using Tween 80, high-shear homogenisation, and ultrasonication, and subsequently integrated with the exfoliated nanoclay to form a hybrid colloidal system. The CEO–MMT nano-hybrid was characterised in terms of particle size distribution, polydispersity index, and zeta potential, confirming good colloidal stability. Encapsulation efficiency was quantified using a centrifugation-based separation method coupled with UV–Vis spectroscopy, demonstrating effective retention of CEO within the nanoclay carrier. The influence of pH on nano-hybrid stability was also examined to assess robustness under conditions relevant to food packaging environments. FTIR spectroscopy was used to investigate molecular interactions between CEO and Na-MMT, providing evidence of successful hybrid formation.

Antimicrobial performance is currently being evaluated using broth microdilution assays to determine the minimum inhibitory concentrations (MICs) of free and encapsulated CEO against representative Gram-positive and Gram-negative foodborne bacteria. The results to date demonstrate the successful formulation of a stable CEO–MMT nano-hybrid system that addresses key limitations associated with essential oil volatility and provides a strong foundation for the subsequent development of biodegradable active and smart food packaging materials.

P18: Effect of oxygen plasma pretreatment on the properties of aqueous barrier coating

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Jia Guo[1], Dr. Emily Boswell[2], Dr. Xiandong Wang[2], Dr. Estefania Lopez-Quiroga[1], Prof. Peter Fryer[1], Prof. Zhenyu Zhang[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Beckett Ridge Technical Centre (BRTC), Procter & Gamble, West Chester Township, United States

While plastic packaging remains widely used, increasing attention is being directed toward more sustainable alternatives. Fibre-based substrates such as paper and cardboard offer advantages in biodegradability and recyclability; however, their porous and hydrophilic structure limits their water vapour barrier performance. This study investigates the use of oxygen plasma pretreatment to enhance the water vapour barrier properties of sustainable paper packaging by increasing surface energy and facilitating coating penetration into the porous fibre network.

Surface energy of the barrier coating was quantified using the Owens–Wendt–Rabel–Kaelble (OWRK) method based on contact angle measurements. The surface and cross-section morphology of the paper substrate were characterised using scanning electron microscopy (SEM) to evaluate coating coverage, defect formation, and penetration depth. White light interferometry (WLI) was used to generate 3D surface topography and quantify surface roughness. Water vapour transmission rate (WVTR) testing was conducted to assess barrier performance under different plasma treatments and coating thicknesses.

Oxygen plasma pretreatment significantly increased substrate surface energy, reaching 76.41 $mN \cdot m^{-1}$ at 40 W compared to 43.22 $mN \cdot m^{-1}$ for untreated paper, resulting in improved wettability. The surface roughness (Sa) of uncoated paper was 1.98 µm, and plasma treatment did not induce noticeable changes in surface morphology, confirming that structural integrity was preserved. Thicker coatings produced uniform, continuous layers and reduced surface roughness to 0.40 µm, while thinner coatings exhibited surface defects, leading to barrier performance (WVTR = 16.824 $g \cdot h^{-1} \cdot m^{-2}$) compared to thicker coatings (WVTR = 3.617 $g \cdot h^{-1} \cdot m^{-2}$). Plasma-treated samples showed improved coating coverage and reduced defect density, indicating enhanced surface integrity and barrier efficiency.

Overall, this study demonstrates that oxygen plasma pretreatment effectively enhances the surface energy of paper substrates, promoting improved wetting and penetration of aqueous acrylic coatings. This reduces pinhole-like defects and significantly improves the water vapour barrier performance of fibre-based packaging materials.

P19: Formulation of a Novel Collagen Food Gel with Different Physico-Chemical Characteristics

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Abeer Hajj Houssein[1,2], Professor Bettina Wolf[1], Professor Richard Greenwood[1], Doctor Stephen Mee[2]

[1]School of Chemical Engineering, University of Birmingham, Edgbaston, United Kingdom,
[2]Devro Limited, Moodiesburn, United Kingdom

Type 1 collagen consists of three polypeptide chains tightly bound into a triple helix held together by hydrogen bonds. It is particularly sourced from bovine hides and valued in food industries for its gelling, emulsifying, and film-forming capabilities. Collagen gels used in the food industry offer formulation flexibility, enabling them to be tailored for both mechanical and specific functional performance. The formation of these gels can be initiated by modifications in pH, temperature, and/or ionic strength that lead to swelling of collagen fibres by water. However, many factors including heredity, environment, feeding regime, and animal age contribute to yield variation in collagen that make it difficult to produce gels with consistent and uniform quality. A poor-quality gel may manifest by a variation of composition and structure, leading to undesirable properties such as different viscoelastic behaviours. Due to complexity, a full factorial design of experiments with 4 factors and 2 levels was developed to understand the main effects of the factors and to optimise the response. The aim of this research is to investigate the effect of pH, mixing speed, time of mixing, and ageing on the final physico-chemical properties of formulated collagen gel.

Initial results indicate that pH measurements are equilibrated with increasing time of ageing. Differential scanning calorimetry revealed differences in thermal transition temperatures and enthalpies suggesting the presence of native or unswollen collagen in some gels. This might be caused by the variation in hides. Scanning electron microscopy uncovered novel microstructure characteristics: a good collagen gel exhibited a void structure linked to properly swollen collagen networks. Images of poor gels showed the presence of reminiscent fibre bundles; these are believed to be unswollen collagen. Finally, rheological experiments revealed that both elastic and viscous modulus increase with increasing pH from 1.5 to 3.0.

P20: Development of a digital platform for the optimised production of sustainable biopolymer products

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Oluwatobiloba Henry[1], Prof Kit Windows-Yule[1], Prof Joseph Wood[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Aquapak Polymers LTD, Birmingham, United Kingdom

The increasing global demand for sustainable materials necessitates the development of efficient manufacturing processes that balance material performance, energy consumption, and environmental impact.

This project investigates the complex flow dynamics and mixing mechanisms within twin screw extrusion systems, with a particular emphasis on the geometrical configuration of elements in a twin screw system and their role in achieving optimal blends of biodegradable polymer blends.

A key aspect of this research is the development on novel mathematical models that accurately describe the geometrical properties of twin screw elements. These models have the ability to describe novel and complex geometries for twin screw system. Through the integration of artificial intelligence (AI)–driven optimisation techniques with simulation techniques, never-before-seen designs can be uncovered and experimentally validated to show improved performance compared to current off-the-shelf/conventional extruder elements, be it kneading or conveying elements. This will lead to improvements in process efficiency, material quality, energy consumption and improved sustainability.

The outcomes of this research will contribute to both fundamental understanding of extrusion science and practical solutions for the large-scale production of biodegradable plastics. This work supports the joint mission of Aquapak polymer Ltd and the University of Birmingham to develop environmentally responsible polymer technologies while advancing the broader field of polymer processing.

P21: Lipid extract from leaves as novel emulsifier for chocolate

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Charlotte Huddart[1], Prof. Bettina Wolf, Dr Fotis Spyropoulos, Dr Josélio Vieira

[1]University of Birmingham, United Kingdom

The aim of this research is to develop a naturally derived replacement for polyglycerol polyricinoleate (PGPR) from cocoa leaves that performs comparably in chocolate formulations. Surfactants are added to chocolate to control the flow properties and prevent sugar aggregation. The two most widely used surfactants are soya lecithin (a viscosity modifier) and PGPR (a yield stress reducer). Lecithin has a good level of consumer acceptance due to it being derived by from common food oils. PGPR is only available as a synthetic substance so is not considered a 'clean label' ingredient and suffers from bad consumer acceptance. This gives incentive for the development of a 'green' alternative. Spinach leaf-derived materials have previously been shown to reduce the yield stress of sugar-in-oil suspensions. (Mohamad, N.J., Gray, D. & Wolf, B. (2020), Sutcharit, P., Wattanakul, J., Price, R., Di Bari, V., Gould, J., Yakubov, G., Wolf, B. & Gray, D.A. (2023). Although encouraging for chocolate innovation, the data reported are constrained by two key limitations: (i) the absence of molecular specificity regarding the active lipid components, and (ii) the use of simplified suspension systems which do not adequately replicate the structural complexity of chocolate. This work established a natural extraction pathway with dried spinach, prioritising industrial feasibility over chemical purity. Compositional analyses of extract prove high lipid content. Addressing the second limitation, chocolate models of increasing complexity were tested using a continuous phase ratio of 30 wt%. Experimental data validates yield stress reducing functionality of both the spinach leaf extract. Spinach leaf extract reduced the yield stress of the model suspension by 87.1% ± 4.2%, highly comparable to PGPR which caused a reduction in the same model by 87.0% ± 5.4%. These results are the first to report the use of spinach leaf extract as a surfactant in suspensions most like chocolate.

P22: Development of high throughput physical characterisation methods for cosmetic products

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Edward Kane[1], Mr Mark Johnson[2], Prof Anthony Metcalfe[1], Dr Tom Mills[1]

[1]University of Birmingham, Edgbaston, United Kingdom, [2]No7 Beauty Company, The Boots Group, Nottingham, United Kingdom

Cosmetic products have traditionally been tested using human volunteers. These techniques are expensive and slow due to their high labour intensity and difficulties arise from differences in skin types and seasonal changes to the skin. Physical characterisation techniques such as tribology, rheology and microscopy offer an alternative to traditional testing methods which allow us to better understand the microstructure of cosmetic products. This encourages the development of novel systems which would previously be overlooked in favour of less adventurous formulations.

Tribology testing has been conducted using a 3 ball on plate rheometer with a stainless steel 3 ball geometry and poly(dimethyl siloxane) (PDMS) skin substitute. Moulds have been developed to consistently produce skin substitute with an appropriate surface roughness to differentiate the lubricating effects of model moisturiser systems ranging from 0-5 % grapeseed and paraffin oils and a purified medium chain triglyceride. These systems do not display full traditional Stribeck curve behaviour with curves starting in the elastohydrodynamic regime instead of the boundary regime as is often observed.

The model systems display shear thinning behaviour with a yield stress which is unaffected across the oil concentrations studied. For this range, the tribological and rheological behaviour of the model systems are independent of each other. Tribology has proven to be an effective technique to characterise and differentiate cosmetics as part of a high throughput testing regime.

P23: Unexpected antagonists within spreading formulations

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Dr Nina Kovalchuk[1], Prof Masanobu Sagisaka[2], Ms Hinata Komiyama[2], Prof Mark Simmons[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Hirosaki University, Hirosaki, Japan

Synergism between fluoro- and hydrocarbon surfactants in spreading formulations is well-known, with the most famous example being aqueous film forming foam (AFFF) used to extinguish fuel fires [1]. Low surface tension is achieved through preferable adsorption of fluorocarbon surfactant at water/air interface and is combined with low interfacial tension at water/oil interface due to preferable adsorption of hydrocarbon surfactant. This enables fast spreading of aqueous film drained from the foam over fuel surface with surface tensions as low as 22 – 28 mN/m. Fluoro- and hydrocarbon surfactants also show synergism in spreading on solid substrate in the case of partial wetting [2].

The aim of this study is thus to explore whether such synergism can be used to promote fast spreading of aqueous formulations over moderately hydrophobic solid substrates in the case of complete wetting. The spreading of aqueous formulations was studied on two commercially available substrates: polyethylene (PE) and polyvinylidenefluoride (PVDF). Studied surfactants included some known commercial superspreaders (enabling complete wetting and fast spreading on the studied substrates), commercial non-superspreaders and a fluorocarbon surfactant sodium bis(1H,1H,2H,2H-perfluorohex-1-yl) sulfosuccinate, 4FG(EO)2 synthesized at Hirosaki University.

Unexpectedly, our study has shown that instead of synergism, antagonistic behaviour was observed. In particular, both 4FG(EO)2 and commercial trisiloxane superspreader BREAK-THRU S 278 (BT-278) demonstrated superspreading on PVDF substrate with spread area being proportional to time. The spread area of 5 mm3 drop reached ~ 400 mm2 for BT-278 and 600 mm2 for 4FG(EO)2 on the time scale of 12 s, whilst mixtures of these surfactants demonstrated only slow spreading with spread area being proportional to the square root of time and maximum spread area < 100 mm2.

References

1. Moody CA, Field JA Environ Sci Technol, 2000, 34, 3864.
2. Kovalchuk N et al. Coll Surf A, 2016, 505, 23.

P24: A hybrid RANS-LES approach for CFD modelling of transitional flow of non-Newtonian fluids in stirred tanks

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Robert Leaney[1], Dr Georgina Wadsley[2], Dr Waldo Rosales[2], Dr Thomas Abadie[1], Dr Joëlle Aubin[3], Prof David Fletcher[4], Prof Mark Simmons[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Unilever, Port Sunlight, United Kingdom, [3]Laboratoire de G´enie Chimique, Tolouse, France, [4]University of Sydney, Sydney, Australia

Applications of computational fluid dynamics (CFD) to stirred tanks in both laminar and fully turbulent flow are widespread. However, many industrial tanks used to manufacture formulated liquid products with complex and/or time-dependent rheology operate in the transitional flow regime, where the flow features are neither fully laminar nor fully turbulent and therefore ”turbulence structures” are difficult to capture.

Recent work has shown good agreement between experimental 2D particle image velocimetry (2D-PIV) measurements and numerical predictions for Newtonian fluids in the transitional regime using a Stress Blended Eddy Simulation (SBES) turbulence model. SBES is a hybrid modelling approach implemented in Ansys that combines a Reynolds-averaged Navier–Stokes (RANS) k–ω SST model near solid boundaries with large-eddy simulation (LES) in the bulk flow. These results were obtained for a stirred tank fitted with an A320 hydrofoil impeller over a broad range of Reynolds numbers within the transitional regime. While previous numerical studies of non-Newtonian transitional flows in stirred tanks have employed RANS or LES methods, the use of SBES for such systems has not yet been reported.

In this work evaluation of the performance of SBES (Ansys 2025R2) is extended to a non-Newtonian fluid in the transitional regime. The simulations were carried out in a stirred vessel of diameter T = H = 0.19 m, with an impeller diameter D = T /2 and clearance C = T /3. The working fluid was a shear-thinning aqueous carboxymethyl cellulose solution (0.6 wt%), corresponding to a Reynolds number of approximately 1900. Predicted flow fields from SBES and from a RANS model (GEKO) were compared with 2D-PIV measurements, the SBES approach was found to provide the closest agreement with the experimental data.

P25: Developing novel sustainable dried capsules for consumer goods applications

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Ms Anjana Madhusoodanan[1], Dr Mariana Cardoso[2], Mr Joel Caragay[3], Dr Jon Preece[4], Dr Zhibing Zhang[1]

[1]School of Chemical Engineering, University of Birmingham, Edgbaston, B15 2TT, UK, [2]Procter & Gamble, Brussels Innovation Centre, 1853, Grimbergen, Belgium, [3]Procter & Gamble, Newcastle Innovation Centre, Newcastle upon Tyne, NE12 9BZ, UK, [4]School of Chemistry, University of Birmingham, Edgbaston, B15 2TT, UK

Microcapsules loaded with fragrance play a critical role in formulation of laundry products because of their ability to deliver actives in a targeted and controlled fashion while enhancing the consumer sensory experience[1]. Silica-shelled perfume microcapsules have potential to be used in laundry detergents as a sustainable alternative to conventional polymeric capsules, which contribute to non-biodegradable polymeric waste[2]. However, current silica microcapsule formulations require large volumes of water in its manufacturing process. Transitioning from liquid to dried particles would reduce associated transportation emissions and enable higher addition levels to detergent product.

This study investigates the drying of silica-based perfume microcapsules to produce low-moisture, high-solid content formulations while maintaining mechanical strength, barrier properties, and adhesion to fabric surfaces. Drying was carried out using a laboratory-scale twin-fluid spray dryer, and the effects of process conditions and residual moisture content on capsule size distribution, morphology, and rupture strength were systematically evaluated [3]. Preliminary results show that spray drying produces free-flowing silica microcapsules with low moisture content and capsule rupture strength was found to be sensitive to drying conditions. These findings demonstrate the feasibility of converting silica microcapsule slurries into dried formulations that align with green chemistry principles by reducing water use, minimising waste, and improving process efficiency, while retaining performance characteristics required for sustainable laundry detergent applications.

References
[1] R. Tekin, N. Bac, and H. Erdogmus, ‘Microencapsulation of fragrance and natural volatile oils for application in cosmetics, and household cleaning products’, Macromol. Symp., 333(1):35–40, 2013, doi: 10.1002/masy.201300047.
[2] Cardoso, M. B. T., Barros, A. M., Nies, P. D., Verstraete, P. D., Wong, V., Smith, S. D. & Smets, J. Capsules., 2020, US20200330949A1.
[3] J. Pidalà, C. Lombardelli, I. Benucci, and M. Esti, ‘Synergistic use of spray drying and fluidized bed in the microencapsulation of food ingredients’, Trends Food Sci. Technol., 165(105323), 2025, doi: 10.1016/j.tifs.2025.105323.

P26: Impact of rheology on the digital optimisation of mixing in soap manufacture

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Rowan Meacher[1,2], Dr Roberto Hart-Villamil[1], Professor Christopher Windows-Yule[1], Professor Mark Simmons[1], Mr Santoshkumar Gupta[2]

[1]University of Birmingham, United Kingdom, [2]Unilever, Bangalore, India

The mixing profile of formulated liquid and solid products such as soap is complicated by an evolving non-Newtonian rheology during saponification, which creates considerable difficulty for optimisation of process conditions and energy use. Poor mixing can result in an incomplete saponification process and a poor-quality end product. Whilst current work by Hart et al has led to the development of a digital optimisation workflow using simplified rheology, scope remains for improving the rheological model to more accurately represent processed material and final product.

The main challenge in measuring soap rheology is the presence of slip on the rheometer geometry walls, making collection of data difficult with poor repeatability and reproducibility. Being unable to measure the rheological profile of soap limits the industry's ability to optimise process, equipment design and process time which collectively limit the ability to control process energy input. This paper describes a scoping exercise to screen the capability of different instruments to measure soap rheology, to thus establish a validated rheological model for the digital workflow. This rheological model will then be compared with torque measurements obtained from a 5-blade ploughshare mixer, modelled on industrial mixers. This mixer contains regions of high shear, low shear, radial flow, and axial flow in close proximity, representing a more complex flow field. This study will thus determine the capability of the torque measurements to determine progress towards process endpoint, using the improved rheological model as a baseline to see whether in-situ determination of the product rheology matches expectations.

P27: Formulation engineering of flavour microemulsions

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Subhashree Patra[1], Prof. Bettina Wolf[1], Dr Fotis Spyropoulos[1], Dr David Garrec[2]

[1]School of Chemical Engineering, University of Birmingham, Edgbaston, B152TT, United Kingdom, [2]Diageo, Unit D Woodside, Dunmow Road, Bishop's Stortford, CM23 5RG, UK, United Kingdom

Emulsions are a widely applied flavour delivery vehicle in beverage applications. Upon combining the formulation ingredients, thermodynamically stable low-turbidity microemulsions with droplet sizes of less than 100 nm form spontaneously. In practice, nanoemulsions formulations are often utilised despite requiring high pressure homogenisation for product stability. The objective of the research presented is the formulation engineering of flavour microemulsion for application in acidic clear beverages via dilution not requiring high pressure homogenisation.

Five flavour oils with varying logP values including 3-methyl-1-butanol, ethyl butyrate, 1-octen-3-one, limonene and eucalyptol were selected and encapsulated individually in 10%w/w dispersed phase formulations. The aqueous phase contained polyoxyethylene (80) sorbitan monolaurate (Tween 80) as a non-ionic surfactant and propylene glycol as the co-surfactant at varying concentrations and surfactant-to-oil ratios (SOR). In addition to formulation parameters, the impact of heating, dilution and pH was investigated. Microemulsions were visually assessed for turbidity and quantitatively for droplet size data via dynamic light scattering. All five flavour oils were successfully encapsulated as judged by the absence of a layer of oil forming on the surface of the emulsion over time. However, over the parameter range considered formulations containing 1-octen-3-one were turbid. The molecular structure of 1-octen-3-one stands out as long extended and appeared to be incompatible with the hydrophobic tail structure of Tween 80. The incompatibility hypothesis was tested by additional experiments with flavour molecules of similar molecular structure but varying chain length.

The findings to-date contribute to developing a rational framework for energy-efficient and scalable flavour delivery systems. By correlating molecular structure with macroscopic stability, this work bridges the gap between fundamental interfacial thermodynamics and practical application in sustainable beverage formulations.

P28: A Novel Amide-Lactone Extraction Agent for Separation of Rare Earth Elements in Nitric Acid Systems

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Yi Chen[1], Miss Ruobing Liu[1], Dr Lina Qiu[1,2], Dr Shangfeng Du[2]

[1]School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing, China, [2]School of Chemical Engineering, University of Birmingham, Birmingham, United Kingdom

Rare earth elements constitute critical strategic resources for modern high-tech and green energy industries, with their efficient and clean separation being central to resource utilisation. Currently, solvent extraction represents the mainstream separation technology within the rare earth industry. Amide-type extractants (such as TODGA) have garnered significant attention due to their favourable coordination selectivity towards trivalent rare earth ions. However, existing extractants generally suffer from excessive acidity dependency. For instance, extraction capacity often diminishes significantly with increasing acidity, or proves insufficient under low-acid conditions. Consequently, practical processes frequently require operation at elevated acidity levels. This exacerbates equipment corrosion, reagent consumption, and environmental pollution, while simultaneously increasing operational costs associated with subsequent wastewater treatment and acid recovery. Consequently, developing novel extractants capable of maintaining high extraction performance across a broad pH range is crucial for advancing rare earth separation technology towards greater efficiency, environmental sustainability, and economic viability.

In this research, a structurally novel amide-capside extractant: 2,2'-((((2,2' oxobis(acetyl))bis(azadiethyl))bis(2-oxoethane-2,1-diethyl))bis(oxy))bis(N,N-dioctylacetamide) is designed and developed. Systematic performance evaluations demonstrate that, in nitric acid media, this extractant exhibits significantly superior extraction capabilities for typical trivalent rare earth ions compared to the conventional extractant TODGA. Notably, its extraction efficiency remains stable across a certain acidity range, exhibiting excellent low acid dependency and maintaining high extraction efficiency even under non-strongly acidic conditions.The extractant developed in this study exhibited excellent acid stability, with its extraction efficiency fluctuating by less than 10% within a nitric acid concentration range of 1 mol/L to 5 mol/L. In contrast, a comparable extractant, TODGA, demonstrated a significant variation in extraction efficiency, exceeding 20%, within the same acidity range. Thus, this research provides innovative insights and robust foundations for the molecular design of next-generation rare earth separation extractants tailored to industrial demands, actively advancing the green and sustainable separation of rare earth resources.

P29: Process contaminant fouling in membranes for CCS applications

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Dr Volatiana Razafindramanana[1], Sean McIntyre[1], Andrew Foster[2], M Vinot[1], Andrew Davies[1], Peter Budd[2], Prof Daryl Williams[1], Dr Paul Iacomi[1]

[1]Surface Measurement Systems, London, United Kingdom, [2]University of Manchester, Manchester, United Kingdom

An attractive type of membrane material for carbon capture applications are polymers with intrinsic microporosity (PIMs), which form flexible and easy-to-manufacture single-component membranes with high gas permeability and selectivity for CO_2 over N_2, O_2, and CH_4, the primary components of flue gas and biogas. Membrane selectivity and permeability are often measured under vacuum or ideal mixture conditions; however, in realistic gas streams, the presence of water vapour and impurities can significantly impact transport properties.

The objective of this work was to develop an experimental method to observe multi-component gas permeation through membranes and to investigate the effects of humidity, contaminants, and process conditions on membrane separation efficiency.

Materials/Methods:
A novel cross-flow membrane permeation device was developed to assess the impact of foulants on gas permeation and selectivity. Membranes of PIM-1 were studied and compared with carboxylated PIM-1 (cPIM-1), Nafion, and graphene-based membranes. Membranes were first exposed to controlled humidity for three hours, followed by permeation experiments using 10% CO_2 in N_2 for simulated flue gas or 20% CO_2 in CH_4 for biogas, while maintaining constant humidity. Dynamic vapour sorption (DVS) experiments were carried out to confirm membrane uptake behaviour, particularly the uptake of water within Langmuir voids and the subsequent impact on CO_2 solubility.

Results and Discussion:
The effect of increasing relative humidity was more pronounced for hydrophilic membranes. cPIM-1 exhibited a 40% decrease in CO_2 permeability compared to a 20% decrease for PIM-1, while the CO_2/N_2 selectivity of cPIM-1 decreased by over 80%, compared to a 16% decrease for PIM-1. For graphene membranes, both humidity and temperature were found to significantly influence CO_2/CH_4 separation. DVS measurements confirmed increased water uptake within Langmuir voids, leading to reduced CO_2 solubility and permeation.

P30: The Science Behind the Sparkle: Surface Insights into Residue-Free Cleaning

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Ms Millie Turner[1], Prof Zhengyu Zhang[1], Prof Peter Fryer[1], Dr Karolina Draper[2], Dr Carlos Amador[2]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Procter and Gamble, Newcastle, United Kingdom

Effective, residue free washing has long been a result sought by automatic dishwasher users. As a result, understanding the formation, composition and adhesion of complex films and residues is necessary to ensure consumer satisfaction. Therefore, employing a wide range of surface analysis techniques, such as AFM, Raman and XPS are necessary.

Preliminary measurements have set the scene to understand different surface mechanisms and dynamics of formation, prevention and removal of residues. These techniques will feed into a more complex system which includes organic (enzymes, food residues) and inorganic (mineral salt mixtures) components, enhancing formulation strategies for residue prevention.

P31: Rheology and Extrusion Behaviour of Zircon-Based Ceramic Pastes for Additive Manufacturing

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Renush Vigneswaran[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]MTC - Manufacturing Technology Centre, Coventry, United Kingdom

Additive manufacturing (AM) of ceramic materials offers significant potential for addressing long standing challenges associated with the manufacture and joining of monolithic, dissimilar, and multi-material systems. Extrusion based AM presents a versatile route for producing complex geometries while enabling greater control over material placement compared to conventional ceramic forming techniques. This focuses on the development of a novel extrusion-based AM capability aimed at progressing from monolithic ceramic components towards multi-material and functionally graded architectures, with the goal of enhancing component performance, extending service life, and improving resource efficiency.

This poster presents current formulation and rheological characterisation work underpinning the early stages of this programme. Zircon-based ceramic pastes were formulated using aqueous binder systems with varying carboxymethyl cellulose (CMC) concentrations and solid loadings. Combining principles from formulation engineering, powder processing, and materials characterisation with mechanical and process design considerations. A key early focus is developing a fundamental understanding of powder/binder interactions relevant to material extrusion and subsequent shape debind-sinter (SDS) processing routes. Current work therefore centres on the formulation and characterisation of ceramic pastes, with particular attention paid to rheological behaviour and extrusion response as enabling factors for reliable additive manufacture.

Rheological measurements were conducted using rotational rheometry to characterise shear-dependent viscosity and yield behaviour of the binder systems. Complementary extrusion experiments, and capillary rheometry were performed to quantify the force-velocity relationship during syringe extrusion of the ceramic pastes across a range of ram speeds. These experiments enable identification of stable extrusion regimes and provide insight into formulation limits associated with pressure instability, flow heterogeneity, and potential phase migration.

By integrating formulation led characterisation with AM process considerations, this research aims to establish a robust foundation for the development of next-generation extrusion based ceramic manufacturing technologies, supporting future applications across advanced structural, thermal, and functional ceramic components.

P32: Regime Map of High-Shear Wet Granulation of High-Surfactant-Content Powders

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Buddy Visetthernrakul[1], Professor Mark Simmons[1], Dr David Bell[2]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Unilever Research & Development Port Sunlight Laboratory, Wirral, United Kingdom

Powder-based personal care products offer benefits such as reduced packaging, lower shipping weight and longer shelf life, but surfactant powders often suffer from poor flowability and dustiness due to their fine particle size. Granulation can mitigate these issues by enlarging particles and improving handling. While high-shear wet granulation (HSWG) is well studied in pharmaceuticals, its application to high-surfactant personal care formulations remains limited. This study investigates the HSWG regime map for a blend of 20% sodium lauryl sulphate and 80% microcrystalline cellulose, using polyethylene glycol 6000 at 33% w/w in deionised water as the binder.

Granulation batches conducted across two impeller speeds and a range of liquid-to-solid (LS) ratios revealed distinct growth regimes that define the HSWG processing space for this high-surfactant formulation. At 1700 RPM, granule enlargement was consistently observed, indicating that moderate shear promotes coalescence and growth. In contrast, operation at 3000 RPM shifted the balance toward breakage-dominated behaviour, demonstrating that excessive mechanical stress can override binder-mediated growth mechanisms. Variation in LS ratio further highlighted the sensitivity of the system to binder availability: LS=0.7 produced rapid growth followed by pronounced breakage, LS=0.5 yielded a steady growth regime, and LS=0.3 exhibited an induction period before growth initiated. Despite this differing growth behaviour, the batches operated at 1700 RPM and LS=0.3-0.7 seems to converge in granule size after approximately 10 minutes of processing, suggesting the presence of a dynamic equilibrium between growth and breakage under these conditions.

These findings have implications for industrial processing, particularly for personal care products using high surfactant powders. They show that increasing impeller speed does not always promote granule growth, beyond a threshold, higher speeds intensify breakage and limit growth. Understanding this balance between growth and breakage is crucial for designing scalable HSWG processes that produce free flowing, low dust granules from high-surfactant content formulations.

P33: Using nuclear imaging, numerical simulation, and lightweight AI to optimise industrial systems

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Professor Kit Windows-Yule[1]

[1]University of Birmingham, United Kingdom

Numerical methods such as the discrete element method (DEM), computational fluid dynamics (CFD), coupled CFD-DEM, and multiphase particle-in-cell (MP-PIC) simulations provide potentially powerful tools for the investigation and optimisation of diverse particulate, fluid, and multiphase systems, including gas-solid systems. However, without rigorous calibration and validation, their outputs may be inaccurate, or even entirely unphysical, and the processes of calibration and validation can prove highly time- and labour-intensive (Windows-Yule, Tunuguntla et al. 2016, Windows-Yule and Neveu 2022).

For many industrial systems – which are typically housed in aluminium or steel, making them optically opaque – it can be highly challenging to extract meaningful dynamical information, and thus provide appropriate ground-truth data for the validation of numerical simulations (Windows-Yule, Buist et al. 2024). For fast-moving systems such as fluidised beds, where the temporal resolution of techniques such as x-ray CT becomes too low for meaningful data reconstruction, the challenge is greater still (Windows-Yule, Buist et al. 2024).

In this talk, we provide an overview of the Positron Emission Particle Tracking technique, and its use as a tool for the calibration, validation, and ultimately optimisation of industrial systems. We provide real industrial case studies conducted with Unilever (Hart-Villamil, Ingram et al. 2024) and Jacobs Douwe Egberts (Che, Al-Shemmeri et al. 2023), demonstrating how PEPT can be used to provide highly-validated, “true to life” simulations of industrial systems, and how these simulations in turn may be coupled to evolutionary AI algorithms to optimise the systems being modelled.

P34: Development of Emulsion-based Confectionery product: Understanding the Role of High Sugar Concentration in Emulsion Formation, Stability and Rheology

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Miss Yanni Yang[1], Dr. Aris Lazidis[2], Dr. Isabel Celigueta Torres[2], Dr. Fotis Spyropoulos[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Nestlé Product Technology Centre, York, United Kingdom

In the food industry, new product development often seeks to expand sensory characteristics, a priority that is particularly important in confectionery where indulgence is central. Emulsion technology is widely used to create distinctive microstructures that govern texture and mouthfeel in products. However, despite its potential, the application of emulsion technology in confectionery remains largely unexplored. Key challenges include the complex rheology associated with high sugar concentrations, their influence on emulsifier performance, and the effects of sugar type and concentration on emulsion formation. Previous studies investigated sugar effects on emulsions, but these have typically focused on a limited range of emulsifiers and sugar concentrations that do not reflect those used in confectionery products.

This study evaluates the effects of high sugar concentration and sugar type on emulsion formation, stability, and rheological behaviour. Three emulsifiers—Tween 20, whey protein isolate (WPI), and pea protein isolate (PPI)—were investigated under varying sugar conditions. Interfacial tension (IFT) and emulsifier structure were analysed using tensiometry and FTIR spectroscopy. Emulsion droplet size, stability, and rheology were also characterised.

Results show that sugar type had minimal impact on IFT, whereas increasing sugar concentration led to distinct changes in IFT, attributed to structural changes in the emulsifiers. Higher sugar concentrations produced smaller droplet sizes and more monodisperse distributions, likely due to increased continuous phase viscosity and differences in emulsifier performance. These effects also influenced emulsion stability. While all emulsions remained stable against droplet size changes over time, higher sugar concentrations improved resistance to creaming, with the exception of 60 wt% PPI emulsions, which exhibited flocculation. Across all formulations, emulsions displayed consistent Newtonian behaviour.

Overall, both sugar type and concentration affect emulsion formation and stability by modifying rheology and emulsifier performance. High sugar concentrations promote finer, more uniform emulsions with enhanced stability, highlighting the potential of emulsion technology for confectionery applications.

P35: Bioleaching of platinum group metals from automotive catalysts: mechanisms, microbial systems, and process integration

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Dr Farid Aiouache[1], **Kuralay Yeskalina**[1]

[1]Lancaster University, Lancaster, United Kingdom

The increasing consumption of platinum group metals (PGMs), particularly platinum (Pt), palladium (Pd), and rhodium (Rh), together with the limited availability of primary mineral resources, has intensified the need for sustainable recycling technologies. Spent automotive catalysts (SACs) represent one of the most important secondary sources of PGMs; however, conventional pyrometallurgical and aggressive hydrometallurgical processing routes are associated with high energy consumption, significant reagent use, and environmental impacts. Biohydrometallurgical approaches have recently emerged as promising environmentally friendly alternatives for the pretreatment and recovery of valuable metals from complex waste materials.

This study investigates the application of bioleaching for the treatment of spent automotive catalyst material using a mixed bacterial culture of Acidithiobacillus ferrooxidans and Acidithiobacillus thiooxidans. These acidophilic microorganisms generate ferric iron and sulfuric acid through biological oxidation processes, promoting the dissolution of base metal components and facilitating structural modification of the catalyst matrix. Such transformations improve the exposure and accessibility of PGMs embedded within the ceramic support, enabling more efficient subsequent recovery.

Experimental work involved mechanical pretreatment of the catalyst material followed by controlled bioleaching under acidic conditions. The evolution of solution chemistry, pH, oxidation–reduction potential, and metal concentrations was monitored throughout the process to evaluate the effectiveness of bacterial activity and the extent of matrix decomposition. The results demonstrate that bioleaching significantly enhances the removal of accompanying base metals and opens the catalyst structure, providing favorable conditions for downstream recovery techniques such as mild oxidative leaching or electrochemical extraction.

The findings highlight the potential of microbial-assisted processing as a green pretreatment technology for recycling PGMs from secondary resources. The proposed approach contributes to the development of sustainable circular economy strategies by reducing chemical consumption, minimizing environmental impact, and improving the efficiency of precious metal recovery from spent automotive catalysts.

P36: Synthesis of aerogels by mimicking natural aerogels of “Money Plant”

Theme: Formulation Engineering, Sustainable Manufacture & Materials

Mr Tianzhou Yuan[1]

[1]Newcastle University, Newcastle upon Tyne, United Kingdom

In our work a novel ambient pressure drying (APD) synthesis methods for the production of cellulose aerogels has been developed and the characterization of the resulting products was carried out. In order to prevent shrinkage during drying of the gel, a novel approach, which utilizes potassium bicarbonate solution that decomposes and generates potassium carbonate and carbon dioxide bubbles withing gel when temperature is between 100 and 120 degrees Celsius have been employed.

This APD method dramatically reduces costs, because commonly used supercritical drying process is complex and has problems such as expensive equipment cost requirements, high energy consumption, low safety, long drying time, and intermittent operation, which significantly increases production costs. To develop aerogel thin films with cellulose at ambient pressure drying condition, the framework of the edges of dried leaves of “money plant” (with no center) were used to make pinned stable aerogel thin films. So far, stable white aerogel films have been produced, which were also characterized by scanning electron microscopy (SEM), and the elemental and structural analyzes of the prepared samples were performed by Fourier transform infrared (FTIR) spectroscopy analysis.

P37: Biocompatible 3D micro-hollow fibre scaffolds as modulators of neuronal extracellular vesicle secretion

Theme: Healthcare Technologies

Mr Luca Adly[1], Dr Richard Moakes[1], Dr Patricia Esteban[1]

[1]University of Birmingham, Birmingham, United Kingdom

Introduction:
Despite technological advances, spinal cord injuries (SCIs) are currently incurable. Due to its complexity, there are no models that can encompass all aspects in a robust and reproducible manner, which hinders the advancement of new treatments. Extracellular vesicles (EVs) are crucial in intercellular communication within the nervous system and are increasingly recognised as important mediators in SCI response. Following injury, neuronal EVs can carry bioactive molecules that influence inflammation, apoptosis, axonal regeneration, and synaptic remodelling. In this work, micro-hollow fibres (MHFs) have been designed to induce cellular alignment of SHSY-5Y cells as seen in vivo. To demonstrate model effectiveness, the microenvironment of 3D cultured SH-SY5Y cells is to be investigated through EV profile analysis.

Methods:
SH-SY5Y cells were cultured on MHFs composed of polystyrene and polycaprolactone and as monolayers. Image analysis provided insight into cell proliferation over time. EVs were collected, pooled, and purified after 3, 5, and 7 days of 2D and 3D cell culture using differential centrifugation and size exclusion chromatography. Samples were analysed using dynamic light scattering and western blotting.

Results:
After 7 days of culture, SH-SY5Y cells exhibited uniform coverage and alignment along the MHFs, indicating successful scaffold population. Preliminary analysis suggests that neuronal cells cultured in 3D produce a greater yield of EVs compared to traditional monolayers, while maintaining a comparable vesicle size distribution, consistent with trends reported in the literature [2]. Protein composition of EVs derived from 3D cultures is anticipated to more closely reflect in vivo neuronal profiles, supporting the potential of this model to better mimic native neural microenvironments.

Conclusion:
MHFs composed of polystyrene and polycaprolactone can induce cell alignment and produce more representative EV profiles. Further work seeks to incorporate the fibres within fluid gels to more accurately represent the mechanical environment of SCI.

[1] DOI: 10.1016/j.tins.2021.01.003
[2] DOI: 10.3389/fimmu.2024.1388769

P38: Digital Twin of the Human Stomach via Physiologically Informed Simulations

Theme: Healthcare Technologies

Ms Thea Davies-Hines[1], Dr Konstantinos Stamatopolous[2], Professor Mark J. H. Simmons[1], Dr Alessio Alexiadis[1]

[1]School of Chemical Engineering, University of Birmingham, Birmingham, United Kingdom,
[2]Biopharmaceutics, DPD, MDS, GSK, Ware SG12 0DP, United Kingdom

The project aims to develop a digital twin of the human stomach by identifying the key physical and biological mechanisms that govern gastric function and expressing them into mathematical relationships. These principles will then be integrated into machine learning driven modelling framework capable of capturing dynamic interactions within the stomach environment.

The long-term goal is to create a model that captures the stomach's mechanical behaviour and predicts how it responds to pharmaceutical tablets, including their mixing, disintegration, and dissolution within the gastric environment, while also integrating the regulatory influence of the autonomic nervous system (ANS). Incorporating ANS control will allow the model to reflect how neural feedback regulates core gastric functions including motility and contraction patterns.

Recent progress has focused on developing the foundational computational tools for this work. A 2D soft-body lattice has been implemented in Python that can eventually be used to model a simplified 2D representation of the stomach, where particles move and interact in response to wall contractions. Using a physics-informed approach, the system models particle deformation and motion through basic force interactions, including simplified collision responses, to produce realistic emergent behaviour.

This preliminary model provides both a technical foundation and a proof-of-concept for particle-based soft-body modelling in Python. The insights gained will support the transition to more physiologically detailed and higher dimensional simulations as the digital twin evolves.

P39: Electrospun PCL–PF127 Scaffolds for Vascular Graft Coatings

Theme: Healthcare Technologies

Dr. Inmaculada De Dios Pérez[1], Ben Cassidy, Amy Morgan, Ílida Ortega Asencio, Patricia Pérez Esteban

[1]University of Birmingham, United Kingdom

Arteriovenous grafts are widely used in long-term haemodialysis, yet their clinical performance remains limited by high failure rates, reaching up to 70% within the first year. From an engineering perspective, insufficient surface wettability and poor early tissue integration are key contributors to thrombosis, leakage, and infection. Addressing these limitations through rational material design is therefore essential.

Poly(ε-caprolactone) (PCL) is a well-established polymer in vascular applications due to its mechanical robustness and processability; however, its intrinsic hydrophobicity restricts early biological interactions. In this work, we explore the incorporation of Pluronic® F127 (PF127), an amphiphilic triblock copolymer, as a strategy to tune both the physicochemical and mechanical properties of electrospun PCL-based scaffolds intended as external coatings for arteriovenous grafts.

Electrospinning solutions containing different PCL–PF127 ratios were prepared in dichloromethane/dimethylformamide and first characterised rheologically to assess their suitability for fibre formation. The resulting electrospun scaffolds were analysed in terms of fibre morphology, mechanical behaviour and surface wettability using microscopy, tensile testing and static contact-angle measurements.

Our results demonstrate that increasing PF127 content significantly enhances scaffold hydrophilicity and modifies fibre diameter and structure. However, excessive Pluronic incorporation compromises mechanical integrity. A 50:50 PCL–PF127 blend provided the best balance between wettability and mechanical performance. Building on these findings, a bilayer scaffold architecture (combining a mechanically robust PCL base layer with a hydrophilic PCL–PF127 surface layer) was developed, achieving optimal overall performance.

These results highlight how polymer blending and scaffold architecture can be used as effective engineering tools to tailor electrospun materials, supporting the development of next-generation vascular graft coatings with improved functional performance.

P40: Spray delivery of anti-fibrotic polysaccharides

Theme: Healthcare Technologies

Miss Jennifer Forbes[1], Jennifer Forbes, Anthony Metcalfe[1], Thomas Robinson[1]

[1]University of Birmingham, United Kingdom

Background and aims:
Almost 45% of deaths globally can be attributed to fibrotic conditions, with 1 in 3 people in the UK currently living with a scar. Despite advances, there is an unmet clinical need for an effective and affordable alternative. Natural polysaccharides isolated from seaweed have shown broad biomedical promise, due to their low cost and low toxicity. Here, we investigated carrageenan spray formulations and their effect on increasingly complex models of fibrosis. We aim to tailor carrageenan sprays for patient compliant delivery, altering their formulation for optimal rheological performance, considering internal microstructure and sprayability. Furthermore, we aim to determine interactions with extracellular matrix components, sequestering Transforming Growth Factor beta 1 (TGFb1), and inhibiting aberrant collagen deposition.

Methods:
Scarring was investigated using in vitro human dermal fibroblasts (HDFs) using immunocytochemistry and scratch assays, to investigate how carrageenan reduced effects of TGFb1-induced myofibroblast transdifferentiating. Carrageenan was formulated into sprayable viscoelastic fluid gels, with key rheological parameters evaluated and spray characteristics quantified. The interaction between TGFb1 and carrageenan was investigated using biophysical methods.

Results:
A successfully formulated carrageenan spray was optimised, showing beneficial cone angle, increased retention, and viscoelasticity. Carrageenan was shown to interact directly with TGFb1, with markers of fibrosis reduced in vitro. Antifibrotic effects are characterised by a reduction in cell based fibrotic markers post biological screening.

Conclusions:
These findings show that carrageenan sequesters TGFb1 and reduces markers of scarring in vitro. Carrageenan may thus be an effective and affordable therapy to reduce the global burden of scaring. The ability to formulate a viscoelastic fluid with both high spray coverage and prolonged retention using regulatory approved materials brings this therapy close to commercial reality and patient benefit.

P41: Multiscale mechanical characterisation of structured hydrogels as artificial biofilm

Theme: Healthcare Technologies

Mrunmayee Joshi[1], Guannan Wang[2], Spring Wang[2], Xu Huang[2], Peter Fryer[2], Zhenyu Jason Zhang[1]

[1]School of Chemical Engineering, University Of Birmingham, United Kingdom, [2]Procter & Gamble, Beijing Innovation Centre, China

Oral biofilms or dental plaque that forms on teeth and soft tissue can lead to many oral diseases such as gingivitis and periodontal disease. It varies from person to person and hence there is an intrinsic variability when investigating these biofilms for research. To improve the consistency of laboratory results, a model system can be used to evaluate mechanical properties such as adhesion, cohesion and elasticity. This work aims to evaluate the physico-chemical properties of structured agar hydrogels across multiple length scales.

Hydrogels with varying mechanical properties were developed using agar and sucrose to replicate biofilms with different growth times (soft to hard). Three different length scales of mechanical characterisation (atomic force microscopy (AFM) at nanoscale, a custom micromanipulation rig at the microscale and a force plate at the macroscale) were used to study mechanical properties.

Results from AFM and micromanipulation showed negligible adhesion and that the Young's modulus of the hydrogels increased with an increase in agar concentration, of which the values ranged from 2-20 kPa – it is of the same order of magnitude reported in literature for biofilms grown from different bacterial species such as Streptococcus gordonii. To validate the hydrogel model, 3-day old biofilm of Streptococcus mutans were grown and the Young's modulus was measured using AFM with values ranging from 1-10 kPa. Hertzian model was applied to analyse the AFM and micromanipulator data.
Understanding mechanical properties of hydrogels as artificial biofilms at different length scales allows us to study molecular interactions, structural deformation and surface detachment. This work contributes to the development of an artificial biofilm model that can help in developing methodologies to removal of oral biofilms.

P42: Dual-crosslinked GAP hydrogels: achieving tissue-mimetic nonlinear mechanics in printed corneal constructs

Theme: Healthcare Technologies

Mrs Hilal Mete Gunaydin[1], Mr Georgios Mikalef[1], Mrs Patricia Perez-Esteban[1], Mr Liam Grover[1]

[1]School of Chemical Engineering, University of Birmingham, Edgbaston, UK, United Kingdom

Hydrogels are increasingly used as tissue surrogates, yet reproducing the nonlinear, viscoelastic behavior of living tissues remains a major challenge in chemical and biomedical engineering. Biological tissues such as skin and cornea exhibit characteristic nonlinear, viscoelastic, and heterogeneous anisotropic properties that is critical for physiological function1. To address this challenge, a gelatin–alginate–PEGDA (GAP) combining controlled dual-crosslinking chemistry. In the present work, this material is applied to bilayered, dome-shaped corneal constructs fabricated via SLAM 3D printing.

GAP hydrogels were formed through ionic crosslinking (alginate-Ca^{2+}) and PEGDA photopolymerization, enabling precise control over gelation kinetics and rheological properties. Component concentration variations provided access to a wide stiffness range. Bilayered corneal domes were SLAM-printed with the GAP layer as mechanical support and an electroactive Mucin-co-AMPS/PEGDA upper layer for non-contact actuation2. Human corneal keratocytes were encapsulated and cultured under standard conditions. Mechanical characterization employed uniaxial compression testing, with stress–strain data fitted to Mooney–Rivlin, Ogden, and Fung hyperelastic constitutive models using MATLAB3.

GAP hydrogels exhibited nonlinear elastic behavior closely matching human skin mechanics. At low strain ($\varepsilon < 15\%$), Young's modulus was ~100 kPa, aligning with dermal tissue. At higher strain ($15\% < \varepsilon < 60\%$), pronounced strain-stiffening occurred with tangent modulus exceeding 1 MPa. Hyperelastic model fits achieved excellent agreement ($R^2 > 0.99$), validating tissue-like mechanical fidelity. SLAM-printed bilayer domes displayed J-shaped stress–strain responses and geometric instabilities characteristic of curved biological shells. Encapsulated keratocytes remained viable and well-adhered throughout the constructs.

The GAP hydrogel successfully replicates the nonlinear mechanical signature of biological tissues through rational design of dual-crosslinking chemistry and network architecture. Combined with SLAM printing and electroresponsive actuation layers, this system offers a controllable, biocompatible platform for corneal biomechanics modeling and stimuli-responsive soft tissue engineering applications.

1 A.Pissarenko et al. Sci., 2021, 120, 100816.
2 G.Mikalef et al. DOI:10.1002/jbm.a.38004.
3 D.S.Nedrelow et al. DOI:10.1016/j.jbiomech.2023.111592.

P43: An electro-active hydrogel system for the creation of a corneal like structure with controllable curvature

Theme: Healthcare Technologies

Mr Georgios Mikalef[1], Ms Hilal Mete-Gunaydin, Dr Zoe Schofield, Dr Patricia Perez-Esteban, Professor Liam Grover

[1]Healthcare Technologies Institute, Birmingham, United Kingdom

Introduction:
Corneal injury and disease can alter the biomechanical properties of the cornea, leading to abnormal bending and deformation that compromise cell viability and visual function. Accurately modelling these changes in vitro remains a considerable challenge. In this study, a novel bilayered construct capable of replicating changes in corneal curvature without direct mechanical contact was developed using SLAM printing. The construct comprised two distinct hydrogel formulations, including an electroactive Mucin-co-AMPS/PEGDA hydrogel.

Results:
Characterization of the electroactive hydrogel by FTIR showed that increasing energy exposure progressively consumed AMPS and PEGDA, indicating polymerization was complete at 2100 mJ/cm². Mechanical compression testing reflected this trend, with the hydrogel modulus reaching 1400 kPa and no further increase beyond 2100 mJ/cm². Higher energy exposure increased stiffness, leading to cracking during actuation. Incorporation of Type II mucin from porcine stomach produced a softer hydrogel with enhanced bending. This hydrogel supported human corneal keratocyte attachment, with viable, well-adhered cells throughout the construct. Using a three-well system, the hydrogel was exposed to varying electric fields, with keratocytes remaining viable after seven days.

Discussion:
Hydrogel bending was driven by asymmetric ionic distribution within the polymer network, generating localized osmotic pressure gradients that induced bending toward an electrode. Increased energy exposure produced higher crosslinking and stiffness, causing cracking. Type II mucin increased porosity and acted as a plasticizer, reducing stiffness and allowing greater bending while presenting bioactive motifs that promoted keratocyte adhesion. Electrode degradation and ROS generation were observed during direct electric field exposure, but the three-well system with salt bridges mitigated this risk, allowing safe electrostimulation.

Conclusion:
These findings highlight the bilayered hydrogel construct as a controllable, biocompatible, and electroactive platform for modelling corneal tissue mechanics and for applications requiring precise, non-contact actuation.

P44: Alcohol Infused Dancing Particles

Theme: Healthcare Technologies

<u>Dr Zoe Schofield</u>[1], Dr Thomas Goffrey[2], Professor Liam Grover[1]

[1]Healthcare Technologies Institute, University of Birmingham, United Kingdom, [2]Centre of Fusion Space and Astrophysics, University of Warwick, United Kingdom

Self-propelling particles move by converting energy from the environment (chemical, electrical, thermal, etc.) into mechanical motion1. Recent interest in them has increased, since they have found use as models of surface swarming by microbes and as toxicity sensors1. They have significant potential for directed drug delivery if their movement could be predicted and controlled. To enable this, it is essential to better understand what drives movement of the particles. Here, we aim to control the speed and behaviour of the particles by altering the surface tension around particle using ethanol as a propellent to push the particle around the environment3. Using 3% (w/v) chitosan solutions mixed with EtOH of varying concentrations (50-100% v/v/) at a 3:1 ratio we were able to observe different propulsion behaviours when dropped into a NaOH bath (3 M, 50 mL). When the chitosan and EtOH solution is dropped into the NaOH bath it undergoes a sol-gel transition2. We found that different concentrations of EtOH alters the surface tension gradient as the EtOH diffuses out of the chitosan, this therefore alters the propulsion behaviour from intermittent motion to a controlled exponential decay (until the EtOH runs out)3. Furthermore, we were able to control the temperature of the NaOH bath which allowed us to control the speed at which the chitosan particles moved throughout the bath. Throughout this work we have demonstrated it is possible to manipulate the surface tension to influence the particle behaviour which could be an attractive tool for biomedical applications.

1Sharma, R., et al., ‘Gel-based self-propelling particles get programmed to dance’, Langmuir, 28, 10128–10135, 2012.
2Kumar, P., et al., Sol-gel transition programmed self-propulsion of chitosan hydrogel. Chaos, 32, 2022
3Kwak, B., et al., Marangoni effect inspired robotic self-propulsion over a water surface using a flow-imbibition-powered microfluidic pump. Scientific Reports, 11, 2021

P45: Structural polymer as suspending media for lightsheet fluorescent microscopy

Theme: Healthcare Technologies

Mr Joseph Weightman[1], Dr Paige White[2], Dr Richard Moakes[1], Dr Thomas Robinson[1], Professor Ferenc Mueller[2], Professor Liam Grover[1]

[1]Healthcare Technologies Institute, University of Birmingham, United Kingdom, [2]Department of Cancer and Genomic Sciences, University of Birmingham, United Kingdom

Recent advances in lightsheet fluorescence microscopy (LSFM) have enabled dynamic 3D and 4D studies across disciplines, from spatial cell organisation to targeted cancer therapy. Nonetheless, long-term temporal imaging of 3D cell models remains challenging due to the lack of suspension materials that are simultaneously compatible with cell culture conditions and LSFM requirements. In this study, we developed optically clear gellan gum fluid gels and assessed their ability to support both cell viability and mechanical stability for extended 4D imaging of colorectal cancer organoids. Low-acyl gellan gum (Kelco) was dissolved at 1–2 w/v% in deionised water containing 5% PBS and 10 mM NaCl, heated to 90°C with mixing until fully dissolved, then autoclaved at 121°C for 1 hour. The hot solution was cooled under agitation at 20°C to form fluid gels and stored at 4°C until use. FUCCI-expressing colorectal cancer organoids were encapsulated in the gels and imaged on a Zeiss Z1 LSFM using 488 and 561 nm lasers, with images processed in ImageJ. Temperature sweep rheology (25–40°C, 1°C/min) on a Malvern Kinexus Ultra+ revealed that all formulations remained elastically dominant with increasing temperature, indicating stable gel networks. Gellan-embedded organoids exhibited continuous growth, preserved key morphological features, and remained immobilised for up to 14 days, enabling repeated imaging of identical regions over multiple cell cycles. Rheological tuning allowed us to modulate microstructure and deformation response, suggesting that gellan gels can be tailored to support diverse biological models. Our findings indicate that gellan gum is a promising platform for long-term live organoid culture and spatiotemporal reporter tracking. Future work will quantify cell viability and extend this approach to in vivo imaging of tissue development.

P46: Sustainable Recycling of Thermoplastics Carbon Fiber Reinforced Polymer (CFRP) Composites using Hydrophobic Deep Eutectic Solvents.

Theme: Chemical recycling of polymers

Mr. Adewale Ajose[1]

[1]University of Birmingham, Birmingham, United Kingdom

The increasing volume of thermoplastic carbon fibre-reinforced polymer waste demands urgent recycling technologies that can recover high-quality fibres while avoiding hazardous solvents. In this work, the thymol: decanoic acid hydrophobic deep eutectic solvent (HDES, 1:1) was investigated as a sustainable medium for the matrix removal of polyamide–6 (PA6)-based CFRP laminates. Batch degradation experiments with silicone oil bath at temperatures between 140 and 160 °C showed complete degradation of PA6 removal under mild conditions, with negligible loss of carbon-fibre thermal stability. Analysis of the PA6 degradation kinetics indicated that early-stage dissolution follows Fickian diffusion-controlled behaviour, with the fractional degradation scaling linearly with t1/2 and yielding an apparent diffusion-controlled activation energy of approximately 100 kJ/mol from an Arrhenius plot of the diffusion rate parameter. A Noyes-Whitney first-order dissolution model produced a substantially higher apparent activation energy (~280 kJ/mol) and a poorer physical description, confirming that bulk solvent penetration and polymer swelling, rather than purely surface-controlled dissolution, govern PA6 removal in the HDES system.

These results show that hydrophobic carboxylic acid-based HDES can serve as an effective, low-volatility alternative to traditional organic solvents for selectively dissolving thermoplastic matrices in CFRP. This enables sustainable recovery of intact fibres and provides a tunable platform for closed-loop composite recycling processes.

Keywords: Carbon fibre polymer composites, deep eutectic solvents, sustainable recycling, thermoplastic degradation, kinetic modelling, circular economy, green chemistry.

P47: Morphology-Controlled Kinetics in the Catalytic Glycolysis of PET

Theme: Chemical recycling of polymers

Mr Joseph Sutton[1], Prof. Andrew Dove[2], Prof Joe Wood[1]

[1]School of Chemical Engineering University of Birmingham, Birmingham, United Kingdom,
[2]School of Chemistry University of Birmingham, Birmingham, United Kingdom

Introduction:
The catalytic glycolysis of poly(ethylene terephthalate) (PET) is a promising strategy to enable a closed-loop PET economy. To realise the recycling of varied real-word wastes it is important to understand how the recycling process operates with different forms of feedstock. While kinetic studies typically emphasise catalyst selection, loading, and temperature [1,2] the influence of PET morphology is rarely quantified. This study examines how PET morphology impacts depolymerisation kinetics under $Zn(OAc)_2$ catalysis. By isolating morphological effects from catalytic ones, it aims to provide predictive insight for reactor design and industrial throughput.

Methods:
$Zn(OAc)_2$ (0.48 g), N-methylpyrrolidone (0.25 mL) and ethylene glycol (30 mL) were charged to a 100 mL round-bottomed-flask and heated to 180°C under reflux. Addition of PET (5 g) initiated the reaction. ^1H qNMR spectroscopy was used to quantify PET conversion. Morphology was examined throughout the reaction using ^1H NMR, optical microscopy, differential scanning calorimetry (DSC), uniaxial compression testing, pycnometry, and particle size analysis.

Results:
PET morphology was found to dictate glycolysis kinetics with an order-of-magnitude variation in depolymerisation rate under identical conditions observed. Accurate prediction of depolymerisation rate for real-world PET waste streams was achieved by utilising shrinking core kinetic models. Sigmoidal conversion profiles arose from morphology evolution with in-situ annealing, chain scission-driven embrittlement, and surface cracking dramatically increasing reactive surface area and accelerating conversion.

Conclusion:
PET morphology exerts a decisive influence on depolymerisation efficiency and reactor energy demand. Even with a robust catalyst such as $Zn(OAc)_2$, kinetics were constrained by substrate geometry, in-line with a shrinking-core kinetic model. Integrating controlled grinding or mechanochemical mixing into glycolysis reactors could therefore deliver substantial gains in reaction rate, energy efficiency, and scalability for PET chemical recycling.

References:

1. Barnard, E. et al; Green Chem. 2021, 23 (11), 3765-3789.

2. Sutton,J et al; J. Chem. Eng. J. 2025, 512, 162400.

P48: Thermoresponsive Polymer-Supported Catalysts for PET Depolymerization

Theme: Chemical recycling of polymers

Dr Laihui Xiao[1], Prof Joseph Wood[2], Prof Andrew Dove[1]

[1]School of Chemistry, University of Birmingham, Birmingham, United Kingdom, [2]School of Chemical Engineering, University of Birmingham, Birmingham, United Kingdom

Poly(ethylene terephthalate) (PET) is a high-performance plastic but poses significant environmental challenges due to its persistent accumulation and resistance to degradation.[1] While mechanical recycling is well established, chemical recycling via depolymerization to monomers or value-added intermediates offers a more sustainable alternative.[2] However, current chemical recycling processes typically require high catalyst loadings (5–20 mol%), creating challenges in catalyst separation, recycling, and reuse.[3] [4] Here, we aim to address these limitations by immobilizing 1,5,7-triazabicyclo[4.4.0]dec-5-ene (TBD) on polymers to develop smart polymer-supported catalysts that integrate the advantages of homogeneous and heterogeneous catalysis. At elevated reaction temperatures, the polymer-supported catalysts fully dissolve, enabling homogeneous catalysis with fast kinetics, while upon cooling they self-assemble into particles, allowing efficient catalyst separation and recycling. The effects of catalyst loading, polymer support composition, catalyst stability, and recyclability were systematically investigated for the catalytic glycolysis of PET to bis(2-hydroxyethyl) terephthalate (BHET). This strategy provides a versatile platform for designing recyclable catalytic systems for polymer depolymerization and other sustainable chemical transformations.

References:

1. C. Jehanno, J. W. Alty, M. Roosen, S. De Meester, A. P. Dove, E. Y. X. Chen, F. A. Leibfarth and H. Sardon, Nature, 2022, 603, 803-814.
2. E. Bezeraj, S. Debrie, F. J. Arraez, P. Reyes, P. H. M. Van Steenberge, D. R. D'Hooge and M. Edeleva, RSC Sustainability, 2025, 3, 1996-2047.
3. S. C. Kosloski-Oh, Z. A. Wood, Y. Manjarrez, J. P. de los Rios and M. E. Fieser, Materials Horizons, 2021, 8, 1084-1129.
4. C. Jehanno, J. Demarteau, D. Mantione, M. C. Arno, F. Ruipérez, J. L. Hedrick, A. P. Dove and H. Sardon, Angewandte Chemie International Edition, 2021, 60, 6710-6717.

P49: Facile Microwave-Assisted Hydrothermal Synthesis of Zinc Phosphate Nanocrystals for Zinc-Ion Batteries

Theme: Energy & Net Zero & LCA

Dr Elochukwu Agudosi[1], Professor Mohammad Khalid[2], Professor Lidija Siller[1], Associate Professor Felipe Sanhueza[3]

[1]Newcastle University, Newcastle upon Tyne, United Kingdom, [2]University of Glasgow, Glasgow, United Kingdom, [3]Newcastle University, Newcastle upon Tyne, United Kingdom, [4]University of Concepcion, Concepcion, Chile

Dependence on renewable energy sources and increased use of green solutions (e.g., electric vehicles) is one of the strategic actions for a sustainable environment in the face of growing fossil fuel consumption and associated environmental impacts. This approach promotes the United Nations Sustainable Development Goals (SDGs) strategy, particularly SDG 7 and SDG 13, on ensuring access to affordable modern energy sources and adapting to climate change, respectively. Exploring suitable and economically efficient cathode materials for zinc-ion batteries plays a vital role in combating current challenges and achieving practical applications. Herein, Zn3(PO4)2 nanoparticles with exceptional battery properties were produced via microwave-assisted hydrothermal synthesis. The synthesis was conducted at different microwave heating times (3, 5, 10 and 15 min) at a fixed temperature of 200 ℃. The structural properties of synthesized Zn3(PO4)2 were studied via XRD, FESEM-EDS and TEM studies, while the electrochemical parameters were evaluated through CV, GCD, and EIS in a standard 3-electrode system with 1M KOH as an electrolyte at room temperature. The electrochemical results show that Zn3(PO4)2 synthesized at 10 min microwave heating time reported the best electrochemical performance with a specific capacity of 38.90 C/g and 31.89 C/g at a scan rate of 10 mV/s and current density of 1 A/g, respectively. Furthermore, a stability test of the synthesized electrode material reported an excellent cyclability of the electrode with 79% retention of the initial value of its specific capacity after 1,000 cycles.

References:

[1]. Agudosi, E.S., et al., Energy Storage, 2024. 6(2): p. e605.
[2]. Agudosi, E.S., et al., Critical Reviews in Solid State and Materials Sciences, 2020. 45(5): p. 339-377.
[3]. Pedersen, C.S., Procedia CIRP, 2018. 69: p. 21-24.
[8]. Zhu, W., et al., Composites Part B: Engineering, 2021. 207: p. 108555.
[5]. Zhou, L.-F., et al., Journal of Alloys and Compounds, 2022. 905: p. 163939.

P50: CO2-Enhanced Oil Recovery for Accelerating Net Zero: A UK-focused Technoeconomic Analysis and Optimisation

Theme: Energy & Net Zero & LCA

Miss Mona Alkhaiyat[1], Dr Vassilis Charitopoulos[1]

[1]Department of Chemical Engineering, The Sargent Centre for Process Systems Engineering, University College London, Torrington Place, London, WC1E 7JE, United Kingdom

Achieving Net Zero by 2050 depends on the coordinated development of hydrogen, electricity and carbon dioxide (CO_2) systems. However, much of the optimisation literature treats these vectors in separately, overlooking the dual role of enhanced oil recovery (EOR) as storage and revenue and neglecting endogenous cost learning, which risks misrepresenting long-term feasibility and costs (Fan et al., 2023; García-Saravia et al., 2025). Recent studies have demonstrated the value of retrofitted CCS (Zhou et al., 2025), hydrogen infrastructure planning (Efthymiadou et al., 2024), and electrification of heat (Charitopoulos et al., 2023). However, a unified national-scale optimisation framework that brings these elements together remains lacking.

This work develops a mixed-integer linear programming (MILP) evolution model designed to address these gaps. The framework is structured as a multi-period optimisation with five-year steps from 2030 to 2050, minimising total system cost while capturing both investment and operational decisions. The aim is to provide an integrated optimisation tool that links hydrogen, electricity and CO_2 infrastructures, enabling a more realistic assessment of strategic pathways for the UK's Net Zero transition. The model incorporates hydrogen production routes, electricity generation and transmission, CO_2 capture and transport, and EOR alongside permanent storage. Retrofitted CCS and Direct Air Capture CCS (DACCCS) is explicitly included to represent the decarbonisation of existing plants, while cost learning is represented through piecewise linear functions linked to cumulative deployment (Heuberger et al., 2017).

A UK national case study demonstrates how the framework can evaluate cost-effective and sustainable infrastructure strategies. By embedding EOR response dynamics, retrofitted CCS, DACCCS and endogenous technology learning into a single optimisation model, this work contributes a practical tool for exploring realistic pathways to Net Zero.

P51: Non-Thermal Plasma Regeneration of Solid Sorbents for Direct Air Capture

Theme: Energy & Net Zero & LCA

Mr Hadi Almusawa[1,2], Dr Jonathan McDonough[1], Professor Adam Harvey[1]

[1]Newcastle University, United Kingdom, [2]Jazan University, Saudi Arabia

Thermal regeneration is a major contributor to the energy penalty and long-term degradation of solid sorbents used in direct air capture (DAC). Non-thermal plasma (NTP) offers an alternative regeneration route by promoting CO_2 release through plasma-induced processes rather than bulk heating. In this work, an NTP-assisted adsorption–desorption process was investigated for cyclic CO_2 capture under DAC-relevant conditions.

A purpose-built dielectric barrier discharge (DBD) reactor was used to study plasma-assisted regeneration of solid sorbents. Sodium carbonate, zeolite 13X, and activated carbon were examined to explore how sorbent chemistry influences regeneration behaviour. The effects of key operating parameters, including plasma input power, cycling frequency, and gas flow rate, were systematically evaluated. System performance was assessed in terms of CO_2 sorption capacity, desorption rate, released CO_2 quantity, and regeneration stability, with online gas analysis used to monitor capture and release behaviour.

Zeolite 13X and Na_2CO_3 showed reproducible CO_2 capture and plasma-assisted regeneration over extended cycling, indicating stable operation under NTP conditions. Regeneration behaviour was observed to vary with both sorbent type and plasma operating parameters. Plasma-based regeneration enabled effective CO_2 release while maintaining adsorption performance, suggesting reduced thermal stress compared with conventional heat-driven regeneration.

Overall, the results align with prior research, which highlighted the potential of NTP-assisted sorption-enhanced reforming and CO_2 conversion as a scalable pathway for integrating plasma technology into carbon capture and utilisation systems [1,2]. The findings highlight the potential of NTP technology to enhance CO_2 capture processes, offering a scalable and sustainable pathway to mitigate carbon emissions.

P52: Optimisation of LNG Supply Chains with Enhanced Fleet Utilisation

Theme: Energy & Net Zero & LCA

Mrs Janaa Al-naemi[1], Prof Lazaros G. Papageorgiou[1]

[1]University College London, United Kingdom

The steady increase in global population and associated economic growth is increasing the global energy consumption. In the early nineteenth century, natural gas was introduced into the market and became a popular primary energy source. For long distances, natural gas (NG) is stored and transported in the form of liquefied natural gas (LNG). LNG is sold via long term contracts (LTC), which are 20 years or more. However, in recent years suppliers would deliver LNG via spot contracts to increase their profit. These spot contracts created challenges to the supplier (Deshpande et al., 2023).

In this work, two mixed-integer linear programming (MILP) mathematical models are developed to optimise LNG supply chain operations under two scenarios: with and without spot market contracts. The models would consider the inventories and berths at both supplier and customer terminals. While ensuring that customer demand is always satisfied with minimal oversupply. The main objective of this model is to minimise the transportation and penalty cost and increasing the LNG carriers' utilisation for the supplier by minimising the total number of ships operated. The proposed formulations are demonstrated through an example and will allow suppliers to evaluate the trade-offs between cost efficiency and fleet utilisation.

The proposed formulations are demonstrated through an illustrative example, which generates satisfactory result. The first model results is able to meet customers demand with minimal oversupply. Then, the resulting optimal cost is then used as lower cost bound for the second model, which focuses on minimising the number of ships used. Moreover, the second model achieves a reduction in the number of ships operated from ten to six. Although this reduction is associated with an increase in the total cost, the improved fleet utilisation enables decision-makers to serve more customers and increase future sales.

P53: Product-Level Absolute Environmental Sustainability Assessment Using Planetary Boundaries: A Soap Bar Case Study

Theme: Energy & Net Zero & LCA

Mr Alex Amin[1]

[1]University College London, United Kingdom

Recent advances in Earth system science are enabling us to quantify the biophysical limits of planetary stability, most notably through the Planetary Boundaries (PB) framework, which defines a safe operating space for humanity. The PB concept, based on nine key Earth system processes and their associated control variables, is attractive because it provides a basis for managing environmental resources at the global scale. Absolute Environmental Sustainability Assessment (AESA) is a novel approach that applies the PB framework to evaluate the environmental performance of anthropogenic activity from an absolute perspective, by comparing its impact against an allocated share of the safe operating space. AESA results reported in the literature have so far varied substantially, highlighting the need for greater methodological alignment. Moreover, its operationalization at sub-global scales, where most anthropogenic impacts occur, remains underrepresented. This study addresses these gaps by applying AESA at the product level, using the latest Planetary Boundaries–based impact assessment method, PB-IA, in combination with Life Cycle Assessment (LCA), a well-established decision-support tool. A cradle-to-grave LCA model was developed in OpenLCA for a soap bar case study, using life-cycle inventory data derived from secondary sources and following ISO 14040/44 standards. Characterisation factors were adapted from PB-IA to quantify environmental impacts across seven Planetary Boundaries and nine control variables. The soap bar's absolute sustainability was estimated by comparing its impact scores to an allocated share of the safe operating space, with multiple allocation principles applied to assess AESA sensitivity. The analysis is expected to identify key life-cycle hotspots and demonstrate how absolute sustainability thresholds could inform product-level decision-making. Preliminary modelling suggests that the raw material sourcing and early-stage processing are likely to be the largest contributors to boundary transgression, making these critical leverage points for intervention.

P54: Preliminary Life Cycle Assessment of textile recycling process and material recovery by enzymatic hydrolysis

Theme: Energy & Net Zero & LCA

Dr Antonia Vyrkou[1], Dr Ali Nawaz[1], Dr Saikat Ghosh[1], Dr Chenyu Du[1], Prof Parikshit Goswami[1], **Dr Athanasios Angelis-Dimakis**[1]

[1]University of Huddersfield, Huddersfield, United Kingdom

The current paper presents the life cycle assessment of the enzymatic hydrolysis of post-consumer textile waste (cotton and PET blend) for the recovery of cellulose, PET and glucose; Cellulose is acetylated for the production of cellulose acetate (which can be of further use in wet and electro- spinning), PET is mixed with virgin material for fibre production (via melt spinning) and glucose can be used as energy supply for the in-house production of cellulase (by fungi cultivation). The calculated environmental impact of the process is compared to traditional ways of post-consumer textile disposal, which are, landfill and incineration.

The Life cycle assessment presented here, is aligned with the ISO14040/44:2006LCA framework using the LCA software SimaPro 9.2 (version 3.6 of the ecoinvent database). The assessment method of choice is Environmental Footprint 3.0, affiliated with the Environmental Footprint initiative. The selected set of midpoint indicators cover a wider range of categories (i.e. global warming, human toxicity, resource depletion etc). The endpoint impact indicator is also calculated as a measure of the total Environmental Footprint of each process.

The goal of this analysis is to understand the environmental impact of the proposed textile treatment process, the location of the environmental hotspots and suggestions for environmentally friendlier adjustments. The main issues that we encountered during the analysis is the lack of data in the Ecoinvent database and a difficulty to characterise the recovered products in accordance with said database. The assumptions made, lead to a total environmental impact for the enzymatic hydrolysis 14 and 17 times higher than the values calculated for incineration and landfill respectively. Therefore, optimisation work is currently done to reduce the use of chemicals and energy consumption that will lead to an environmentally friendlier process.

P55: Intensified Solvent Extractions for Lithium Enrichment

Theme: Energy & Net Zero & LCA

Mr Freddie Broomhead[1], Mr Duan Cong[1], Mr Malik Olasinde[1], Professor Angeli Panagiota[1]

[1]University College London, London, United Kingdom

Enriched lithium 6 is important for deuterium-tritium (DT) fusion reactors, where it is used to breed tritium [1]. Enriching lithium 6 from a natural abundance of 7.25% to the >30% is of paramount interest but challenging because of the similarity in chemical properties between isotopes. Solvent extraction with crown ethers has been shown to enrich lithium, but in conventional extractors, long residence times and low fractionation currently limit the industrial use of the technology.

Small channel contactors have been demonstrated to reduce residence time and enhance mass transfer of two-phase solvent extractions [2]. This technology was applied to the two-phase enrichment of lithium using a crown ether / ionic liquid system as the extracting phase.

Using small channel contactors, it was found that the residence time of the reaction could be drastically reduced to as low as 20 seconds and a mass-based difference in diffusion coefficients between lithium isotopes, harnessed by tight residence time control, significantly increased the fractionation [3]. Fractionation factor, defined as the relative abundance of lithium 6 in the extracted phase over the initial phase, was found to be as high as 1.07, with extraction percentage as high as 50%. Extractions in a scale-out manifold consisting of 5 parallel channels showed similar results to a single channel, demonstrating the potential for rapid enrichment cycles of large quantities of lithium 6.

Acknowledgements. This work has received funding and academic expertise from UKAEA. F. Broomhead also acknowledges UCL for his studentship.

References:
[1] T. Hoshino et al., Journal of Nuclear Materials, vol. 417, no. 1–3, pp. 684–687, Oct. 2011, doi: 10.1016/j.jnucmat.2010.12.128.
[2] P. Angeli, Chemical Engineering and Processing - Process Intensification, vol. 206, p. 110045, Dec. 2024, doi: 10.1016/j.cep.2024.110045.
[3] C. Duan et al., Sep. Purif. Technol., vol. 362, p. 131525, Jul. 2025, doi: 10.1016/j.seppur.2025.131525.

P56: Techno-economic assessment of methane pyrolysis for low-carbon hydrogen from Nigeria’s natural gas

Theme: Energy & Net Zero & LCA

Mr Promise Chukwu[1], Dr Orla Williams[1], Dr Ioanna Dimitriou[1]

[1]Faculty of Engineering, University of Nottingham, Nottingham, United Kingdom

For a gas-rich nation like Nigeria, advancing low-carbon hydrogen technologies is essential to realising sustainable value from its natural gas resources. This study investigates methane pyrolysis as a route to low-carbon hydrogen, evaluating its techno-economic viability and environmental performance in a Nigerian context. Three methane pyrolysis scenarios are analysed and benchmarked against conventional steam methane reforming (SMR): (i) pyrolysis without flue-gas CO_2 capture, (ii) pyrolysis with CO_2 capture (CC) from the process-heater flue gas, and (iii) pyrolysis driven by concentrated solar thermal (CST) energy for process heat supply. Process models for the three methane pyrolysis scenarios were developed in Aspen HYSYS for a 100 Nm^3 day^{-1} hydrogen plant, incorporating detailed mass and energy balances, heat integration, and auxiliary systems. The process modelling supported a comprehensive economic assessment, which estimated key cost and profitability indicators, including capital investment, operating costs, the levelised cost of hydrogen (LCOH), and internal rate of return (IRR). This was complemented by sensitivity analysis to evaluate risk exposure, focusing on variations in natural gas price, hydrogen selling price, discount rate, and other key parameters. The LCOH of the base pyrolysis case shows a moderate increase to \$2.86 kg^{-1} H_2 compared with \$2.4 kg^{-1} H_2 for SMR. Slightly higher LCOH values are observed for the CST-based (\$3.07 kg^{-1} H_2) and CC-integrated (\$3.56 kg^{-1} H_2) configurations. Despite higher hydrogen costs, methane pyrolysis achieves significant CO_2 emission reductions of approximately 70–92% relative to SMR. The results indicate that, although production costs remain higher than SMR, methane pyrolysis could serve as a viable low-carbon hydrogen pathway in Nigeria and other gas-rich countries. The base pyrolysis case, in particular, offers a balance between cost and emissions performance, indicating potential for deployment as a transitional technology as costs decline with scale and technological maturity.

P57: The value and limits of carbon circularity for net zero in the petrochemical industries

Theme: Energy & Net Zero & LCA

Dr Jennifer Hawkin[1], Dr Fanran Meng[1], **Dr Jiacheng Sun**

[1]University of Sheffield, United Kingdom

Context:
Circularity has become a prominent concept across academia, policy, and industry, and has been particularly embraced by the petrochemical sector. Here, carbon circularity promises continued production, products, and business models while reducing greenhouse gas emissions towards net-zero. Carbon circularity refers to the recapture, recycling, or substitution of carbon (both fossil and non-fossil) to form closed-loop systems that reduce fossil dependence and waste generation.

Petrochemical materials are embedded across approximately 95% of manufactured goods, some of which underpin essential societal services. In this context, carbon circularity appears attractive, yet its feasibility at scale remains uncertain. Previous critiques frame petrochemical circularity as a mitigation deterrent or as lacking systems-wide consideration, but do not quantify its constraints or identify priority applications.

Approach:
This work develops a framework to assess the role of carbon circularity in the petrochemical sector. It (1) quantifies constraints on carbon circularity, considering technological maturity, deployment gaps, infrastructure constraints, and sustainable resource availability; (2) contrasts sector-internal circularity with cross-sector and demand-targeted strategies; and (3) proposes a prioritisation framework for deploying carbon circularity alongside higher-impact alternatives.

Findings and significance:
The analysis shows that petrochemical carbon circularity faces deep structural constraints that limit its contribution to near-term climate mitigation. Across five key technologies, current capacities meet less than 1% of existing demand, indicating that carbon circularity cannot feasibly scale to offset continued growth in petrochemical production. A realistic pathway therefore, requires rebalancing circularity efforts. Carbon circularity should be applied selectively where alternatives are unavailable or where it can reduce impacts associated with essential services. Greater mitigation potential lies in demand reduction, reuse systems, and business-model innovations that reduce material throughput. A targeted role for carbon circularity, embedded within broader demand-side and cross-sector strategies, provides actionable guidance for aligning petrochemical systems with sustainable and equitable decarbonisation.

P58: Ethanol photo-reforming for hydrogen generation in a slurry batch reactor under simulated solar illumination

Theme: Energy & Net Zero & LCA

Mr Israila John[1], Professor Asterios Gavriilidis, Dr Maria Mourkou, Dr Xinjie Luo, Dr Xiyi Li, Associate Professor Yang Lan

[1]University College London, London, United Kingdom

Photocatalytic ethanol reforming for green H2 production over 1 wt.% Pt/TiO2 was studied in a slurry batch reactor to examine the influence of key parameters including light intensity, slurry depth, temperature and photocatalyst concentration. Experiments were carried out utilising a quartz glass top reactor under solar light simulator of varying light intensity. H2 production was measured using an inverted burette and offline gas chromatography equipped with BID. Liquid products were analysed with gas chromatography equipped with FID. The evaluated order, n of H2 generation rate power-law dependence on light, R∝I^n, had a value of n = 0.5 under constant temperature conditions, and an apparent value of n = 1.3, when the temperature varied between 298 - 313 K. An effective strategy for increasing the H2 generation rate involves using an optimal slurry depth that receives sufficient illumination from the light source. Under this slurry depth, the H_2 production rate of 0.4906 mL h-1 cm-2 or 43.72 mmol h-1 g-1 observed at 121 mWcm-2 was comparable to 44.53 mmol h-1 g-1 reported for 154.5 mWcm-2 sunlight in literature [1]. Other dehydrogenation products like acetaldehyde and C-C cleavage products like CH4 and CO2 [2] were also obtained. An activation energy of 19.4 kJ mol-1 was calculated by varying the slurry temperature in the range 298-328 K. This value is considerably low revealing the photocatalytic nature of the process, rather than photothermal effects. Studies on the effect of photocatalyst concentration demonstrated that H2 generation increased with higher concentrations, reaching a peak value before declining. This behaviour is attributed to the greater number of active sites available at higher concentrations, and ultimately a shielding effect and increased slurry turbidity, hindering efficient light utilisation beyond the optimal concentration. The results obtained in this work showed promising H_2 generation, setting a benchmark for future efficiency gains.

P59: Integrated Capacity Design and Year-Long Scheduling Optimisation of Green Ammonia Production Systems

Theme: Energy & Net Zero & LCA

Ruitao Sun[1], **Dr Jie Li**[1]

[1]The University of Manchester, United Kingdom

Green ammonia is emerging as a key vector for decarbonising fertiliser production and enabling long-duration energy storage, whilst its economic viability remains strongly constrained by renewable intermittency, storage requirements, and limited process flexibility. This study presents a fully integrated optimisation framework to minimise the levelized cost of ammonia (LCOA) for renewable-powered ammonia production while explicitly accounting for operational dynamics and location-dependent renewable resources.

Unlike sequential design approaches that daily scheduling is optimised after an optimal capacity design [1], this work simultaneously optimises wind and solar capacities, battery storage, process unit sizing, and hourly operation over a full year (8760 h). Critical operational constraints such as minimum load and ramp-up limits of electrolysers instead of instantaneous start-up [2], air separation units (ASU), and the Haber-Bosch (HB) synthesis loop are explicitly modelled. Site-specific renewable power profiles are derived from historical weather data. The economic basis for HB process is based on our previous cost estimation using rigorous modelling and detailed equipment sizing and costing [3]. The resulting mixed-integer nonlinear programming (MINLP) problem is implemented in GAMS and solved using the DICOPT solver, with penalties applied for curtailment, gas venting, and frequent start-ups.

Results show that integrated optimisation leads to markedly different and more cost-effective system configurations compared to commonly used sequential methods. Enhanced flexibility of the ammonia synthesis loop substantially reduces storage requirements and lowers LCOA, particularly in regions with pronounced seasonal variability. The balance between operational flexibility and storage investment is found to be strongly location-specific.

P60: MFM-300(Al) for SO2 Adsorption from Flue Gas to Enable Cyanobacterial Carbon Capture

Theme: Energy & Net Zero & LCA

Mr Milad Mousavi[1], Dr Sean Craig[1], Dr Andrea Laybourn[2], Dr Begum Tokay[1], Dr Samantha Bryan[1]

[1]Department of Chemical and Environmental Engineering, University of Nottingham, Nottingham, United Kingdom, [2]Institute of Process Research and Development & School of Chemistry, University of Leeds, Leeds, United Kingdom

Keywords:
MOFs, cyanobacteria, carbon capture

Purpose / Objective:
Metal–organic frameworks (MOFs) such as MFM-300(Al) are promising adsorbents for selective toxic gas (e.g. SO2) removal from flue gas emitted from industries, enabling downstream use of the toxic-free gas in cyanobacterial carbon capture. In addition to evaluating MFM1300(Al) for gas purification, it is important to understand its compatibility with cyanobacterial cultures, particularly in the event of accidental particle carryover or contamination from the adsorption system.

This study investigates the stability and biological compatibility of MFM-300(Al) with Synechococcus sp. PCC 7002, alongside ongoing work integrating an adsorption column with a photobioreactor to assess the impact of SO2 removal on cyanobacterial growth. Materials / Methods: MFM-300(Al) was synthesised and characterised using X-ray diffraction. Batch cultures of PCC 7002 were exposed to MFM-300(Al) particles (0.1–1 mM), and cell growth and culture pH were monitored. MOF stability was assessed after incubation. Furthermore, a fixed-bed adsorption column has been constructed to evaluate SO2 removal from simulated flue gas streams. This column is being coupled upstream of a photobioreactor containing PCC 7002 to compare cell growth and photosynthetic performance in purified versus unpurified gas conditions.

Results:
Cyanobacterial cultures maintained normal growth and photosynthetic activity in the presence of MFM-300(Al) at concentrations up to 1 mM, indicating good tolerance to potential contamination. However, structural analysis showed that MFM-300(Al) began to degrade when culture pH exceeded 8.5, due to increased photosynthetic activity and alkalinisation of the media.

Conclusion:
These findings demonstrate that MFM-300(Al) is compatible with cyanobacterial cultures at relevant concentrations even at pHs higher than 8.5 in which the MOF degrades. Ongoing integrated adsorption–photobioreactor experiments will determine how the upstream SO2 removal using MFM-300(Al) affects cyanobacterial growth. This study provides insight into the feasibility of integrating MOF-based gas purification with cyanobacterial carbon capture systems.

P61: Sustainable mechanochemical synthesis of Molybdenum and Tungsten dichalcogenides for the Hydrogen Evolution Reaction

Theme: Energy & Net Zero & LCA

Mr Joseph Parkinson[1], Dr Bonity J. Lutton Gething[2], Prof. Tomislav Friščić[2], Dr Neil Rees[1]

[1]School of Chemical Engineering, University of Birmingham, United Kingdom, [2]School of Chemistry, University of Birmingham, United Kingdom

Transition Metal Dichalcogenides (TMDs) have seen extensive research into their activity towards the Hydrogen Evolution Reaction for the last 2 decades, with focus given to materials such as molybdenum and tungsten disulfide (MoS2 and WS2).Compared to platinum as the industry standard cathode, these materials boast lower costs, more sustainable production, and ease of modification, though lack activity in their bulk state due to an inactive basal plane. [1]

Despite this, microstructuring techniques can help remedy this inherent inactivity, for instance by preferentially exposing certain active sites, formation of heterostructures or doped species, or exfoliation to monolayers. [2,3] Mechanochemistry has been used to great effect exploring top-down modifications of the bulk, but synthesis and modification from the bottom-up remains unexplored, despite key advantages of bottom-up synthesis on catalytic activity, and recent precedent for the synthesis of similar materials despite molybdenum and tungsten varieties remaining elusive. [4,5,6] Such a method would demonstrate a versatile, sustainable, energy-efficient and scalable mechanochemical method to produce these essential catalysts; aligned with the key principles underlying Green and Sustainable Chemistry. [7]

Hence, we present investigations into the bottom-up mechanochemical synthesis and modification of TMDs, using combined solvent-free and Liquid-Assisted approaches in an attempt to synthesise a range of chalcogenides. Synthetic conditions were varied to explore the optimal reaction pathway, along with characterisation of intermediates, for a more complete mechanistic and electrocatalytic understanding.

1. Manyepedza, T. et al, Appl. Mater. Today, 2025, 42, 102582
2. Li, G. et al, J. Am. Chem. Soc., 2016, 138, 16632–16638
3. Liu, Y. et al, Adv. Mater., 2022, 34, 2203615
4. Floyd, K. et al, RSC Mechanochemistry, 2024, 1, 289–295
5. G. A. Vinnacombe-Wilson et al, Chem. Rev., 2023, 123, 8488–8529
6. E. Dutkova et al, Crystals, 2025, 15, 511
7. Anastas, P., Eghbali, N, Chem. Soc. Rev., 2010, 39, 301-312

P62: Hybrid Vapour-Compression Cooling Configurations for Sustainable Cold-Chain Applications

Theme: Energy & Net Zero & LCA

Diah Ayu Almaas Salwa[1]

[1]School Of Chemical Engineering, University Of Birmingham, Birmingham, United Kingdom

Cold-chain refrigeration is essential for maintaining the quality of food and temperature-sensitive medical products, but it is also associated with high energy consumption. Conventional vapour-compression (VC) systems can experience efficiency limitations under demanding operating conditions, motivating interest in hybrid cooling approaches that combine VC cycles with active alternative technologies to improve system performance and temperature control. This work presents a systematic review of VC-based hybrid cooling systems applied in cold-chain refrigeration. A PRISMA-informed search and screening process was conducted using a validated Boolean strategy, resulting in the selection of 38 relevant studies. The reviewed literature was analysed to identify dominant hybrid configurations, integration architectures, research methodologies, and reported performance metrics. The results indicate that VC–absorption and VC–thermoelectric hybrids are the most commonly investigated configurations in cold-chain applications. Absorption-based hybrids exhibit diverse integration strategies, including cascade and parallel arrangements, reflecting their suitability for medium- and large-scale refrigeration systems. In contrast, thermoelectric hybrids are typically implemented as auxiliary or cascaded components, supporting compact and portable cold-chain applications where temperature stability is critical. Across all hybrid configurations, performance evaluation approaches remain inconsistent, limiting direct comparison between systems. These findings highlight the need for greater consistency in performance reporting and further experimental validation to support the development of energy-efficient and reliable hybrid cold-chain refrigeration technologies.

P63: The Influence of Vessel Aspect Ratio on Internal Dynamics and Mixing Efficiency in Resonant Acoustic Mixing

Theme: Energy & Net Zero & LCA

Hazal Sezer[1]

[1]University of Birmingham, United Kingdom

To test how the fill level and the vibrational acceleration to which it is exposed affect mixing efficiency, we ran some experiments imaging a simple material, microcrystalline cellulose (MCC) within a RAM mixer using positron emission particle tracking (PEPT) and we observed that there is a clear, monotonic, positive relationship between acceleration and mixing efficiency. However, while we observed that fill level has a clear effect on mixing efficiency, the form of this relationship is currently unclear [1].

The present study examines the effect of vessel aspect ratio on internal particle dynamics and mixing efficiency. Previous studies showed that aspect ratio (AR) influences mixing dynamics and heating, but no systematic study has been performed [2,3]. To clarify the effect of aspect ratio on mixing quality and efficiency we decided to study this relationship further by using 3 different aspect ratios for mixing vessel: 0.25, 1, and 4 with constant volume using Positron Emission Particle Tracking (PEPT) with 3 different accelerations 100g, 65g and 30g within the constant 20 % fill level with a simple material, microcrystalline cellulose (MCC).

References:
[1] Sezer, H., Werner, D., Sykes, J.A., Bazin, N., Bolton, P. and C.R.K. Windows-Yule (2025). Exploring the internal dynamics of resonant acoustic mixing using positron emission particle tracking. Chemical Engineering Science, pp.121166–121166. doi:https://doi.org/10.1016/j.ces.2024.121166.
[2] Coguill, S. and Martineau, Z. (2012). Vessel Geometry and Fluid Properties Influencing Mix Behavior for ResonantAcoustic ® Mixing Processes. In: The 38th International Pyrotechnics Seminar. [online] Available at: http://dx.doi.org/10.13140/RG.2.2.28890.64964.
[3] Miller, J.T., Bode, D.A. and Coguill, S. (2010). ResonantAcoustic® Mixing; Design and Process Considerations Concerning Vessel/Case Geometry and Mix versus Cure Time When Preparing Composite Solid Propellant. [online] JANNAF 36th Propellant and Explosives Development and Characterization Joint Subcommittee Meeting. Available at: https://www.researchgate.net/publication/270216392_ResonantAcoustic_R_Mixing_Design_and_Process_Considerations_Concerning_VesselCase_Geometry_and_Mix_versus_Cure_Time_When_Preparing_Composite_Solid_Propellant.

P64: Exploring the Formation of Active Sites in Transition Metal and Nitrogen Doped Carbon Catalysts toward Oxygen Reduction Reaction

Theme: Energy & Net Zero & LCA

Ms Qingxiu Shi[1], Mr Chao Wu[1], **Dr Yujun Si**[1], Professor Shangfeng Du[2]

[1]Sichuan University of Science and Engineering, Zigong, China, [2]University Of Birmingham, Birmingham, United Kingdom

Transition metal and nitrogen co-doped carbon materials (M-N-C) are being developed as the promising candidates to replace the Pt-based oxygen reduction reaction (ORR) catalysts owning to the remarkable catalytic performance, easy availability and low cost. The catalysts are typically prepared by pyrolyzing precursors different types of transition metal-nitrogen-carbon reagents. The diversity of precursors and the commonality of ORR activity of M-N-C inspire two questions: (1) What are the active sites of the M-N-C catalysts? (2) How are the active sites formed? Currently, the first question has been well answered by experimental and theoretical evidence. However, regarding the 2nd one, it is difficult to in situ monitor the formation of active sites due to the complicated carbonization process in the preparation of M-N-C, which hinders the rational design on the catalyst.

Aim to this topic, an N-doped carbon catalyst (FeAMeC-A2) to ORR is prepared by pyrolyzing a precursor using agar as carbon source and melamine as nitrogen source in this work. The formation mechanism of the active sites is simulated by using ammonia as a probe gas inspired by the fact that the N-contained melamine would be decomposed to ammonia, further achieving the doping of N into the carbon grids during the carbonization process. The results indicate that the nitrogen atoms are preferentially doped into the carbon matrix below 400 °C when the precursor is being carbonized, facilitating the formation of active sites. This study addresses a practical problem frequently encountered in the field of M-N-C catalyst and presents a strategy to identify the formation mechanism of active sites.

P65: Towards easy co-adsorption measurement via a gravimetric-integrated gas analysis method

Theme: Energy & Net Zero & LCA

Dr Jiacheng Sun[1], Dr Gabriela Ferreira[2], Dr Thabang Selalame[1], Dr Zhenxi Li[1], Dr Rick Lupton[2], Prof Anthony Ryan[1], Dr Nixon Sunny[3], Dr Marwan Sendi[3], Dr Amir Abdul-Manan[3], Dr Fanran Meng[1]

[1]University of Sheffield, Sheffield, United Kingdom, [2]University of Bath, Bath, United Kingdom, [3]Saudi Aramco, Dhahran, Saudi Arabia

Global trade is viewed as a lever for decarbonising plastics industry by relocating production to regions with lower greenhouse gas (GHG) emission intensities. However, the achievable mitigation scale, its interaction with regional energy systems, and the risk of carbon leakage remain uncertain. This study develops an integrated multi-regional material flow analysis (MFA) and life-cycle assessment (LCA) framework to evaluate the net-zero potential and structural limits of international and intra-regional trade across the plastics value chain. A cradle-to-gate LCA boundary covers feedstock extraction and processing, steam cracking and polymerisation, utilities provision, and intermediate transport. Region-specific emission factors are parameterised using electricity grid carbon intensities, thermal energy sources, and process efficiencies to enable consistent cross-regional comparison under alternative energy-transition pathways.

Foreground inventories are constructed for major commodity polymers and intermediates, while background datasets are harmonised from established databases and literature. Multi-output refinery and cracking units apply mass-based allocation, with economic allocation tested in sensitivity analysis. Uncertainty is represented through Monte Carlo sampling of emission factors, capacity utilisation, and trade elasticities. Scenarios explore renewable electricity penetration, feedstock switching, circularity improvements, and policy-driven trade rerouting, supporting both attributional and consequential LCA perspectives.

Results show that, even under optimistic assumptions, trade-driven reallocation offsets only around 8–20% of projected plastics-related GHG emissions by 2030. Most reductions stem from differences in upstream energy mixes and process efficiencies rather than transport emissions. Mitigation potential is further constrained by entrenched trade imbalances, rapid demand growth in emerging economies, and limited low-carbon production capacity. Uncoordinated regional climate policies risk carbon leakage, shifting rather than reducing emissions. For several major consuming regions, over 70% of incremental demand must still be met domestically even in high-trade scenarios. Overall, trade alone is insufficient for net-zero alignment; coordinated strategies integrating low-carbon energy deployment, circular material flows, and leakage-aware industrial and trade policies are essential.

P66: Assessing the limitations of gravimetric methods for CO2 capture under humid conditions

Theme: Energy & Net Zero & LCA

Miss Emily Walford[1,2], Dr Mijndert Van der Spek[1], Professor Susana García-López[1], Dr Paul Iacomi[1,2], Mr Connor Hewson[2], Dr Aamir Hanif[2], Dr Lisa Sun[2]

[1]Heriot Watt University, Research Centre for Carbon Solutions, Edinburgh, United Kingdom, [2]Surface Measurement Systems, London, United Kingdom

To mitigate rising global temperatures, carbon capture and storage (CCS) is widely expected to play a significant role in reducing CO_2 emissions and decarbonising the industrial sector. Point Source Capture (PSC) targets the removal of CO_2 from industrial effluent streams, for which solid sorbents, such as zeolites, are a promising option due to their efficiency and scalability. The design of such adsorption processes relies on accurate predictions of adsorption behaviour under realistic conditions. These predictions rely on mechanistic adsorption isotherm models, obtained from accurate adsorption equilibrium data. In addition to CO_2, flue gas streams are often saturated with humidity, which can introduce competition for adsorption sites and thus complicate interpretation of adsorption data. Gravimetric methods are one of several techniques available for measuring adsorption and offer high precision and low material requirements.

However, true multicomponent data from accurate co-sorption experiments is essential to determine the extent to which competitive adsorption with water inhibits CO_2 capture. While co-sorption experiments can be run in a gravimetric instrument, the method only reports total mass uptake, rather than the quantitative uptake of each component. Current methods therefore provide insufficient information to fully close the component balance around the adsorbent sample. These limitations mean that obtaining essential co-adsorption data from prospective sorbents using gravimetry is experimentally challenging.

This work forms the first phase of a PhD project aimed at improving gravimetric methods by integrating a flow-through gravimetric adsorption balance with additional instrumentation to measure the instrument outflow and gas-phase composition. This method will be applied to a wide range of sorbents and enable simultaneous measurement of inlet and outlet compositions, thus identifying the component responsible for the observed mass increase during adsorption. Our recent study of zeolite 13X for PSC has suggested a promising avenue for measuring CO_2-water co-sorption using gravimetry.

P67: Environmental Assessment of Repurposing Decommissioned Offshore Platform

Theme: Energy & Net Zero & LCA

Dito Winanda[1], DR Andrea Paulillo[1]

[1]University College London, London, United Kingdom

The number of offshore oil and gas platforms in Indonesia entering the decommissioning phase will continue to increase in the coming years. This has sparked discussions about appropriate decommissioning methods and the search for repurposing alternatives. This is not without reason. Offshore decommissioning is a complex process which involves high operational risk, high cost, and potential environmental impacts. Leaving the infrastructure in situ or reutilizing it for other facilities will affect these aspects. Therefore, environmental assessment is needed to obtain comprehensive sustainable end of life decision.

This study applies Life Cycle Assessment (LCA) approach to quantify the energy and environmental impacts of decommissioning bottom fixed offshore platforms – considering both full and partial removal - and compares it with repurposing scenarios, including installation of wind turbines. The system boundaries for the offshore decommissioning process includes marine transportation, fuel consumption, cutting operations, heavy lifting operations, and waste management. Meanwhile the system boundaries for reusing the platform for wind turbines consist of material fabrication, transportation, installation, operation phase, until decommissioning (cradle to grave). Regarding data sources, this study uses primary data from an offshore platform in the Java Sea, Indonesia, and secondary data obtained from previously reported cases in the literature.

Given that heavy lifting, cutting operations and marine transportation generate substantial environmental impacts, it is expected that these impacts will be counterbalanced by the benefits of recycling steel – the primary component of offshore platforms – as well as the recycling capacity available in the region. It is also projected that repurposing offshore platform for wind turbine installation will only give environmental advantages if specific operational lifetime of the turbine is attained. The findings of this study are expected to support decision making on sustainable end of life strategies for offshore platforms under increasing demand of decommissioning and renewable energy deployment.

P68: Tri-Objective Optimization for Integrated Electricity-Heating System Scheduling: Balancing Cost, Carbon, and Comfort

Theme: Energy & Net Zero & LCA

Dr Hui Yan[1], Prof Sara Walker[1]

[1]University of Birmingham, United Kingdom

Energy transition to net zero is reshaping the operation of power and heating systems, which increases the need to consider emissions in scheduling decisions. The growing electrification of district heating networks (DHNs) also enables valuable demand-side flexibility. However, flexibility should not degrade comfort of occupants. This study proposes a tri-objective scheduling model for an integrated electricity–heating system. The DHN and energy storages are the flexibility providers. Heat is supplied through an energy hub that includes a boiler, a combined heat and power plant, and a heat pump. The model minimizes operating cost, carbon emissions, and thermal discomfort. The thermal comfort is evaluated with the Predicted Mean Vote (PMV) index. Apart from the direct emission from gas consumption, the time-varying grid carbon-intensity are considered to assess the carbon emission of the integrated system. Simulations are conducted on an integrated system consisting of a 33-node distribution network and a 51-node DHN, which validate the effectiveness of the proposed framework. With $|PMV| \le 0.5$ ensured, DHN-provided flexibility reduces carbon emissions by 8.33% and decreases the operating cost by approximately 1.86% compared with a no-flexibility baseline.

P69: Pretreatment and fermentation of digestate

Theme: Energy & Net Zero & LCA

Ms Deborah Mathias[1], Dr Sharon Velasquez-Orta[1]

[1]Newcastle University, Newcastle upon Tyne, United Kingdom

The growing popularity of anaerobic digestion necessitates the need to find safer and sustainable ways of containment of the resultant digestate. Digestate cannot be discharged directly due to some environmental and legislative concerns. Digestate has been used to amend soil and animal bedding extensively. However, there is accumulation of anaerobic digestate as some farmers tend to be conservative and prefer to use conventional fertilizers. Also, farming is seasonal hence digestate is required at certain period. This study aimed to investigate the mechanism of three pre-treatment measures and yeast fermentation of digestate; to evaluate the changes that occur in the digestate. Digestate was diluted 25% and 50% then pre-treated separately by hydrothermal (HT), ozonolysis (OZ) and thermal (TM) methods. Responses such as disinfection of the digestate, chemical oxygen demand, ammonia nitrogen (NH_4^+ N), phosphate, nitrate, nitrite, volatile fatty acid, total carbon, compounds formed were evaluated. The pre-treated digestate was supplemented with glucose then inoculated with Saccharomyces cerevisiae and fermented for six days, afterwards responses including bioethanol production, yeast biomass growth and glucose utilisation were analysed. Pretreatment made the most significant change in the digestate composition in reducing NH4+–N concentrations by an average of 64.9% relative to the baseline 5100 mg L−1. Subsequent fermentation for six days removed an additional mean decrease equal to 19.7% of the pretreatment value. At 25% digestate concentration, NH4+–N removal following pretreatment and fermentation averaged 80.8%, while at 50% averaged 62.7%. Compared with an initial concentration of 10,339.83 mg L−1 phosphate, 25% digestate concentration removed an average of 75.7% while 50% digestate 47.2%. Nitrogen removals had more consistency in results, while phosphate removals had more variability with increasing pretreatment severities. In conclusion, this work showed digestate treatment conducted by different pre-treatment steps and the subsequent feasibility to be utilised as a nutrient additive to facilitate fermentation.

P70: Rheological Characterisation andCFD Modelling of Non-Newtonian Soap Flow in a Co-Rotating Twin-Screw Extruder

Theme: Process Modelling, Reactions & Simulation

Mr. Fawad Ahsan[1]

[1]Phd Researcher, Sheffield, United Kingdom

Extrusion processes are well understood for Newtonian fluids; however, industrial soap formulations typically exhibit strongly non-Newtonian behaviour, with rheological properties that evolve under processing conditions. In soap extrusion, viscosity and flow response are influenced by temperature, shear stress and shear rate, moisture content, and formulation-dependent constituents. These coupled effects are critical for achieving target product attributes, notably final soap hardness, yet they significantly complicate both experimental interpretation and predictive modelling.

This work addresses these challenges through rheological characterisation of industrial soap formulations and the development of a staged CFD framework implemented in ANSYS FLUENT. In the first phase, benchmark simulations of laminar flow between fixed, parallel plates were used to support constitutive model selection and verification of shear-dependent viscosity behaviour over representative processing ranges. Building on this, a hierarchical set of CFD simulations was performed, progressing from benchmark flows to simplified screw-driven models and, subsequently, to 3D single-screw and twin-screw extruder geometries. Parametric studies were conducted over a controlled screw-speed range to assess pressure generation for Newtonian and yield-stress fluids.

The simulations successfully captured the rheological behaviour of soap-like materials and established a clear relationship between pressure rise and screw speed. Pressure was found to increase monotonically with RPM for all cases; Newtonian fluids exhibited near-linear ΔP–RPM scaling, whereas yield-stress and strongly shear-thinning materials generated substantially higher pressure with reduced sensitivity to RPM. Diagnostic analysis showed that pressure rise is dominated by static (viscous) contributions, with dynamic pressure effects being comparatively small.

The study further indicates that flow behaviour within the intermeshing region of co-rotating twin-screw extruders is not fully resolved using steady, isothermal CFD alone, motivating future work involving further modelling and targeted experimental validation. Overall, the work establishes a robust and physically interpretable CFD foundation for analysing soap extrusion and for extending the methodology toward DiPP-scale twin-screw systems.

P71: Modelling of CO_2 Capture by Temperature Swing Adsorption in a Packed-Bed Reactor

Theme: Process Modelling, Reactions & Simulation

Mrs Israa Alghurabi[1], Dr Helena Navarro, Dr Tongtong Zhang, Professor Yulong Ding

[1]The University of Birmingham, United Kingdom

Temperature swing adsorption (TSA) is a promising technology for post-combustion CO_2 capture due to its compatibility with moderate-temperature heat sources as well as heat re-utilization through thermal energy storage. In this work, a two-dimensional dynamic model is developed to investigate CO_2 adsorption and regeneration in a packed-bed reactor operating under TSA conditions, aimed to understand fundamental flow, heat and mass transfer processes and their interactions, thus contributing to efforts to reduce carbon dioxide emissions and support carbon neutrality.

While regeneration strategies and two-dimensional TSA models have been studied separately in previous work, limited attention has been given to the comparison of practical heating approaches within a dynamic framework relevant to different TSA systems at different scales. Zeolite 13X is selected as the model adsorbent owing to its high CO_2 selectivity and adsorption capacity. The packed-bed adsorber is described using transient mass, energy, and momentum balances. The model is implemented in COMSOL Multiphysics and simulates both the adsorption and thermal regeneration steps of the TSA cycle. Adsorption equilibrium is represented using the Langmuir isotherm, while adsorption and desorption kinetics are modelled using a linear driving force (LDF) formulation. Thermal regeneration of the packed bed is achieved using external band heaters, mimicking a lab-scale experimental system under construction for the model validation. The use of hot purge gas heating is also examined, to compare different regeneration strategies. These heating approaches are relevant to solar-assisted TSA systems, where low- to medium-temperature heat can be supplied. The work also provide basis for future thermal integration through thermal energy storage of excess process heat.

Preliminary simulations establish a physically consistent TSA model resolving axial–radial transport and adsorption kinetics. The impact of two-dimensional transport and regeneration strategy will be quantified using outlet breakthrough metrics and specific energy per kilogram of CO_2 captured, supporting future experimental comparison.

P72: Digital twin of a Solid Oxide Fuel Cell

Theme: Process Modelling, Reactions & Simulation

Mrs Zahraa Aljazaeri[1], Dr Yousif Al-Sagheer[1], Pro Robert Steinberger-Wilckens[1]

[1]University of Birmingham, Birmingham, United Kingdom

Digital Twin of a Solid Oxide Fuel Cell
Zahraa Al-Jazaeri, Yousif Al-Sagheer, Robert Steinberger-Wilckens
School of Chemical Engineering, College of Engineering and Physical Sciences, University of Birmingham, Birmingham, United Kingdom

Purpose / Objective:
Solid Oxide Fuel Cells (SOFCs) operate at high temperatures with tightly coupled electrochemical, thermal, and fluid processes that influence efficiency, durability, and safety. Experimental optimisation of these interactions is complex and costly. This work develops a dynamic digital twin framework of a high-temperature SOFC system to analyse fuel utilisation, heat generation, and system-level behaviour under realistic operating conditions.

Materials / Methods:
A system-level digital twin was developed in MATLAB/Simulink using Simscape multi-domain libraries. The SOFC stack model combines electrochemical voltage losses (activation, ohmic, concentration) with species transport in anode and cathode gas channels. Hydrogen consumption and oxygen reduction are dynamically linked to electrical load. A thermal network represents stack heat capacity and internal heat generation. An afterburner sub-model accounts for oxidation of unreacted fuel in the anode exhaust, adding a secondary heat source. Balance-of-plant elements, including gas flow paths and a cooling loop, were included to represent realistic system architecture. Parameters are based on literature values for high-temperature SOFC operation.

Results:
The digital twin establishes multi-physics coupling between electrochemical reactions, mass transport, and thermal dynamics within a unified simulation framework. The model enables dynamic interaction among load demand, fuel utilisation, and heat generation, and supports transient analysis. Full numerical convergence and experimental validation are ongoing.

Conclusion:
This work provides a structured digital twin foundation capturing the coupling among electrical load, species consumption, and heat distribution in a high-temperature SOFC. The framework supports future studies on thermal management, start-up and load-following behaviour, and integration with monitoring systems for predictive control and performance optimisation.

P73: Hydrodynamic and reaction studies in an axially ribbed Taylor vortex reactor

Theme: Process Modelling, Reactions & Simulation

Mr Sotirios Andrianos[1], Dr Mrityunjay Sharma[1], Professor Federico Galvanin[1], Professor Asterios Gavriilidis[1]

[1]Department of Chemical Engineering, University College London, Torrington Place, London, WC1E 7JE, UK, London, United Kingdom

Taylor vortex reactors (TVR) exhibit tuneable residence time distribution and intensified heat and mass transfer[1]. A TVR of annulus volume 10 ml, equipped with a ribbed rotor, with ribs parallel to the axis of rotation, was characterised in terms of macro-mixing behaviour, reactant conversion and heat transfer performance. Macro-mixing was studied using step-input experiments by monitoring the tracer's concentration (Rhodamine B) with inline UV–Vis spectroscopy. Residence time distribution (RTD) analysis showed good agreement with theoretical predictions based on the tanks-in-series model. The number of ideal CSTRs in series ranged from 3 to 7. The effect of space time on the number of ideal CSTRs in series was stronger than the rotor speed under the experimental conditions investigated (space time 1-7 min, rotor speed 100-300 rpm), as supported also by partial least squares modelling. Conversion was evaluated using n-benzylidenebenzylamine synthesis from benzaldehyde and benzylamine in methanol as a model reaction, since it has well-documented kinetics[2]. The imine synthesis experiments were conducted simultaneously with RTD successfully. Experimental conversion was determined using inline Raman spectroscopy by monitoring the benzaldehyde peak and applying the adaptive iteratively reweighted penalized least squares baseline correction method. Conversions of 55-98% were obtained for residence times 1-7 min and inlet jacket temperatures 5-25 ℃. Heat transfer experiments using methanol as the working fluid and deionised water as the thermal fluid showed that higher axial velocity and rotor speed enhanced heat transfer. The highest productivity and the lowest raw material and energy costs were obtained for the experiment with the highest total volumetric flow rate.

References:
[1] Schrimpf, M., Esteban, J., Warmeling, H., Färber, T., Behr, A., & Vorholt, A. J. (2021). AIChE Journal, 67(5).
[2] Grammenou, E., Friso, A., Dawes, S., Snead, N., Gkogkos, G., Besenhard, M. O., Mourkou, M., Galvanin, F., & Gavriilidis, A.React. Chem. Eng., 2026,11, 148-159.

P74: Spatially Resolved Analysis of Gas Concentrations and Temperature in Emission Control Catalysts Using SPACI-MS

Theme: Process Modelling, Reactions & Simulation

Mr Theo Bockmuehl[1]

[1]Johnson Matthey, Sonning, United Kingdom

Purpose/Objective:
Traditional catalytic testing for automotive aftertreatment relies on packed-bed, structured reactors and requires extensive testing across various conditions, including engine testing. Spatially Resolved Capillary Inlet Mass Spectrometry (Spaci-MS) enables real-time, axial measurements of gases and temperatures along catalytic channels, providing detailed insights into conversion, selectivity, and temperature changes throughout a monolith. This technique reduces testing time and uncovers kinetic behaviours where exotherms are relevant by masking the rate of reaction orders.

This work will showcase how I have applied Spaci-MS during my Industrial Placement for applications such as H2-ICE and other novel sustainable applications to abate high global warming GHGs (not reported for brevity).

Material/Methods:
A 3” Pd-coated monolith was evaluated in steady-state tests within a 1” OD reactor, using a feed of 0.4% hydrogen, 0.025% nitric oxide, 10% oxygen, and 5% water in argon. Inlet temperatures ranged from 100-250°C to study effects on conversion and reaction zones. Axial gas concentrations were measured via capillary-coupled mass spectrometry, and temperature gradients were recorded using 0.25-micron thermocouples.

Results:
Hydrogen oxidation at all three temperatures, showed full conversion within the first 20% of the monolithic reactor. The conversion profile was consistent, with higher temperatures causing a slight shift toward the front. NO found in internal combustion engine exhaust, was partially converted - highest at 150°C and lower at 250°C - suggesting NO reduction occurred where hydrogen oxidized, likely due to changing oxidation states within the initial 2cm. These experiments demonstrate that SPACI can reduce material use and provide useful parameters for integrating this unit into future NOx aftertreatment systems, as well as heterogeneous structure catalysis.

References:

Lanza et al. Catalysis Today, 437, 114775. https://doi.org/10.1016/j.cattod.2024.114775.

Touitou et al. (2012) ‘An in situ spatially resolved method to probe gas phase reactions through a fixed bed catalyst’, Catalysis Science & Technology, 2, pp. 1811–1813.

P75: Influence of novel container geometries on resonant acoustic mixing

Theme: Process Modelling, Reactions & Simulation

Mr. Mark Jakob Elbre[1], Mr. Jack Richard Grogan[1], Prof. Christopher R. K. Windows-Yule[1]
[1]University Of Birmingham, Birmingham, United Kingdom

Resonant acoustic mixing (RAM) is a method for mixing solids and/or fluids based around oscillating materials vertically at the system's resonant frequency, potentially allowing faster, lower-cost mixing than other technologies.

To date, the vast majority of academic and industrial applications of RAM utilise cylindrical container geometries.

This presentation illustrates how modifying container geometry impacts RAM mixing performance for particulate materials.

We present a full-factorial study of the state space of superellipsoids as RAM containers, utilising the discrete element method (DEM).

Results suggest cylinders are suboptimal for both low-acceleration/high-fill and high-acceleration/low-fill mixing conditions.

These findings may prove highly valuable in diverse industries using RAM, facilitating faster mixing from vessel geometry optimisation alone.

P76: Feasibility Analysis of Sorption Enhanced Chemical Looping Steam Methane Reforming for Intensified Blue Hydrogen Production

Theme: Process Modelling, Reactions & Simulation

Dr Theodoros Papalas[1], Mr Athanasios Arampatzis[2], Dr Andy Antzaras[2], Prof. Angeliki Lemonidou[3]

[1]School of Chemical Engineering, University of Birmingham, Birmingham, United Kingdom,
[2]School of Chemical Engineering, National Technical University of Athens, Athens, Greece,
[3]Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki, Greece

Hydrogen stands at the forefront of the global energy transition, but its dominant natural gas reforming production pathway remains carbon- and energy-intensive, highlighting the need for more sustainable alternatives. This study evaluates a novel intensified technology, called Sorption Enhanced Chemical Looping Steam Methane Reforming (SE-CL-SMR), which couples calcium looping and chemical looping of a NiO-based oxygen carrier (OC) with natural gas reforming. This process enables in situ CO_2 capture and autothermal reforming at 600°C, producing high-purity H_2 (~98 vol%), without requiring downstream water-gas shift reactors. The exothermic OC oxidation supplies the energy needed for regenerating the CO_2 capture material and releases a high-purity CO_2 stream (~96vol%), suitable for sequestration. A detailed process design of 850 kg H_2 h^{-1} capacity and 20-year lifetime is developed, followed by a comparative technoeconomic analysis of SE-CL-SMR to the incumbent steam methane reforming (SMR). The SE-CL-SMR technology requires higher fixed capital investment (~\$56M) compared to SMR (~\$42M), mainly due to the use of pure oxygen to drive the OC oxidation. However, SE-CL-SMR attains lower levelised cost of H_2 production (\$3.61 kg^{-1}) than SMR (\$3.77 kg^{-1}).This arises from the benefits of process intensification, including equilibrium shifting through in situ CO_2 capture, autothermal reformer operation without external fossil fuel combustion, and enhanced heat integration strategies, resulting in 78-85% reduction in CO_2 emissions. Therefore, implementing a generalised carbon tax of \$120 per tonne of emitted CO_2 can increase the SMR cost by more than 35% and cause minimal impact on SE-CL-SMR due to its low-emissions profile, while reducing the H_2O/CH_4 reformer feed ratio from 3 to 2 can further lower CO_2 emissions by ~5%. Overall, SE-CL-SMR provides a scalable, cost-competitive, and low-carbon pathway for H_2 production, highlighting the transformative potential of process intensification for sustainable H2 systems.

P77: Green synthetic route to produce metal nanoparticles coated with hydrophobic ligands in 100% water and their biomedical applications: combined simulation and experimental approach

Theme: Process Modelling, Reactions & Simulation

Mr Pranav Pazhamukku Premdas[1], Mr Miguel A. Ruiz-Fresneda[2], Mr Mohamed Larbi Merroun[2], Dr Jesus Ojeda Ledo[1], Dr Yon Ju-Nam[1]

[1]Swansea University, Swansea, United Kingdom, [2]University of Granada, Granada, Spain

Our positively charged lipophilic gold nanoparticles (AuNPs) have demonstrated strong bacterial inhibition and show significant potential as active interfaces in biosensing platforms for the early detection of neurodegenerative disease biomarkers. This work reports a green synthetic strategy for the production of cationic lipophilic AuNPs and their associated organic intermediates. Aspen Plus was used to design and simulate fully water-based reaction pathways for the synthesis of hydrophobic ligands used to functionalize the AuNPs, enabling optimization of reaction conditions while minimizing solvent use, waste generation, and experimental trials. Thermophysical properties unavailable in the Aspen database were estimated using the Joback method to support reliable process modelling prior to experimental validation. All intermediates and ligands were synthesized experimentally using a novel 100% water-based route that eliminated organic solvents such as acetonitrile. Structural confirmation was achieved by ATR-FTIR spectroscopy through identification of characteristic functional groups associated with triphenylphosphonioalkylthiosulfate ligands. Green strategies were further applied to AuNP synthesis and surface functionalization by removing dichloromethane, a hazardous solvent used in conventional methods. The formation of positively charged lipophilic AuNPs in water was confirmed by UV–visible spectroscopy, showing characteristic surface plasmon resonance peaks between 516 and 525 nm. TEM revealed monodispersed AuNPs with sizes of 3.13–8.01 nm (2), strongly dependent on reaction conditions. Successful surface functionalization was verified by XPS through detection of metallic Au(0) and thiol–gold bonding, while the resulting colloids exhibited excellent stability in aqueous media for over 12 months. In addition to physicochemical characterization, the functionalized AuNPs displayed notable antimicrobial activity against selected bacterial strains similar to commercially available antibiotics such as penicillin and kanamycin. Furthermore, a label-free electrochemical biosensor was developed using these AuNPs for Tau protein detection, where AuNP modification increased the electroactive surface area by 82.5%.

P78: Performance evaluation of the PC-SAFT, Soave-Redlich-Kwong and Peng-Robinson Equations of State in Modelling Vapour-Liquid Equilibria of Binary CO2 + 1-Alkanol Mixtures

Theme: Process Modelling, Reactions & Simulation

Dr Luis Roman, Prof Gary Leeke

[1]London South Bank University, United Kingdom

CO2 + alcohol mixtures are important in industries such as the chemical, pharmaceutical and the food industry. These mixtures appear for instance, in the extraction of natural products and pharmaceuticals using supercritical CO2 with the alcohol as a cosolvent, in the chemical synthesis of CO2 to alcohols, in reactions between CO2 and an alcohol to produce high-value chemicals, and in biodiesel production. Therefore, the understanding of the phase behaviour of these mixtures is important for reactor and process design.

In this work, a comparison of the performance in modelling the vapour-liquid equilibrium of CO2 + 1-alkanols with the Perturbed Chain Statistical Association Fluid Theory (PC-SAFT) equation of state (EoS), the Soave-Redlich-Kwong (SRK), and the Peng-Robinson (PR) EoS was made by means of the Average Absolute Relative Deviations in bubble pressure and vapour phase composition.

Different versions of the PC-SAFT equation were considered: to account only for the dipolar moment of alcohols (PCP-SAFT-D); to account only for the quadrupolar moment of CO2 (PCP-SAFT-Q); the non-polar version of the equation (PC-SAFT); and the polar and non-polar versions of the equation but considering induced association (I) between the molecules (PCP-SAFT-ID, PCP-SAFT-IQ and PC-SAFT-I). The association term was considered in all versions. Classical mixing and combining rules were employed in SRK and PR. A single binary interaction parameter was used in all models.

Results showed that the induced association approach improved the representation of these systems compared when only polar interactions are considered. The best results were obtained with the PCP-SAFT-IQ equation, which also required a lower binary interaction parameter for most temperatures. Surprisingly, the results with SRK and PR were similar than those obtained with PCP-SAFT-Q, even with a better performance over the dipolar and association versions, with or without induced association.

P79: Integration of DAC into industrial clusters and renewable energy systems

Theme: Process Modelling, Reactions & Simulation

Fatemeh Salmanpour[1], Fariborz Shaahmadi, Katia Piscina, Mijndert Van der Spek, Susana Garcia Lopez

[1]Heriot-watt University, Edinburgh, United Kingdom, [2]Heriot-watt University, [3]Heriot-watt University, Edinburgh, United Kingdom, [4]Heriot-watt University, Edinburgh, United Kingdom, [5]Heriot-watt University, Edinburgh, United Kingdom

Large scale direct air CO2 capture needs to counter greenhouse gas emissions from ‘hard to abate’ sectors including certain industrial activities. While direct air capture has the potential to reach the carbon removal scale required, its deployment is currently hindered by high energy consumption and costs. Synergistic integration with industrial and renewable energy systems can be one measure to reduce these.

To this end, this project combines solid-sorbent DAC process modelling with energy and industrial systems modelling to develop least energy and least cost DAC deployment scenarios. Moreover, it explores flexible operation strategies of Integrating DAC into renewable energies to overcome the challenges related to intermittency of renewable energy systems. In this regard, this work focuses on developing the adsorption modelling framework as a first step towards modelling DAC-energy/industrial system integration. A monolith contactor is selected to i) help decreasing the electrical energy consumption of air transport through the bed by providing lower pressure drop, ii) enhance mass transfer into the sorbent, and iii) enable faster adsorption cycles. The adsorption system was modelled via a system of coupled partial differential equations describing the component, energy, and momentum balance along the contactor length, solved using finite volume methods. We used this approach to model a temperature vacuum swing adsorption cycle. Our first results compare the use of a monolith contactor with using a thin fixed bed contactor and highlight the difference in adsorption breakthrough curve and time cycle.

P80: Tailored Refrigerants for High Temperature Heat Pumps

Theme: Process Modelling, Reactions & Simulation

Mr Finlay Sandham[1], Mr Andrew Muumbo[1], Mr Kenneth Mathew[1], Mr Sarthak Sinha[1], Dr Smitha Gopinath[1]

[1]School of Chemical, Materials, and Biological Engineering, University Of Sheffield, Sheffield, United Kingdom

High temperature heat pumps (HTHPs) are an emerging technology that will be instrumental in decarbonising industry. The most common type of heat pump (HP) uses a subcritical vapour compression cycle. This cycle uses a working fluid (the refrigerant) to absorb heat from a heat source at low pressure (such as a waste heat stream) through evaporation, and then deliver heat at a high pressure to a heat sink (some heat consuming process, e.g. a distillation column or reactor) through condensation. To enable this, a pressure difference is maintained by a compressor. The performance of a HP can be measured using the coefficient of performance (COP), which is the ratio of heat delivered by the condenser to energy consumed by the compressor. It can also be measured using the volumetric heating capacity (VHC), which is the amount of heat delivered by one unit volume of the refrigerant, calculated using the volume at the compressor inlet. Different refrigerants allow for better performance at different source and sink temperatures. An optimisation program is presented that uses the computer aided molecular & process design (CAMPD) methodology to design optimal refrigerant molecules for a given heat source temperature, heat sink temperature, and design objective. HP designs were obtained for a range of heat source-sink temperatures. Using an Intel Core ultra 9 185h CPU, the CAMPD method was able to find optimal molecules from a search space of ~7.68e+20 feasible molecules out of 1022 possible integer combinations in under 3 minutes for the VHC and under a minute for the COP. In 27 out of 30 cases, the designed molecules outperformed 4 benchmark molecules already used in HTHPs.

P81: Exploration of the vibro-packing process in complex geometries using the Discrete Element Method

Theme: Process Modelling, Reactions & Simulation

Mr Aaron Wiggin[1], Mr Freddie Barter[1], Dr Thomas Abadie[1], Dr Shirley Fong[2], Dr James Mainwaring[2], Dr Oliver Phillips[2], Dr Christopher Windows-Yule[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]AWE plc, Reading, United Kingdom

Vibro-packing is a technique used to fill moulds with granular particles to a high degree of packing fraction using vibration. After vibration, the mould can then be backfilled with a suitable binder (e.g. epoxy resin) to produce a high quality, homogeneous composite material in the shape of the mould tool. Existing research into the understanding and optimisation of the vibro-packing process focuses primarily on either the effect of particle properties or vibrational properties. However, many industrial applications require the production of composite materials in shapes other than the standard geometries used in literature (boxes, cylinders). There are numerous changes in system behaviour that can arise from changes in mould geometry, such as node formation around fixtures and unique flow patterns, that will not be observed in the mould shapes used in literature. The ability of numerical methods such as the Discrete Element Method (DEM) to investigate systems across wide parameter spaces allows for a comprehensive comparison of system behaviour between different mould shapes at various excitation and fill levels, without incurring significant cost and time expenses. This presentation will discuss ongoing work studying the effect of key process parameters on the resultant packing fraction and homogeneity of a vibro-packed system in more complex mould shapes, by comparing a simple cylindrical shape to ones of greater complexity. This work aims to address the following questions: How similar is system behaviour across different mould geometries? How much potential knowledge transfer is there from existing literature to complex geometries? How similar are the optimal vibration parameters between mould geometries? The results of this work contribute towards a greater understanding of the vibro-packing process in complex geometries, enabling the production of high-quality composite materials in shapes that are of specific interest across a wide range of industrial applications.

P82: Mesoscale Modelling of Cleaning Surfaces through Hydrodynamic Removal of Foulants

Theme: Process Modelling, Reactions & Simulation

Antoni Zingas[1], Dr Thomas Hubbard[2], Dr Ian McRobbie[2], Prof Zhenyu (Jason) Zhang[1], Dr Amin Rahmat[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Innospec Ltd, Ellesmere Port, United Kingdom

Surface cleaning is a fundamental process in a wide range of areas however, despite extensive research, some knowledge gaps remain; particularly, the understanding of microscale interactions between cleaning agents and foulants. Hence, a computational framework is being constructed focusing on modelling the physico-chemical cleaning processes and interactions of cleaning agents and foulants on a surface, with a focus on the micro- and meso-length scales.

The computational models being developed to simulate surface cleaning are a combination of several mathematical particle-based methods with the current focus being on Smoothed Dissipative Particle Hydrodynamics (SDPD). SDPD solves the Navier-Stokes equations over particles with the addition of thermal fluctuations. This method has been used to create numerical models for surface cleaning in the mesoscale length range. Using this, the dissolution of both a homogeneous and heterogeneous foulant is being modelled, with the impact of varying shear rates having been investigated. In these, the foulant removal rate is seen to increase with increasing shear rate. Additionally, scenarios involving shear rate being added and removed at set intervals have been created. This results in a clear difference between the regions with shear rate and without, showing the significance of shear for foulant removal.

Building on these simulations, the complex physical structure of real foulants on substrates will be modelled through extracting data for various parameters (such as adhesive and cohesive properties) from available experimental and in-house data. From this data, the simulations will be modified to recreate realistic cleaning scenarios of different foulants.

P83: Enhancing Digital Literacy in Chemical Engineering through a Sustainable, Student Centred Coding Club Initiative

Theme: Education

Dr Sakiru Badmos[1], **Dr Solomon Bawa**[1]

[1]University College London, United Kingdom

The accelerating pace of digitalisation is reshaping engineering practice, with data driven decision making, automation, and computational modelling becoming indispensable in academia and industry. Within chemical engineering, proficiency in Python has become increasingly important. Although computational tools are embedded withing the chemical engineering curriculum at UCL, it has been observed that students prioritize grades over long-term relevance of the programming skills. To address this, a Coding Club initiative was developed to shift the focus of the students from assessments to the relevance of the tools beyond their undergraduate program and to enhance their digital competencies for the emerging paradigm of Industry 5.0, which emphasises human–machine collaboration, intelligent systems, and sustainable innovation.

Preliminary consultations across multiple student cohorts revealed a clear enthusiasm for programming. They perceived coding skills as essential for future professional practice, which was further reinforced by a Mentimeter survey involving students from Year 1 to MSc levels. Approximately 87% of respondents agreed that the Coding Club would improve their data analytic competency, and 47% believed it would strengthen their problem solving skills. Only a small minority (7%) questioned the relevance of coding for career readiness.

One of the central challenges identified in the early stages was variation in prior Python experience: 50% of respondents had never used Python, 36% identified as beginners, and 14% reported intermediate proficiency. A tiered learning structure was then proposed allowing students to progress at an appropriate pace without diminishing engagement for more experienced learners.

Overall, early findings indicate strong student motivation and a recognition of the significance of the skills. The Coding Club will continue to evolve through iterative feedback, with the overarching aim of fostering digital literacy, enhancing employability, and supporting a culture of innovation within the department.

P84: We know students use GenAI, but do we know how they use it?

Theme: Education

Dr Eleni Routoula[1]

[1]University of Sheffield, Sheffield, United Kingdom

Three years after Generative AI's (GenAI) mainstream appearance, academic Institutions have accepted the fact that GenAI is here to stay, and they have rolled out guidelines with the aim of controlling and regulating the use of such tools. However, the presence of GenAI tools has added another level of complexity to the already complicated issue of teaching critical thinking skills. With answers to complex questions being retrieved more easily than ever with the press of a few buttons, how can engineering students learn to identify meaningful GenAI outputs and use GenAI tools to sharpen their critical thinking skills?

At the University of Sheffield, School of Chemical Materials and Biological Engineering (CMBE), we have been working towards understanding how students use GenAI tools and how we can support critical use of such tools. Starting with a survey deployed two years ago gathering student views on GenAI, ways of using it and expectations from the University, we designed materials to help students understand appropriate use of GenAI tools, and also developed open-ended ways for students to inform us of their GenAI practices.

Analysing results from four student cohorts across two modules and three programmes on how students used GenAI tools, revealed a preferred type of GenAI tool. When it came to activities students used GenAI tools for, the two most often declared ones were the need to get feedback prior to coursework submission, and to summarise existing information found elsewhere. While the second use is expected, the use of such tools to provide feedback reveals perhaps an opportunity that could be further explored by educators.

This work showcases the progress of CMBE towards the understanding of students' approach towards GenAI tools and shares practical steps we have implemented to support the development of critical thinking skills.

P85: From Lab Preparation to Reflection: Integrating AI Across Pre- and Post-Lab Learning Activities

Theme: Education

Dr Wennie Subramonian[1], Mr Afiq Husaini Bin Rozali

[1]The University of Manchester, United Kingdom

Traditional laboratory learning is fundamental to chemical engineering education, yet existing AI applications in this space address only isolated stages of the laboratory experience. This project aims to design and evaluate a comprehensive AI-assisted learning framework that closes the loop by connecting pre-lab preparation and post-lab reflection across the full laboratory learning cycle. The framework addresses key gaps identified in current literature such as limited support for visualising experimental setups, lack of exploratory "what-if" scenarios, insufficient connection between experimental work and industrial applications, and absence of structured frameworks integrating AI across complete learning cycles. Four AI-assisted learning activities were designed and delivered through pre-lab and post-lab focus groups using ChatGPT, Co-Pilot, and Gemini. Activities integrate AI as a Socratic tutor adopting various professional roles including Laboratory Manager, Project Manager, Senior Safety Engineer, and Client to mirror realistic engineering communication. The first pre-lab activity focuses on pipeline design and reasoning, where students develop process flow diagrams with industrial symbols, conduct cost-evaluation tasks, and explore "what-if" scenarios. The corresponding post-lab activity applies Hazardous Area Classification with scaled-up industrial scenarios. The second pre-lab activity addresses packed column selection through industrial decision-making simulations, while the post-lab activity involves mechanical design feasibility assessment considering real environmental conditions. Throughout all activities, structured socratic prompts require students to justify and critically evaluate AI-generated reasoning, promoting critical thinking and ethical AI use. Findings from focus groups indicate that the integrated framework successfully supports students across the full learning cycle with improved comprehension of experimental setups and enhanced ability to connect theoretical concepts to industrial applications. The framework promotes inclusivity by providing personalised support for diverse learners while strengthening critical thinking as students learn to evaluate AI-generated reasoning rather than accepting outputs uncritically, establishing a novel approach that bridges theoretical knowledge with industrial practice.

P86: Use of Tea Leaves and Banana Peels for the removal of Copper (II) Ions in a Laboratory Scale Fixed Bed Adsorption Column

Theme: Bioprocessing & Biotechnology

Mr George Artell-Cram[2], **Dr Abdullatif Alfutimie**[1]

[1]MEng degree, Manchester, United Kingdom, [2]Senior lecture, Manchester, United Kingdom

As a consequence of rapid technological advancement and industrialisation, copper consumption has increased substantially, leading to the improper disposal of copper-containing materials and subsequent freshwater contamination. Major sources include electronic waste and corroded industrial infrastructure, which release Cu^{2+} ions into aquatic systems. Elevated copper levels in drinking water pose serious health risks, including abdominal pain, jaundice, and hematemesis. To promote sustainable water treatment strategies, this study evaluated the performance of two low-cost bio-adsorbents—waste tea leaves and banana peels—for the removal of Cu^{2+} from aqueous solutions.

Experiments were conducted in a fixed-bed column with a bed volume of 290.5 cm^3 to investigate the effects of flowrate (70 and 130 mL min^{-1}), solution pH (4 and 6), and contact time (5–150 min) on copper removal efficiency (η). Synthetic wastewater was prepared by dissolving copper(II) sulfate pentahydrate ($CuSO_4 \cdot 5H_2O$) to obtain an initial Cu^{2+} concentration of 20.36 mg L^{-1}. Residual copper concentrations were quantified using Inductively Coupled Plasma Optical Emission Spectrometry (ICP-OES), with calibration standards prepared in-house.

Tea leaves exhibited superior adsorption performance, achieving a maximum removal efficiency of 79.79% at pH 4 and 70 mL min^{-1} after 30 minutes of contact time. Banana peel showed lower overall efficiencies, with optimal performance (55.01%) at pH 6 and 70 mL min^{-1}. Structural and functional characterisation using Fourier Transform Infrared Spectroscopy (FTIR) and X-ray Diffraction (XRD) indicated that O–H, C=C, C–H, N–O, and C–N functional groups contributed to copper binding. Shifts in FTIR peaks and reduced transmittance below 500 cm^{-1} suggested surface complexation. XRD patterns confirmed predominantly amorphous structures, with notable surface modifications observed in banana peel after adsorption. Overall, tea leaves demonstrated greater potential as an effective, sustainable bio-adsorbent for copper removal from contaminated water.

P87: Characterisation of Biochar Derived from Sidr (Ziziphus spina-Christi) Biomass

Theme: Bioprocessing & Biotechnology

Mr Abdulaziz Ebrahim[1], Dr. Xiaoan Mao[1], Dr. Amin Osatiashtiani[1], Dr. Ali Hassanpour[1]

[1]University of Leeds, Leeds, United Kingdom

Nitrate (NO_3^-) and nitrite (NO_2^-) in water are priority pollutants, commonly linked to fertiliser use and industrial wastewater discharge. Many countries follow the World Health Organization (WHO) benchmark limits of 50 $mg \cdot L^{-1}$ for nitrate (as NO_3^-) and 3 $mg \cdot L^{-1}$ for nitrite (as NO_2^-). This work investigates whether biochar produced from Sidr (Ziziphus spina-christi) biomass can be developed into an adsorbent for nitrate and nitrite removal, with a focus on fixed-bed column treatment and meeting WHO benchmarks by optimising flow rate, bed depth, and influent concentration. Sidr biomass was collected in Kuwait, dried, shipped to Leeds, then chipped and sieved into different size fractions. Baseline “pristine” biochars were produced by slow pyrolysis under nitrogen at 450 °C. Two initial runs gave similar biochar yields (35.9% from fine material and 37.9% from larger cubes), suggesting repeatable production. Preliminary characterisation established a baseline before adsorption testing. SEM imaging showed pores and channels in the raw biomass. TGA-based proximate analysis across three Sidr size fractions gave moisture contents of 6.34–8.36%, volatile matter of 65.46–69.58%, fixed carbon of 19.42–20.85%, and ash of 1.48–5.18%, with broadly similar thermal behaviour across sizes. Surface-area analysis indicated strong microporosity after pyrolysis: N_2 BET values were low (0.396–6.101 $m^2 \cdot g^{-1}$), whereas CO_2 NLDFT analysis gave micropore surface areas of 320.16–322.39 $m^2 \cdot g^{-1}$ with micropore volumes of 0.0889–0.0909 $cm^3 \cdot g^{-1}$.

P88: Designing Microbiome-Compatible Skin Cleansers: Multiscale Effects of Surfactant Chemistry

Theme: Bioprocessing & Biotechnology

Miss Zaineb Kamal[1], Dr Patricia Esteban[1], Dr Emma Shore-William[2], Dr Peter Fryer[1], Dr Ian McRobbie[2], Dr Zhenyu Jason Zhang[1]

[1]University of Birmingham, Birmingham, United Kingdom, [2]Innospec Inc, Ellesmere Port, United Kingdom

This study investigates how surfactant chemistry shapes skin-associated microorganisms across molecular, cellular, and community scales to inform the rational design of microbiome-compatible cleansing systems. We combine in vitro single-species and coculture assays with a controlled human study to define structure–microbiome relationships for mild versus sulfate-based surfactants. In vitro assays quantify growth, viability, membrane integrity, ultrastructure, and transcriptional responses in key bacterial and fungal taxa using growth curves, flow cytometry, electron microscopy, RT-qPCR, and RNA-seq. Coculture experiments resolve species-specific and community-level responses, linking surfactant physicochemical properties to gene-expression signatures and functional resilience. In humans, three regimens—a mild surfactant, an SLS-based surfactant, and a surfactant-free control—are compared for effects on skin lipidome, chemistry, microbial composition (16S/18S rRNA sequencing), and host–microbial transcriptional responses via tape-strip sampling. Preliminary data reveal charge- and envelope-dependent growth inhibition, with SLS inducing stronger membrane stress than mild surfactants, supporting the hypothesis that cell-envelope architecture and surfactant class jointly determine microbiome impact. Collectively, this work establishes human-relevant criteria for designing mild surfactants that preserve skin barrier function and microbiome homeostasis while maintaining cleansing performance.

P89: Multifunctional PEG-based pH- and Redox-Dual-responsive Nanogels for Oral Drug Delivery

Theme: Bioprocessing & Biotechnology

Peiyu Kong[1], Bowen Yu[1], Jiayi He[1], Qianyi Zhao[1], You Cheng[1], Yeting Jin[1], Dr Rongjun Chen[1]

[1]Imperial College London, London, United Kingdom

Oral administration remains one of the most preferred routes of drug delivery because of its convenience, high patient compliance and suitability for self-administration. However, effective oral delivery is often compromised by the harsh and dynamic gastrointestinal (GI) environment, including strong acidity, digestive enzymes, and food-related variability that can reduce the stability and bioavailability of drugs. Stimuli-responsive hydrogels can protect payloads in the stomach and enable release in the intestine; nevertheless, conventional bulk hydrogels may exhibit limited efficiency for small-molecule delivery because their relatively large mesh sizes may cause premature diffusion and unintended leakage. In contrast, nanogels provide improved encapsulation and controlled release, and their higher surface-area-to-volume ratio can enhance dispersion and promote closer contact with the mucosal layer. Here, we report a novel nanogel system synthesised through crosslinking of a multifunctional PEG polymer for oral drug delivery.

We systematically investigated how solvent composition and polymer concentration influenced nanogel formation, swelling behaviour, pH/redox-triggered release of model payloads. Fourier-transform infrared spectroscopy (FTIR) confirmed covalent crosslinking and successful payload encapsulation. Dynamic light scattering (DLS), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) were used to characterise particle size, dispersity, and morphology. Using fluorescein and doxorubicin as representative payloads, the optimised formulation exhibited pH/redox dual-responsive release profiles, providing gastric protection and accelerated release under intestinal-like conditions. Haemolysis assays revealed pH-mediated membrane activity, and in vitro cytotoxicity studies demonstrated favourable cell tolerance. Therefore, this multifunctional PEG-based dual-responsive nanogel system offers a novel strategy for oral delivery and shows promise for gastrointestinal disease therapy.

P90: Identification of Aromatic Phytochemicals from Sustainable Horticulture Waste via Supercritical Carbon Dioxide Extraction: A Comparative Study

Theme: Bioprocessing & Biotechnology

Miss Rebecca Still[1], Professor Parimala Shivaoprasad, Professor Ray Marriott

[1]University of Nottingham, United Kingdom

Climate change, resource constraints, and increasingly fragile global supply chains are reshaping how chemicals, materials, and fragrances must be produced; placing sustainability at the centre of future industrial viability. Despite this, horticultural waste streams such as rejected and surplus flowers remain under-utilised despite their rich phytochemical content. This study explores the valorisation of discarded Hyacinthus orientalis flowers through the selective recovery of aromatic compounds using supercritical carbon dioxide ($scCO_2$) extraction, a green, and advanced chemical separation technology. Volatile profiles were first characterised by solid-phase microextraction and GC–MS, revealing colour-dependent differences in aroma composition and identifying phenylethyl alcohol (PEA) as a key floral compound. A fractional factorial Design of Experiments was employed to assess the effects of pressure, temperature, CO_2 flow rate, and extraction time. Pressure emerged as the dominant factor influencing both extract yield and PEA concentration, while extraction kinetics demonstrated rapid initial solute recovery followed by diffusion-limited behaviour. Supercritical CO_2 extraction produced extracts enriched in delicate floral volatiles while mostly excluding non-volatile lipids, waxes, and thermally degraded compounds common with solvent-based and distillation techniques. Importantly, $scCO_2$ enabled direct extraction from fresh flower biomass, eliminating energy-intensive drying and pre-treatment steps. This reduces environmental impact and operational costs while preserving delicate phytochemicals. Overall, the results demonstrate a viable pathway for transforming low-value horticultural waste into high-value aromatic ingredients, supporting circular economy principles, and resilient production.

P91: Process intensified continuous-flow enzymatic transesterification of rose geranium oil via coiled flow inverter (CFI) microreactors

Theme: Bioprocessing & Biotechnology

Miss Alisa Wikaputri[1], Miss Rhea Satpute[1], Mr Shyam Rana[1], Professor Derek Irvine[1], Professor Robert Stockman[2], Professor Volker Hessel[3], Dr Parimala Shivaprasad[1]

[1]University of Nottingham, Department of Chemical and Environmental Engineering, Nottingham, United Kingdom, [2]University of Nottingham, Department of Chemistry, Nottingham, United Kingdom, [3]University of Adelaide, School of Chemical Engineering, Australia

The UK produces approximately 34,000 tonnes of flower waste annually, most of which is landfilled despite containing crude flower oils rich in citronellol and geraniol, key precursors for terpene esters widely used in the flavour and fragrance industries. Conventional batch biocatalysis faces major engineering challenges when converting these oils, including slow kinetics, enzyme deactivation, and limited scalability, leaving this renewable feedstock underexploited. Overcoming these barriers could transform UK floral waste into a high-value circular-economy feedstock, addressing the growing demand for sustainable fragrance ingredients, with global markets projected to exceed USD 42 billion by 2029.

We introduce a solvent-free, biphasic continuous-flow platform for enzymatic transesterification of crude rose oil into multi-terpene esters, employing a Coiled Flow Inverter (CFI) microreactor and Pseudomonas fluorescens lipase. The CFI integrates process intensification and microreactor engineering, enhancing heat and mass transfer and generating a narrow residence-time distribution for precise bioprocess control. The biphasic system improves enzyme recyclability, accelerates reaction rates, and maintains catalytic activity six-fold higher at temperatures that deactivate lipases in batch systems (>55 °C).

Under optimised conditions, we achieved a maximum 93 % citronellyl ester and 100 % geranyl ester within five minutes, significantly increasing the productivity from 45 g/day to 1631 g/day using 90 % less reactor volume. Moreover, this 90 % water-based formulation enables a safe and scalable operation. Recently, we developed the first the first multi-substrate kinetic model for the solvent-free rose oil transesterification which will be extended to this scaled-up version, capturing substrate competition and turnover dynamics. This platform and kinetic framework offer a scalable approach to valorise UK floral waste into high-value chemicals, and a methodology transferable to other biomass-derived, terpene-rich feedstocks to reduce dependence on fossil resources.

P92: Techno-Economic Analysis of an Air-Source Heat Pump System Integrated with Phase Change Material for Decarbonising Residential Buildings in the UK

Theme: Energy & Net Zero & LCA

Dr Sajan Preet[1], Professor Jonathan Radcliffe[1]

[1]University of Birmingham, Birmingham, United Kingdom

The decarbonisation of residential buildings is essential to reduce space heating energy demand and associated greenhouse gas emissions in the United Kingdom. As electricity-based heating systems become increasingly prevalent, innovative solutions are required to minimise electricity consumption while maintaining indoor thermal comfort and enhancing system flexibility. In this context, the present study proposes an advanced residential heating system that integrates an air-source heat pump (ASHP) with latent thermal energy storage using a phase change material (PCM). The incorporation of PCM provides operational flexibility to the ASHP by enabling thermal energy storage, load shifting, and decoupling heat generation from demand. The performance of the integrated ASHP–PCM heating system installed in a semi-detached residential building is investigated to assess its potential to reduce electricity demand for space heating. The system is designed to store thermal energy during off-peak periods and release it during periods of peak demand, thereby increasing flexibility in response to time-varying electricity prices and grid conditions. A comprehensive techno-economic and environmental analysis is conducted to evaluate the performance of the ASHP–PCM system relative to a conventional standalone ASHP and a gas boiler.

Authors list