Chemical Engineering Day UK 2021
University of Bradford, 7/8 April 2021, Online

LIST OF ABSTRACTS FOR SESSIONS 1,2,3 &4

1. Process Modelling 2. Advanced Materials 3. Energy & Sustainability 4. Learning & Teaching

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1.1: Modelling and simulation of multi effect distillation and solar powered multistage humidification-dehumidification hybrid process for seawater desalination

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Abstract

Desalination, by convention, is defined as the process of removing dissolved solids and other minerals from water. The process is becoming necessary as per capital increase in demand for fresh water caused by population growth, urbanization and industrialization outpaces availability of high-quality water. Not only that, but also the global water stress caused by the effects of climate change. It is estimated that up to 2.8 billion people will face water stress or scarcity by 2025 globally and that number could reach 4 billion people by 2050 if alternative sources of water are not found.

There are several desalination technologies suitable for water purification. These includes multi effect distillation (MED) and solar powered Multistage humidification-dehumidification (HDH) desalination. MED is a distillation process consisting of multiple stages or "effects". In each stage the feed water is heated by steam in tubes, usually by spraying saline water onto them. Some water evaporates, and this steam flows into the tubes of the next stage (effect) for heating and evaporating more water. Humidification-dehumidification is a thermal desalination cycle that operates by heating saline water using solar energy, evaporate the heated water using humidifier and finally condenses the water vapor into fresh water.

In order to improve performance and reduce operating costs for desalination systems many researchers have suggested coupling of these individual processes. However, little attempts have been made to analyze performance and operating costs for the combined multi effect distillation (MED) and Humidification-dehumidification desalination processes. Therefore, this research focuses on investigating several design options of the coupled MED and HDH system. To achieve this goal, detailed mathematical models for the two individual processes will be developed and independently validated against literature and experimental data. Then the integrated model will be used to investigate the performance and operating costs of several configurations of the MED and HDH processes for the hybridized system. The performance indicators will include fresh water productivity, energy consumption, fresh water purity, and recovery ratio.

The outcome of this project will be the hybridized water desalination model that can be used for designing and analyzing technical and economical aspect prior to construction of the real plant. This model will have advantages of lowering the cost and time for designing desalination plants.

Keywords: *Humidification, Dehumidification, multi effect distillation, desalination, mathematical models.*

1.2: A Novel Lagrangian Recurrence-Based Approach for Local and Global Description of Mixing in Multiphase Flow

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Abstract

Mixing aims to enhance the homogeneity of a single phase or multiphase system through input of mechanical energy to achieve a desired process result. This is an important industrial operation which is often conducted in a mechanically agitated vessel and is critical to the successful manufacturing of numerous products including fine chemicals, pharmaceuticals, personal/home care products, paper and pulp, polymers, food, and the formulation of products for these sectors. The design of mechanically agitated vessels, however, is still often as much an art as a science and for many applications it cannot be carried out from first principles. Therefore, theoretical methodologies for evaluation of mixing performance are vital. Traditional mixing indices are generally based on Eulerian data which are often unable to capture the detailed features of what is intrinsically a Lagrangian process. A mixing index which is based on Lagrangian trajectories of fluid elements or particles can potentially provide a better description of the relevant mixing phenomena which determine the degree of mixedness. Over a long period of time, the trajectory of a particular phase in mixing system tends to recur repeatedly in a form close to that of its initial state. On the basis of this principle, Lagrangian experimental data obtained by a technique of positron emission particle tracking (PEPT) have been used to develop a new methodology for the evaluation of mixing performance in agitated vessels. The PEPT technique can provide the long-term three-dimensional trajectories by tracking particle or fluid elements in space over an extended period of time. By considering the recurring states of the PEPT trajectories and the positions at which these recurrences occur, a new data-driven approach has been developed for the description of mixedness in a multiphase flow. For this purpose, a windowing recurrence quantification analysis of the trajectories is performed based on the Shannon entropy of the probability distribution of diagonal lines of recurrence structures, which leads to a detailed ‘pointwise’ description of mixedness in the flow. The implementation and potential of this new method are demonstrated by analysing a wide range of experimental PEPT trajectories in single-phase liquid as well as solid-liquid suspensions. Detailed information is obtained on local mixedness, allowing the identification of well-mixed and poorly-mixed cells in a vessel agitated by a pitched blade turbine (PBT) operating in both up- and down-pumping configurations over a range of rotational speeds.

Keywords: *mixing, agitated vessel, PEPT, recurrence, entropy*

1.3: Integration of digital technologies for engineering, operation and maintenance of process plants

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Abstract

The digital twin of a process plant is seen as a central lever for more productivity and higher added value. An essential prerequisite for this is the combination of data from various software tools for engineering, simulation and automation across the entire process plant life cycle. For this combination, suitable interfaces between the various software tools are necessary, which are used across the plant life cycle. One of these interfaces connects the process simulator, which is used for design simulation and process optimization, with a simulation platform that enables virtual commissioning and operator training. The relevance and the technical implementation of this interface will be shown in the context of this presentation using a demonstrator.

Keywords: digital twin, process modelling, co-simulation, model integration, OPC-UA

1.4: Lagrangian Stochastic Modelling of Three-Dimensional Particle-Liquid Flows

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Abstract

Stochastic models are used to predict various outcomes of a system by utilising random perturbations on pre-determined variables. As many processes are not deterministic, stochastic models can be used to give the probability of a certain result. This use of probability can be used, for example, to model the Brownian motion of particles or fluid parcels, and has previously been used to predict diffusion in oceanography, atmospheric pollutants, and dissipation of odours. To construct deterministic models for complex flow systems is challenging and computationally expensive to execute. Stochastic models use a simplified structure instead, greatly reducing computational time, whilst predicting complex flow characteristics. We propose a Lagrangian stochastic approach to model liquid and particle trajectories in a multiphase stirred vessel system. In a Lagrangian stochastic model (LSM), fluid or particle positions are advanced in space over a given time step and are subject to random perturbations. Depending on the order of the model (zeroth, first, second), different flow parameters (position, velocity, acceleration) are affected by this random increment. The random increment is defined by the Wiener process and the LSM, a data-driven model, utilises a velocity flow field extracted from Lagrangian experimental trajectory data.

The predictive capability of different order LSMs has been evaluated by comparing 3D theoretical trajectories in a two-phase particle-liquid flow inside a stirred vessel, using Eulerian and statistical analysis, with 3D Lagrangian experimental trajectories obtained by a technique of positron emission particle tracking (PEPT). It is found that the first order LSM is the most suitable for this flow. The LSM has also been compared to numerical computational fluid dynamics (CFD) simulations. Unlike numerical Eulerian-Eulerian or Eulerian-Lagrangian methods, LSMs are not computer intensive and long trajectories can be obtained in a short time. Trajectories predicted by LSM have shown good agreement with both Eulerian-Eulerian and Eulerian-Lagrangian simulations.

Keywords: Lagrangian flow, stochastic modelling, stirred vessel, PEPT

1.5: Investigating the Effect of Elevated Pressure on the Flow Characteristics and Regime Transition in a Pressurized Fluidized Bed by Electrical Capacitance Tomography Measurements

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Abstract

Gas-solids fluidized beds have been widely used in the process industries, due to their excellent mixing and heat/mass transfer performance. Many industrial processes require high pressure operation to improve the throughput and reduce the size of the reactors. However, despite the considerable studies performed on atmospheric fluidized beds, understanding the effect of elevated pressure on flow characteristics and regime transition is still quite insufficient, due to the difficulties in visualization and measurements of pressurized fluidization systems.

In this research, the advanced electrical capacitance tomography (ECT) technique is introduced to provide non-intrusive and real-time measurements of a cold pilot-scale pressurized fluidized bed. The experiments are performed at four pressure conditions from 0.2 to 1.3 MPa, and a wide range of fluidization velocities, to cover the flow regimes from bubbling to fast fluidization. The temporally- and spatially-resolved particle volume fraction (PVF) distributions are obtained from ECT image reconstruction, and the bubble properties and flow regime transition velocities are further characterized by means of detailed statistical analyses. Some key conclusions on the effect of operating pressure are given and discussed.

The results show that for the experimental Geldart B particles, the concerned flow regime transition velocities, namely, the values of: the minimum fluidization velocity (Umf), the onsets of turbulent flow (Uc) and fast fluidization flow (Uk) show significant decrease with the pressure increase. However, the corresponding critical fluidization numbers (i.e. Uc/Umf, and Uk/Umf) almost stay consistent in various pressure conditions, indicating its validity as a criterion for flow regime classification in pressurized fluidized beds.

The bubble properties, including bubble size and rising velocity at elevated pressure condition are also investigated. The equivalent bubble diameter, estimated by the reference cut-off values of PVF, increases as the gas velocity increases. In addition, the average bubble rise velocities calculated from two methods of cross-correlation analyses, based on the dual-plane ECT sensor, also increase with the gas velocity increase. Furthermore, the pixel-by-pixel correlation gives the velocity distribution across the cross-section, from which the uneven distribution feature between the center and near-wall region is clearly observed.

This work demonstrates the high suitability of ECT technique, applied to a gas-solids pressurized fluidized bed, for the real-time measurement without intruding the flow field. The experimental results, in terms of the pressure effect on gas-solids flow characteristics, bubble properties and regime transition are believed to provide some useful information for the proper design and optimization of pressurized fluidization apparatus in the future.

***Keywords**: pressurized fluidized bed, flow regime transition, bubble properties, electrical capacitance tomography*

1.6: Process Modelling Improvements for Yield Stress Sludge and Slurry Handling at Sellafield

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Abstract

Significant effort has been made at Sellafield in recent years to improve modelling of Liquid-Solids Sludge handling and Slurry Transfer Systems. This work is supporting existing and future operations and design projects addressing retrieval and treatment of sludge from legacy facilities. Process Modelling and a brief description of test rig work to underwrite the modelling will be described including:

· Solids-liquid handling in a feed lute to a vacuum evaporator. Solids transfer can result in significant solids accumulating in the lute after a feed trip. This work looked at re-suspending solids within blocked lutes and showed existing theoretical models gave reasonable prediction for transfer rates and pressures required to unblock the lutes.

· Pulse Jet solids re-suspension testing and modelling within flat-bottomed tanks and dish-end tanks. The developed Sellafield Theoretical Model has been validated at several scales and is also the basis of a current Hanford Model.

· Solids handling in dished end vessels using Pulse Tube Mixing, which is an area of current modelling work.

· Solids-Liquid transfer and wash-out in long and short transfer lines. There is ongoing experimental work looking at slurry transfer

· Crater Collapse and Shape Modelling for Grab Emptying of Sludge Tanks and general slumping of Yield Stress Solids.

· Process Modelling of Grout Feed Lines to Encapsulation Plants cleaning by pneumatically driven pigs to support control, design and operational studies.

This work has variously developed new process modelling theory and under-written existing published theory for some scenarios.

Keywords: Yield Stress, Sludges, Slurry, Pigging, Slumping

1.7: ON THE EXISTENCE OF THE YIELD STRESS IN GELS

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ABSTRACT

Waxy crude oils are pumped hot but upon power cut, pumping stops, the oil cools leading below the wax appearance temperature to precipitation of the wax and the formation of a gel throughout the pipe. In such a situation, what is the minimum pressure required to restart *flow*, not to merely deform the gel or break it? This paper provides a solution to this problem using rheological data conducted in constant stress mode under controlled temperature and cooling conditions and restart experiments in laboratory pipelines replicating the rheometric conditions and deviations from them to inform large diameter operation in the field. We found from the rheological data that these oil gels can appropriately be described as elasto-visco-plastic but with subtle features at the very beginning (consolidation) and at the very end (fragmentation) before entering into viscous flow. Neither of these features have been reported before. We suggest from these results that "*indeed everything flows*" but yielding and yield stresses are real and measurable. We identified τ_f (the stress at fragmentation of the gel) as the pertinent parameter as far as restart and tested this in a pipeline rig using a small diameter pipe, effectively acting as a capillary rheometer with uniform cooling. We assessed deviations from uniform cooling using a larger diameter pipe. The important conclusion is that τ_f , the threshold stress signalling the release of the oil trapped in the gel structure, is the most accurate predictor of re-start pressures. Further underpinning of this conclusion is provided by microscopic observations to explain the strengths that an oil gel can display through the variation of the sizes of the crystals formed with cooling rates and temperatures.

Key words: *waxy crude oil, rheology, re-start pressure yield stress, crystallisation.*

1.8: Optimal cleaning schedule of air coolers in concentrated solar power plants

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Abstract

Solar radiation is a renewable source of energy available all over the surface of the Earth. One alternative to convert it into electricity is a combination of concentration technologies and heat transfer fluids. Concentrated solar power (CSP) plants concentrates the solar radiation using a heliostat field, and storage it as thermal energy using a heat transfer fluid. That fluid is used to produce steam, which generates power in a turbine. Then, steam is recovered in a cooling system. Most cooling systems involve wet cooling towers, but water is scarce in areas where solar radiation is high and the efficiency of CSP plants is maximum, hence it may limit the operation of CSP plants. Dry cooling systems use air instead but consume a significant percentage of the electricity generated. In addition, air coolers, being exposed to atmospheric conditions in dry areas (e.g. desserts), are subjected to particulate fouling, which deteriorates their performance. To ensure feasibility and profitability of CSP plants in regions where water is a limitation, it is paramount to optimally design, operate, and plan maintenance of the air coolers.

In a previous work we developed accurate models, and efficient algorithms for the optimal design of A-frame heat exchangers in CSP plants considering seasonal variability. Now, the optimal operation and cleaning schedule of the cooling system is considered. Assuming that the cooling system is optimally designed, and can be operated in a modular fashion, we develop a model, and a mathematical formulation for its optimal operation and cleaning schedule. The problem is formulated as a large scale multi period MINLP that includes the monthly variability and covers a time scale of 10 years of operation. The main decision variables are the air flow rate to each section of the cooling system, the power required by the fans, the total steam condensed, and the timing of the cleanings of each module. The MINLP problem is solved using a generalized Benders decomposition approach where the relaxed master problem is the cleaning scheduling problem (MILP), and the primal problem is the optimal operation given a cleaning schedule (NLP).

A case study of a CSP plant located in Dubai with a production capacity of 18.9MW/year is used to demonstrate the benefits of the method. In addition to particulate fouling, this location presents regular sandstorms that cause an acute loss of efficiency of the system because of the large deposition of sand over the heat transfer surfaces. Sandstorms are modelled as a stochastic process based on atmospheric and historical data available for the region. Compare to the normal operation, the optimal solution generates savings of $ 2.3 M without considering sandstorms. When sandstorms are introduced the operation is infeasible without any maintenance action (the system cannot fully condensate the steam flow rate during summer months), while the optimal alternative is always feasible, and reacts in the best way to the large disturbance considering the economics of the process.

Keywords: optimal cleaning schedule, particulate fouling, concentrated solar power, air coolers, MINLP

1.9: A novel combination of scale-down techniques and design of experiments to identify operating regions for the process-scale recovery of intracellular proteins

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Abstract

UCL and Biocatalysts Ltd are collaborating in a Knowledge Transfer Partnership focussed on improving yield of enzyme products across the primary recovery stages.

In this presentation a combination of design of experiments and ultra scale-down techniques has been utilised to identify operating regions for the primary recovery of intracellular proteins from E. coli broth homogenate. This is to establish the basis for the study of the recovery of individual enzymes.

A process sequence of dilution, flocculation, centrifugation and depth filtration stages is considered. An integrated study is made of three process variables; the concentration of a modulating agent, of a flocculant and the dilution factor during flocculation. Bench-scale centrifugation is used in a fashion to mimic pilot scale operation. The impact of these three process variables on the supernatant turbidity and its protein content and the sediment volume fraction is recorded. These measurements are used to estimate the filter demand to clarify the supernatant and the predicted protein recovery at scale. While the resultant predicted protein yield is only moderate (~ 60%) subsequent studies have inferred that much of the loss is of colloidal protein and the predicted yield for an individual enzyme might be considerably greater (~80%).

Conditions achieving both acceptable predicted protein yield and low filter demand, required high flocculant concentration and high dilution and there is a potential role for a modulating reagent. Operating widows are presented to demonstrate such relationships.

Keywords: *Flocculation. DoE. Optimisation. Ultra scale-down. Microbial.*

1.10: NUMERICAL SIMULATION OF PARTICLE PIPE TRANSPORT IN VISCOUS NEWTONIAN LIQUIDS

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Abstract

A vital challenge for modern engineering is the modelling of the multiscale complex particle-liquid flows at the heart of numerous industrial and physiological processes. Industries dependent on such flows include food, chemicals, consumer goods, pharmaceuticals, oil, mining, river engineering, construction, power generation, biotechnology and medicine. Despite this large range of application areas, industrial practice and processes and clinical practice are neither efficient nor optimal because of a lack of fundamental understanding of the complex, multiscale phenomena involved. Flows may be turbulent or viscous and the carrier fluid may exhibit complex non-Newtonian rheology. Particles have various shapes, sizes, densities, bulk and surface properties. Our fundamental understanding has so far been restricted by huge practical difficulties in imaging such flows and measuring their local properties. Mixtures of practical interest are often concentrated and opaque so that optical flow visualization is impossible. We address this problem experimentally by using a technique of positron emission particle tracking (PEPT). In PEPT, radiolabeled particles are used as flow followers and tracked in 3D space and time through positron detection. Thus, each component in a multiphase particle-liquid flow can be labelled and its behavior observed. Compared with leading optical laser techniques (e.g. LDV, PIV), PEPT has an enormous and unique advantage that it can image opaque fluids and fluids inside opaque apparatus with comparable accuracy. Computationally, we study the viscous pipe flow of dense (up to 40% v/v) particle suspensions in turbulence Newtonian regions using an Eulerian-Eulerian CFD model. The predicted flow fields of the continuous and discrete phases are successfully validated by accurate experimental measurements of velocity profiles obtained from PEPT. The effects of various flow parameters are investigated including particle size, density and concentration, and carrier fluid properties. Varying the particle concentration changes the behavior of the flow velocity profiles of both phases. Moreover, particle size and concentration have a significant effect on the particle radial distribution.

Keywords: *Eulerian-Eulerian CFD, Pipe, velocity profile, solid distribution, PEPT*

1.11: Steam-Oxygen Gasification of Refuse-Derived Fuel in Fluidized Beds: Modeling and Data Validation

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Abstract

Gasification is the thermochemical conversion of solid feedstock into syngas, and can be accomplished through several reactors configuration. Feedstock containing high ash and moisture fractions, such as refuse derived fuel (RDF) produced from municipal solid waste (MSW), are mostly treated in fluidized bed reactors, which are particularly suitable due to their flexibility with respect to feedstock and operating conditions. Waste derived fuels are generated from a number of sources and influenced by a wide range of factors that create a complex mixture of materials, resulting into an extensive variability in RDF composition and, therefore, process operating conditions. The complexity of the phenomena, which occur simultaneously during RDF gasification, and the lack of experimental data in the literature, require a mathematical model that correlate the effects of process variables with the product gas composition. In this study, a model of steamoxygen gasification of RDF in a bubbling fluidized bed gasifier has been developed. The model incorporates the complex reaction network of gasification with the hydrodynamics of a bubbling fluidized bed. In particular, the entire reactor is divided into a finite number of compartments of appropriate height, and variations only occur along the axial direction. The bed zone is modelled according to the two-phase theory, with both heterogeneous and homogeneous reactions taking place; the fluid-dynamic and the kinetics of each reactions are embedded into the mass balances, which consider also the enhanced mass transfer between the phases, solved for each compartment. The freeboard zone is modelled as a non-isothermal plug flow reactor to describe variation of syngas quality at different heights. The model was validated by comparing gas outlet concentration and temperature profile with experimental data from a demonstration plant. Finally, the effects of the operating conditions on gas yield and process efficiency were evaluated, as well as the most appropriate fuel feeding height, equivalent ratio and the relative amount of steam to inject.

Keywords: Waste Gasification, Fluidized beds, 1-D Model.

1.12: Autonomous self-optimising reactors based on low-cost sensors

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Abstract

Automated chemical reactors allow for product complexity unimaginable even 30 years ago. The automated reactors relieve the burden of routine operations from the experimenter and allow to focus on the key elements of the process. This is possible with reactors that incorporate closed-loop feedback algorithms; these in turn are enabled with online sensors to analyse the reactor performance and feedback algorithms to compute and adjust the experimental conditions to reach the desired outcome. Such automation, however, is hardly applied in the area of heterogeneous catalysis. Moreover, conventional process analytical tools cost above 10k rendering their application costly. The work presented shows the application of low-cost process analytics sensor to assist process and catalyst development.

The hydrogenation experiments were performed in an automated system controlled with an OpenFlowChem [1] software and contained two systems: (i) the flow reactor, (ii) and a control system containing the optical sensor and the sample collector. The flow reactor included two HPLC pumps, the gas flow rates were set with a set of mass flow controllers. The reaction was performed in catalyst-coated tube reactors (1.27 mm inner diameter, 1.6 mm outer diameter) provided by Stoli Catalysts Ltd placed inside an oven follower by a back-pressure controller. The liquid products were collected using an automated sample collector and analysed offline with a gas chromatograph (Shimadzu GC-2010) equipped with a flame ionisation detector and a Stabilwax column.

The self-optimising reactor equipped with the optical sensor was studied in the reaction of nitrobenzene hydrogenation to aniline. A flow of nitrobenzene was combined with a hydrogen flow. The hydrogenation reaction was performed in a tube reactor wall-coated with a 5 wt% Pd/SiO2 catalyst. The reaction system was controlled with a proportional-integral-differential (PID) algorithm which adjusted the nitrobenzene concertation as well as the proportional hydrogen flow rate to obtain the constant liquid fraction in the product stream.

This approach works for a broad range of compounds, catalysts, reaction temperatures and pressures [2]. It could be applied to time-on-stream experiments. This approach provides optimal reaction conditions form the catalytic reaction even despite changes in the catalyst activity. As a result, a turn-over number of 10^6-10^7 can be achieved – 1,000 times above typical values observed in batch even with catalyst recycling.

We further improved the sensors and developed a proof-of-concept prototype of a wireless stirrer that incorporates a modular architecture that provides a possibility for measuring electrical conductivity of the solution, its temperature, colour of the ambient light reaching the sensor in red, greed, blue and combined components, as well as light scattering and fluorescence of the solution, linear acceleration, angular momentum and magnetic field in 3 axes. These data are transferred wirelessly onto an external receiver/data recorder. These sensors were demonstrated in titration experiments.

References:

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2. Cherkasov, N.; Exposito, A.; Bai, Y.; Rebrov, E. V.; React. Chem. Eng. 2019, 4, 112.

Keywords: Process analytical tools; PAT; Internet of things; sensor; process conditions

1.13: Benchmarking the performance of oxygen-carrier materials in a thermodynamically limited chemical looping process for hydrogen production from the water-gas shift reaction

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Abstract

Chemical looping is the concept whereby a gas-phase reaction is broken down into multiple sub-reactions via the use of a solid intermediate carrier material. The water-gas shift reaction for hydrogen production ($CO + H_2O \rightleftharpoons CO_2 + H_2$) can be carried out in a chemical looping reactor to produce separate hydrogen and carbon dioxide streams, thereby reducing the need for downstream separation associated with current widely used processes that operate on mixed feeds.

Non-stoichiometric perovskite oxides have been identified as promising carrier materials for the chemical looping water-gas shift process as they can be engineered to allow for rapid oxygen uptake kinetics and take on a range of oxidation states. Previous work has demonstrated how a fixed-bed chemical looping reactor, with the non-stoichiometric perovskite $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ as the carrier material, was able to overcome the chemical equilibrium constraints associated with the water-gas shift reaction [1]. However, this material is held back by its limited oxygen capacity in the active range of oxygen partial pressures that, assuming a constant temperature, sees the greatest extent of reaction of the water-gas shift reaction (roughly 10^{-20} bar to 10^{-15} bar). Higher oxygen capacity in this range would mean less material would have to be used in a fixed bed reactor, leading to improved scale-up potential.

In this work a TGA investigation found that the substitution of 33% Mn onto the B-site of $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ results in an almost threefold increase in the oxygen capacity of the material in the active oxygen partial pressure range. Additionally, the cycling performance of $La_{0.6}Sr_{0.4}Fe_{0.67}Mn_{0.33}O_{3-\delta}$ was investigated in a laboratory-scale integral reactor. Consecutive counter-current streams of carbon monoxide and water vapour in a balance of argon were flowed through a fixed bed at 1093 K. Stable hydrogen production was observed using 0.01 mol (2.2g) $La_{0.6}Sr_{0.4}Fe_{0.67}Mn_{0.33}O_{3-\delta}$ for over 200 cycles with feed lengths of up to 5 minutes, and water and carbon monoxide conversions of >80% were obtained. For comparison, conversions using $La_{0.6}Sr_{0.4}FeO_{3-\delta}$ dropped to ~52% at shorter feed lengths of only 2 minutes.

The improved performance of $La_{0.6}Sr_{0.4}Fe_{0.67}Mn_{0.33}O_{3-\delta}$ can be explained by focusing on the effect on conversion of the relationship between the oxygen non-stoichiometry of the carrier material and the oxygen partial pressure of the gas phase. The case for a hypothetical material which arises from the thermodynamics of the water-gas shift reaction is proposed. This can be applied as a benchmark to aid in predicting the conversion performance of new oxygen carrier materials, provided that they have sufficiently fast kinetics to make the process thermodynamically limited.

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Keywords: *Chemical looping, water-gas shift, perovskite, non-stoichiometry, oxygen capacity*

1.14: Numerical Study of Thermophoresis Mass Transport in Binary Fluid Mixtures Using OpenFOAM

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Abstract

In homogeneous fluid mixture systems under the influence of temperature gradients, mixture components tend to concentrate at specific regions of the systems. This phenomenon is caused by the mass transfer process known as thermophoresis or thermal diffusion mass transport. It depends on some physical properties of the systems, including the concentration and the molecular weight of each component, as well as the temperature field distribution. The understanding of the mass transport process is crucial for its applications for instance in separation processes. Experimental study of the transport of components under the effect of thermophoresis in such mixture systems in various flow conditions can be very challenging. A numerical approach that helps to overcome these difficulties is proposed. As the primary focus of the current work, a computational fluid dynamics (CFD)-based methodology to analyse the mechanism of thermophoresis in binary fluid mixture processes has been specifically developed. Details of the implementation of the newly developed solver, which is based on the Open Source toolkit OpenFOAM, are laid out. This development accounts for pure diffusive and convective binary mixture systems, where temperature gradients are derived from different sources. Several simulations were performed, and results agree well with the analytical solutions and experimental data available, demonstrating that the developed tool is effective for the investigation of the species separation in complex fluid mixture systems using thermophoresis.

Keywords: Thermophoresis, CFD, Binary Mixtures, Mass transfer, OpenFOAM

1.15: A model-based understanding of degradation in solid oxide electrolysis cells during syngas production

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Abstract

In order to prevent global warming and climate change caused by the rapid increase of CO_2 emissions into the atmosphere, most governments have planned to lower CO_2 emissions so that to limit the global temperature to 1.5℃. In addition to carbon capture and storage technologies, there has been a growing interest in evaluating the economic value of the captured CO_2 through utilisation. High-temperature solid oxide electrolysis cells (SOECs) are promising devices for efficient CO_2 and H_2O co-electrolysis into syngas ($CO + H_2$) which can be further converted into a wide range of chemicals and fuels. Although SOECs have been tested for durability under co-electrolysis, degradation phenomena occurring within the cell is still of great concern for commercial deployment. Importantly, to the best of our knowledge, there is no previous studies which combine process modelling and SOEC degradation to assess long-term cell performance and operating strategies at micro level. The present work addresses the gap and report a multi-physics model for SOEC degradation. The model incorporates electrochemical reactions, particle transport and microstructure evolution for a typical SOEC material set: Ni-YSZ cathode, YSZ electrolyte and LSM-YSZ anode. The SOEC degradation model has been validated for different current densities (0.25 – 1.5 A/cm^2) and operating temperatures (800, 850℃). Performance analysis showed that increasing the current density enhances syngas production but also leads to higher degradation rate. It was observed that electrolyte degrades rapidly the first 500 hours of operation due to cubic to tetragonal phase transition then remains almost constant. Therefore, electrolyte degradation does not significantly contribute to SOEC degradation regarding long-term performance. Long-term SOEC degradation is mostly due to oxide scale growth and anode delamination with a degradation rate of 13.9 %/kh after 1000 hours of operation at 800℃, 1 bar and 1.5 A/cm^2. Applying an anti-oxidant layer at the interconnect between the anode and cathode electrodes could considerably reduce the degradation rate by roughly 63% on the anode side.

Keywords: *CO_2 utilisation; Solid oxide electrolysis; Co-electrolysis; Modelling; Degradation mechanism*

1.17: Novel Feasible Path Optimization Algorithms for Process Flowsheet Optimization using Rigorous Models

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Abstract

The feasible path optimization algorithm is widely used for process flowsheet optimization in which each optimization step requires to solve a process simulation problem.[1] Therefore, its performance strongly relies on the convergence of the process simulation, which is difficult to guarantee in the equation-oriented (EO) environment. The pseudo-transient continuation (PTC) modeling approach can significantly improve the convergence performance of the process simulation and hence enable the feasible path optimization algorithm to solve many challenging process flowsheet optimization problems.[2]

There are two existing optimization algorithms using PTC modelling approach for process flowsheet optimization including the time-relaxation-based optimization algorithm[2] and the PTC model-assisted steady-state optimization algorithm.[3] The former often leads to computational inefficiency due to a time-consuming dynamic simulation required at each optimization step, while the latter could be more computationally efficient but may fail to converge in some cases. We propose three new optimization algorithms that could guarantee both the convergence performance and computational efficiency. In the 1st algorithm we improve the steady-state feasible path optimization algorithm through using the feasible starting point before line search to guarantee the convergence of the process simulation during the line search. The 2nd algorithm improves the time-relaxation-based optimization algorithm through using the tolerance-relaxation-integration method for the PTC-based simulation. In the new integration method, a large convergence tolerance is used at the beginning of the dynamic simulation and the simulation is integrated to a point close to the steady-state solution after a long enough integration time, while the required tight tolerance is used at the latter phase of the simulation. A long enough integration time is used to guarantee the dynamic solution after the initial integration period has been close to the final steady-state solution so that the latter integration using tight tolerance can be fast. The 3rd algorithm is a hybrid algorithm which integrates the steady-state simulation and the PTC-based dynamic simulation. In this hybrid algorithm, the steady-state simulation is replaced by the PTC-based dynamic simulation once it fails to converge, which could significantly reduce the number of PTC-based simulation runs required and hence improve computational efficiency.

We use four examples to illustrate the capability of the proposed algorithms. All examples are related to process flowsheet optimization problems using rigorous models. The computational results demonstrate that the proposed algorithms could solve Examples 1-2 with much less computational effort compared to the existing PTC model assisted steady-state optimization algorithm and time-relaxation-based optimization algorithm. Furthermore, the proposed algorithms can even solve Examples 3-4 which are extremely difficult to solve while the existing algorithms fail to solve without trial-and-error adjustment of parameters. Among the three new algorithms, the improved feasible path optimization algorithm took the least computational time but it had the most number of optimization steps. The hybrid algorithm generally used a similar number of optimization steps to the improved time-relaxation-based optimization algorithm, while it took only one third of the computational time compared with the latter.

Keywords: *Process flowsheet optimization, PTC simulation, feasible path optimization.*

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2.1: Numerical Modelling and Simulation of Volume Variation of pH Sensitive Anionic Hydrogels

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Abstract

Over the years, smart hydrogels have received significant attention in pharmaceutical and biomedical disciplines. Main reason is their potential use in drug delivery devices and tissue scaffolds, of particular interest due to their ability to respond to external triggers, such as pH variations in the body, and alter their conformation (swell and/or collapse) accordingly. To modulate smart hydrogel properties, a broader understanding of the underlying mechanism yielding their behaviour is required. To achieve this, mathematical modelling and simulation studies were pursued in place of expensive empirical approach. The classical Poisson-Nernst-Planck (PNP) equations and equilibrium mechanical equation, can mathematically model the interplay of chemo-electro-mechanical fields for hydrogels exposed to ionic environment. However, this continuum model is not amenable to analytical solutions, and the complex geometry involved makes finite difference method unsuitable for the numerical simulation. Therefore, finite element approach is employed to develop a numerical model that approximates the earlier mentioned mathematical model.

In this modelling study, a cylindrically shaped anionic hydrogel immersed in a buffer solution has been used as a case study. All relevant information, defining hydrogel and its environment, was obtained from the literature. A two-dimensional axial symmetrical domain using Finite Element Method implemented in COMSOL Multiphysics software was employed. In the software, the transport of diluted species interface representing the Nernst Planck equation (captures the diffusion and migration of ionic species), electrostatics interface under AC/DC module (represents the Poisson equation, which describes the distribution of the electrical potential in the subdomains) and the solid mechanics interface (describing the deformation of the gel) were all coupled and solved using Direct-PARADISO linear system solver.

Parametric studies for transient and equilibrium simulations were performed to determine the effects of material properties (such as concentration of the fixed charge group at the backbone of the hydrogel, modulus of elasticity, and initial dimensions of the hydrogel) and the surrounding external conditions (such as ionic strength, composition and pH value of the buffer solution) on the volume change of the pH responsive hydrogel.

The results obtained from the simulation were compared with experimental work in the literature for hydrogels fabricated in a microchannel, confined to deform only in the radial direction. The predictions are in good agreement; hence, the model has the potential to offer predictions for volume changes as a function of pH changes in the surrounding medium.

Keywords: *pH-responsive hydrogel, numerical model, simulation, volume-variation behaviour, finite element method, COMSOL Multiphysics.*

2.2: Foam stability under external electric fields

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Abstract

Nanofluidics present unique opportunities in the field of electrokinetic separations [1], allowing for screening of analytes by shape and size, in addition to electrical charge. Liquid foams can be considered as networks of micro and nanofluidic channels, with film thicknesses reaching down to the order of 10s of nanometers [2]. Liquid foams can provide a quick, simple and inexpensive method to produce large networks of micro/nano channels with high interfacial area to volume ratio that can be used to enhance separation of charged biological entities such as proteins, DNA etc. Liquid foams present unique challenges; a major limiting factor of foams is their instability. As fluid is removed from the films by gravity drainage or capillary action, the films become more likely to rupture and disrupt the structure of the foam. The impacts of electro-osmotic flow on foam stability are not entirely understood [3]; therefore, knowing the effects of applied electric fields on foam stability and their behaviour will be vital in developing any foam-based electrophoresis device.

A 35 mm x16 mm x 2 mm foam cell is constructed by sandwiching two parallel electrodes between two glass slides with the electrodes aligned along the long edges. A monolayer of foam produced using different types of surfactants (anionic surfactant, SDS; cationic surfactant, MTAB; non-ionic surfactant, Triton X-100 and zwitterionic surfactant, SB3-14) were subjected to an external electric field and their stability was measured. All surfactant solutions used were at critical micelle concentration (CMC) and mixed with 50% glycerol to increase the solution viscosity. Initially during the setup stage, the foam chamber was held vertically, and 0.3 ml of surfactant was injected into the base. Then, air was injected at constant pressure and flowrate for a set time, until the chamber is fully filled with monodisperse 2D foam. The chamber was then placed horizontally to negate the effects of gravity driven drainage. An electric potential difference of up to 32V was applied across the foam chamber and a time-lapse video of foam collapse was recorded.

Application of the electric field (0-2000 V/m) resulted in different effects depending on the surfactant type used and strength of the electric field. Anionic surfactant (SDS) showed a reduction in lifespan from over 6 hours to approximately 20 minutes with the increasing electric field, while cationic surfactant (MTAB) exhibited an extended lifespan from 20 minutes to 3 hours with increasing electric field. Non-ionic surfactant (Triton X-100) did not exhibit any significant effect to increasing electric current. Zwitterionic surfactant (SB3-14) stability was increase from 10 to 30 minutes with increasing field strength. The analysis carried out in this study is invaluable in design, fabrication and operation of a foam separation system based on electrokinetics.

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Keywords: *Electrokinetics, foam, surfactants, nanofluidics, electrophoresis*

2.3: Simulations of carbon fibre reinforced composites

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Abstract

Carbon fibre reinforced composites are used in a wide variety of applications that take advantage of their mechanical, thermal and electrical properties. These materials are traditionally composed of a polymer matrix, usually a thermoplastic or thermoset combined with the reinforcement fibre. Both components have widely different properties on their own and adhesion between them poses is a key factor in determining the properties of the composite. It is likely that the presence of the interface affects the network formation of the polymer, thus affecting the adhesion of the polymer matrix to the carbon fibre. Experimental observation of the interface between the polymer matrix and fibre surface at a molecular level and the impact of the interface on polymer network formation (crosslinking) is extremely challenging, hence molecular simulations are often employed to gain insight and an understanding of these systems.

Bead-spring polymer models have been used extensively in molecular dynamics simulations to study the properties of polymer materials in bulk and near surfaces. However, their application to reactive systems where crosslinking is involved is still in its early stages. We have developed a bead-spring model capable of replicating the formation of a 3D crosslinking polymer network and we will use it to investigate fibre-surface interactions, including the effect of the carbon fibre on the network formation and structure of the resulting polymer matrix.

Keywords: polymer simulations, crosslinking, toy models, composites.

2.4: Analysis of Physio-chemical Properties of Salt

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Abstract

There are a wide variety of table salts that can be used to season and flavour the foods that are available in the market and used daily. It is claimed that some salts are healthier than other salts as they are packed with natural minerals which provide health benefits. As a result, certain salts are much more expensive than the others and some have even gathered a very big following.

This study seeks to identify if these claims are factual or not by exploring the physio-chemical properties of three samples of salt. The salts used in this study are two rock salts, Himalayan and Shah Alamdar and a sample of sea salt. Initially, the surfaces of the salts are studied by using a scanning electron microscope. Also, it is suggested that some salts contain iodine naturally and so chemical testing allowed presence to be detected. Iodine is essential to consume since the human body does not produce it and is required to produce thyroid hormones. Moreover, through numerous laboratory techniques, such as EDX, XRD, TGA, DSC and FTIR spectroscopy, the samples were characterized and analyzed in detail by identifying organic and inorganic elements and its impact on the health. Trace elements found through analysis were Mg, Si, S, Cl, K, Ca, Br, Fe, O and C. The impacts of impurities on the human body are discussed.

Keywords: *Sodium Chloride, Trace elements, Impurities, Analysis, Health, SEM, EDX*

2.5: Microencapsulation of fish oil for tableting

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Abstract

Fish oil as a dietary supplement is beneficial to human health. Soft gelatin capsules are currently used on the market for loading fish oil. However, they tend to generate strong fishy odour and are easily oxidized although the gelatine shell can stabilise the fish oil to some extent. Moreover, the gelatin shell dissolves quickly in the stomach, which releases the oil and can cause “fishy burp”. In contrast, tablet is the most widely used dosage form of medicine for oral delivery. The tablet with right formulations may provide an additional barrier to stabilise the fish oil, prevent “fishy burp” and contain different active ingredients (e.g. whey protein, vitamin and flavour) to enhance its functionality. This study aims to encapsulate fish oil in microcapsules, which should be mechanically strong, and can potentially be compacted into tablet as a final dosage form. Gelatin and gum Arabic were used as wall materials. Microcapsules were produced using two different encapsulation techniques: spray drying coating (SPC), and coacervation followed by spray drying coating (CC-SPC). The size of the microcapsules was measured using Malvern Mastersizer 2000. Their morphology and structure were characterised using scanning electron microscopy (SEM) and transmission electron microscopy (TEM), and mechanical properties were measured using a micromanipulation technique (Sun and Zhang, 2001; Zhang et al., 2009). The encapsulation efficiency and payload of the active ingredient were quantified by a UV spectrophotometer at a wavelength of 315 nm (Chatterjee and Judeh, 2015; Yu et al., 2017).

From the SEM images of the microcapsules prepared by the two techniques, they were nearly spherical in shape and intact with no cracks. Their SEM and TEM images indicate that the microcapsules produced by SPC had a matrix structure, and those by CC-SPC possessed a core-shells structure. The corresponding mean diameter D [4,3] of microcapsules prepared by SPC was 10.4 ± 0.2μm, and that by CC-SPC 13.9 ± 0.2 μm. The mechanical properties data of the microcapsules are as follows: The mean rupture force of the microcapsules prepared using CC-SDC was 1.3±0.1 mN, which is approximately 3 times as great as those by SDC (0.44±0.05 mN). The corresponding mean nominal rupture strain and nominal rupture stress of the microcapsules produced using CC-SPC were 22±2 % and 6.2±0.2 MPa, and those using SPC 14.5±0.9 % and 3.2±0.2 MPa. These results indicate that the microcapsules with a core-shells structure prepared using CC-SPC were significantly stronger than those using SPC. The flowability of the microcapsules and the storage stability of the encapsulated fish oil have also been investigated, and the detailed results will be presented. The microcapsules will be mixed with industrial excipients, which will be compacted into tablet, and the fate of the microcapsules after tableting and the long-term storage stability of the fish oil will be studied in the future.

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Keywords: *Fish oil; formulation; mechanical properties; microcapsules; micromanipulation; tablet.*

2.6: Predicting Crystal Breakage in Pharmaceutical Agitated Dryers

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Abstract

Crystal breakage is an issue of great concern to the pharmaceutical industry. Conservation of the desired particle size distribution (PSD) throughout downstream processing is extremely important, as PSD changes are known to affect properties such as bulk density, solubility and flowability. Active Pharmaceutical Ingredients (APIs) are, in the majority, organic high aspect ratio crystals and are typically filtered and dried before subsequent secondary processing.

Understanding and predicting the breakage of elongated particles in agitated drying systems remains a challenging and active area of research. Computational methods, such as Distinct Element Modelling (DEM), have been used to simulate the flow of particle beds for various stress conditions [1] and a range of particles aspect ratio [2]. The contact forces between particles induces an internal stress which is responsible of particle breakage: bending is known to be the main breakage mechanism of elongated particles [3]. Therefore, to elucidate the fracture phenomenon of elongated particles in agitated drying, the bending stress of individual crystals needs to be determined within a bed of particles.

In this study, a shear cell is built in DEM and mimics the stress experienced by particles in dryers using moving parallel walls and periodic boundaries. Elongated rigid particles are modeled with clumped spheres and experience stress due to the shear application in the box. The particles interactions are governed by Hertz-Midlin contact model with no cohesion to simulate a dry system. The bending stress of individual particles is calculated during the simulation and a bending stress distribution is obtained for the given stress condition (normal, shear). The mechanical properties of a sample of Beta-Glutamic Acid (β-LGA) crystals are assessed with a novel 2-point cantilever bending method using Atomic Force Microscopy [4]. The simulated bending stress distribution is combined with the experimental breakage strength distribution of the β-LGA sample: this novel probabilistic approach allows the estimation of the extent of breakage within the particle bed during the shearing phase, which is found to increase exponentially with the normal stress acting on the shear layer.

Future work consists on investigating the influence of particle alignment and aspect ratio on the bending stress distribution. Correlation analysis will allow the development of a breakage kernel to be used in a population balance model for the prediction of PSD in industrial agitated dryers.

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Keywords: *Breakage, Elongated particles, Shear cell, Organic crystals, Agitated drying, DEM.*

2.9: Two-Phase Fluid Displacement in Microchannels with Pure Viscoelastic Fluids

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Abstract

In everyday chemical processes, displacement is a crucial phenomenon. Many fundamental but critical applications such as medical administration of drugs, apparatus cleaning and oil recovery involve the displacement of a liquid by another fluid. Frequently, the initial liquid within the channel is more viscous, causing an instability during the displacement process. This would result in branching of the leading interface of the fluid, also known as viscous fingering effect, as reported by Saffman and Taylor (1). This instability often leads to inefficient cleaning and removal of liquid from a channel as a liquid film remains trapped at the wall (see Fig. 1). Numerous studies have been done to characterise this instability involving two Newtonian fluids but there is little to no knowledge available when the liquid is substituted by a complex fluid.

This research involves the employment of a pure viscoelastic fluid (more commonly known as Boger fluid) to displace an immiscible organic phase within a microchannel. A dilute polymer solution of polyethylene oxide (PEO) and polyethylene glycol (PEG) is used to displace the Newtonian silicone oil. Initially, the main scope of the study is to observe the effect of fluid elasticity on displacement efficiency, but the peculiar effect of a purely viscoelastic fluid in a microchannel has led to more research into the internal mixing characteristics within the phases. This internal mixing is due to the effect of elastic instability, which can be characterised by a wave function. Thus, internal circulation is enhanced and high degree of mixing can be achieved, even at low Reynolds numbers (2). To characterise the mixing, the velocity fields in both phases are obtained with a two colour μ-PIV imaging technique (see Fig. 2). In addition, high-speed imaging is employed to visualise the displacement and the flow patterns within the microchannel.

2.8: The Arabinoxylan Story

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Abstract

Arabinoxylans (AX) are potentially a valuable co-product of biorefineries, offering a new class of functional food ingredients and non-food materials, and facilitating the introduction of commercially viable biorefineries. The first step in the AX story was to establish that commercial production of AX could be economically viable through integration with bioethanol production, with bioethanol pinch analysis being developed to enhance the economics. The diverse range of potential AX feedstocks and products now gives rise to challenges of characterising these materials, defining processes to produce a range of fractions, and creating markets and end-uses for those fractions. Wheat bran, sugarcane bagasse and oat husks have been explored as promising feedstocks giving AX fractions of different molecular weights, structures and functional properties. The identification of prebiotic AX oligosaccharides as one promising fraction has helped to push the agenda forward in terms of analytical capabilities, greater scope for process integration, and commercial opportunities.

Keywords: *arabinoxylans, bioethanol, biorefinery integration, oligosaccharides, food ingredients*

2.9: Advancing the nucleation of peptides using organic templates: The case study of human insulin

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Abstract

The crystalline form of insulin and many other bio-active polypeptides offers significant pharmacokinetic advantages, such as better release control and higher bioavailability [1]. One of the main challenges of peptide crystallisation is the lack of controllability of the nucleation. Nucleation is a stochastic event and strongly depends on the interaction peptides form between each other. However, very little has been done in tailoring controlling strategies for nucleation to achieve a consistent and reproducible crystallisation process.

In our recent studies, it has been shown that amino acids can act as an organic template and have a significant impact on the ability to control insulin nucleation. In this presentation, the impact of types and amount of amino acids on the crystallisation performance of insulin will be reported. Insulin comprises of 2 peptide chains, A and B, with a combined 51 amino acids and a molecular weight of 5.8 kDa. Citrate buffer with a pH between 5 and 7 was used with zincsulphate as the precipitant. The impact of amino acids on crystallisation is evaluated by means of measuring induction time, crystal yield and size distribution as a function of time. The experiments were carried out in batch crystallisation (milliliter-scale) and the insulin concentration was measured via UV-vis absorption every 20-30 mins. Amino acids that exhibit electrically charged residual-groups for the relevant buffer conditions were investigated. Both insulin and amino acids concentrations were varied to determine the optimal concentrations and ratio. Additionally, crystalliser volumes between one milliliter to multiple milliliters were investigated.

Our results show that amino acids can reduce the induction time of insulin crystallisation by up to 40% when compared to the induction time with no amino acids. The reduce in induction time implies an impact on the crystal growth rate, which tends to increase with amount of amino acids added. The charged residual-groups of the added amino acids lead to an increase in the stability of the tertiary structure of insulin by altering the physio-chemical surface properties of insulin which result in a faster nucleation. It was also found that the investigated amino acids do not alter the solubility of insulin, as for example an additional precipitant would do. As the crystallisation occurs faster, a yield of 90% can be achieved within 2 hours when amino acids were added. While the use of amino acids has no significant impact on the mean crystal size (~20 µm), adding amino acids leads to a narrower crystal size distribution as a result of a more controlled crystallisation. The insulin crystals obtained with amino acids show a smaller span and more uniform crystal size distribution. The above described impacts of adding amino acids could be confirmed for multiple crystalliser volumes, from one milliliter to multiple milliliter.

Amino acids as organic templates have been demonstrated to have the potential of improving the controllability of crystallisation. These include a significant reduction in the induction time and an increase in the crystallisation yield. Additionally, amino acids increase the consistency of the crystal shapes and sizes.

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2.10: Parametric Study of Paper-based Al-Air Battery

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Abstract

Paper-based Al-air battery is a potential power source for mini-watt applications such as wearable electronics. A low cost paper-based Al-air battery is generally fabricated with porous cellulose paper as an electrolyte substrate, a low-grade Al foil as anode and a carbon paper as cathode. The porous microstructures of the cellulose paper greatly affect the battery performance, thereby understanding the fundamentals of electrochemical and mass transfer inside paper microstructures help design and optimise the battery structure.

In this study, we developed a numerical model for paper-based Al-air battery that includes a series of important transport phenomena and electrochemical reactions. The model was firstly validated and showed reasonable agreement with experimental data. Subsequently, we employed this model to study the effects of different geometric parameters of porous papers (such as thickness and porosity) and operating parameters (such as electrolyte concentration) on the battery performance. It was found that the battery performance was improved as the paper porosity and thickness increased. This is because higher porosity and higher thickness of paper can store larger volume of electrolyte. As the thickness increased from 50 μm to 250 μm, the improvement of battery performance was weak. The battery performance was improved with increasing the electrolyte concentration and reached a peak when the concentration is 5 M.

It is concluded that the geometric and operating parameters need to be optimised to improve the battery performance and the present model provides a powerful tool for this purpose.

Keywords: *Al-air battery; porosity, electrolyte concentration; numerical model; parameter study*

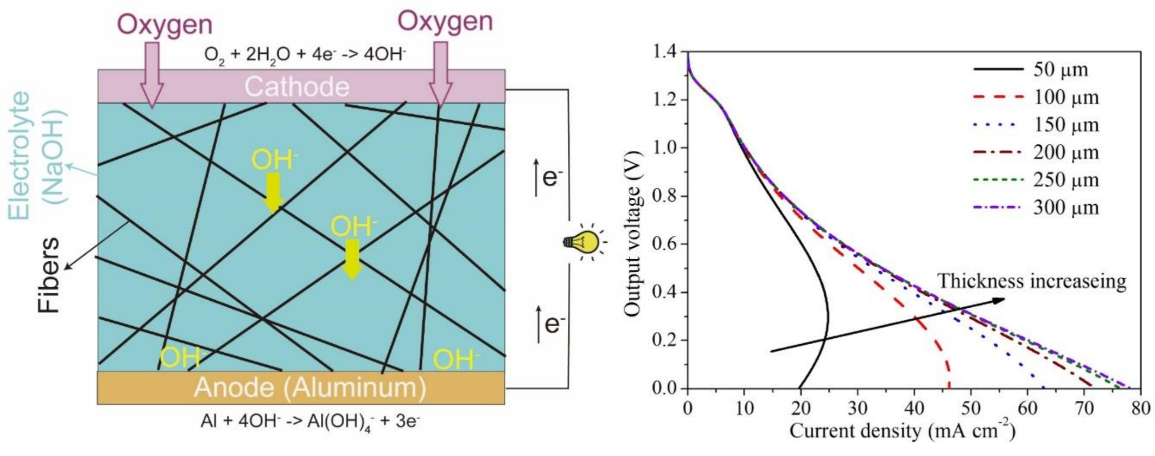

Figure 1 (a) Schematic of paper-based Al-air battery and (b) effects of paper thickness on the battery performance.

2.11: The Influence of Counterion Selection on Electrostatic Properties of Pharmaceutical Salts

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Abstract

Salification of an active pharmaceutical ingredient (API) is an approach effectively utilised to modify physicochemical properties of acidic and basic drugs, including solubility, dissolution rate, stability and hygroscopicity. It is commonly reported that approximately 50% of drugs are administered in the salt form, and this continued popularity of salt formation supports the need for sustained research to discover entities with the greatest physicochemical and material handling properties to help reduce the cost of manufacturing. However, little work has been carried out to determine the effects of salt formation upon the tribo-electrification propensity of the resulting material. Tribo-electrification can influence material handling properties, whereby powder handling operations can induce a charge upon the particles, resulting in an increase in tendency of particles to adhere to themselves and the walls of the processing equipment.

The aim of this study was to investigate the influences of solvent selection and ratio of counterion to active pharmaceutical ingredient to determine the effects on the final form in terms of crystal habit and tribo-electrification propensity as a result of solvent selection.

The experimental results show the magnitude of ratio selection and solvent selection upon the crystal habit, and the solvent selection upon the tribo-electrification propensity. Three carboxylic acid drugs were used namely flurbiprofen, felbinac and biphenyl-4-carboxylic acid, due to their similar structures along with three counterions; cyclopropylamine, cyclobutylamine and cyclopentylamine. The results show that significant differences were observed in physicochemical properties including reduction in solubility with an increase in the carbon chain length of the counterion, as well as the extremely low charging propensity of biphenyl-4-carboxylic acid, potentially improving powder handling properties.

This work demonstrates the potential of investigating the salt formation on physicochemical and tribo-electrification property relationship in pharmaceutical materials.

2.12: Process induced surface property variation for crystalline pharmaceutical solids

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Abstract

Particle surface properties are affected by the processing approaches and conditions employed for each unit operations. The transformations in surface properties of crystalline solids, in turn, could influence powder processing, particle handling and particle performance. Surface analytical techniques like Inverse Gas Chromatography (IGC), is a versatile tool to detect even small changes at the surface level of the solids through the surface energy determination. In a series of studies, we show the surface property evolution in crystalline solids subjected to processes like milling, sieving, mixing and surface modification.

Milling is an important unit operation during powder processing and a range of milling induced surface changes can occur in crystalline solids. The results highlighting the influence of milling induced surface energy heterogeneity changes in D-Mannitol and α-lactose monohydrate powders were reported through IGC studies. The results suggested an increase in the surface energy heterogeneity post milling. We show that crystalline materials are anisotropic and milling results in the generation of new surfaces exposing different crystal facets varying in facet specific surface energy. Investigating the breakage behaviour of powders using finite dilution inverse gas chromatography (FD-IGC), it is argued that crystals fracture along the weakest attachment energy planes, which are also shown to be the most hydrophobic. Furthermore, an approach to decouple the effect of the contribution of milling induced increase in surface area and surface energy was presented through a series of work by functionalising of the crystal surfaces. Surface silanisation resulted in normalisation of the surface energy heterogeneity for unmilled and milled powders. The α-lactose monohydrate powders produced by both milling and sieving were also investigated. The sieved samples were divided into a top, middle and bottom fraction, each showing some degree of heterogeneity. The sieved bottom fraction exhibited higher heterogeneity with higher dispersive (γ^d) surface energy values ranging from 42.5 mJ/m^2 45.9 mJ/m^2 compared to the top and middle fractions. Here, we show that sieved fractions of the same material could exhibit different surface properties due to exposure of different crystalline facets upon milling. The coarse lactose powders showed lower γ^d values 43.1 mJ/m^2 to 45.0 mJ/m^2 compared to the fine powders, produced by milling, with γ^d values ranging from 43.2 mJ/m^2 to 46.5 mJ/m^2.

From the mixing studies with D-Mannitol and glass beads compositions, it was shown that the structuring of component particles in binary compositions affects the solid-solid interfacial properties. Three different scenarios viz. structured, random and segregated systems of the binary powder composition were considered for the analysis in the IGC column. Binary mixtures with large size disparity between the components produced structured mixtures exhibiting a guest-host type of interactions and energetic homogeneity irrespective of the energetics of the finer component.

Thus, our work confirmed that processes like milling, sieving, surface functionalisation and mixing affect the surface energy of the particulate solids due to the changes in properties like size, shape, exposure of internal cleavage planes and interparticle structuring and the surface energy heterogeneity determination using FD-IGC helped in characterising these changes.

Keywords: *Mixing, Milling, Sieving, Surface functionalisation, Surface Energy, Interparticle structuring*

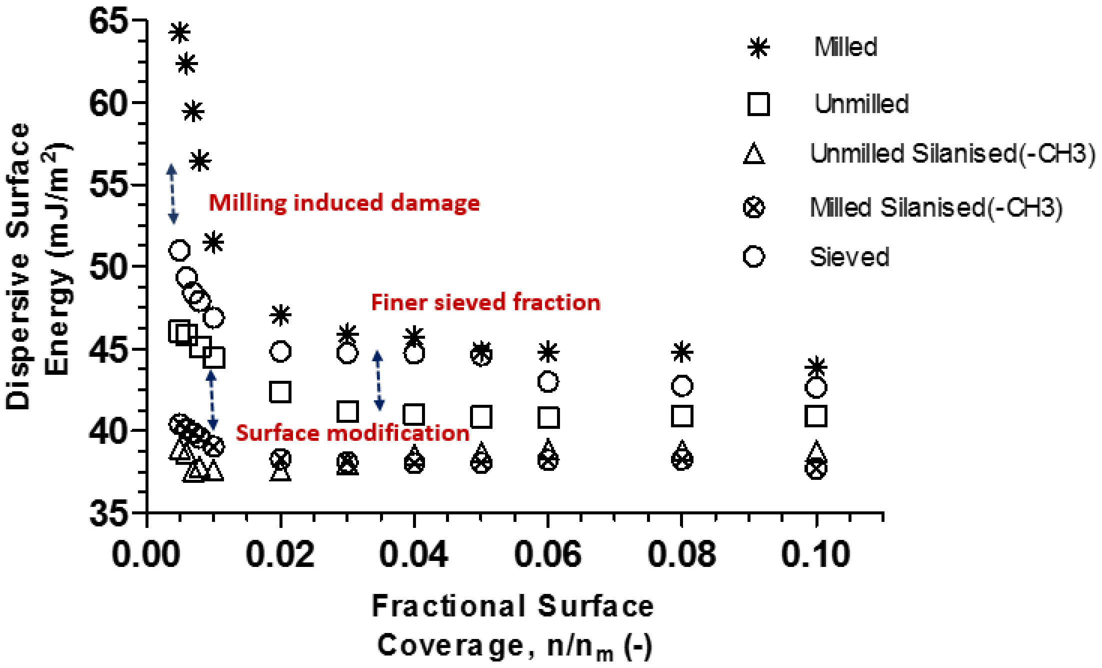

Figure. 1 Surface energy heterogeneity profiles of milled, sieved and surface functionalised powders

2.13: Functionalised Nanoparticles Assisted Enhanced Oil Recovery

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ABSTRACT

In spite of the improvement has been made on renewable energy, hydrocarbons and fossil fuel are still the world's main energy source. In the meantime, great amounts of discovered oil deposits remain unrecoverable after several applications of traditional oil recovery methods. The main target of Enhanced Oil Recovery (EOR) operations in general, is to change the properties of both fluid and rock formations for purpose of minimizing the oil saturation value below the residual oil after water flooding process as a traditional technique. Thus, innovative EOR operations have been evaluating over the years which have managed to involve the nanotechnology to be part of the required solution of the trapped oil problem.

This study is aiming to introduce a novel combined EOR process, by employing the nanotechnology to improve a traditional water flooding operation. This will be achieved by involving and utilizing special surface-functionalised NPs in EOR operations, as these functionalised NPs have not been studied for EOR applications before, while the nanotechnology generally and functionalised NPs specifically, have been successfully presented in many manufacturing and science areas including drug delivery, catalysis substances, optical instruments, adsorbent, and water purification. Functionalizing the surface of NPs by chemical materials (functional groups; carboxylic acids CO_2H, carbonyls C=O, esters CO_2R, alcohols -OH, sulfonate acids SO_3H and amines NH_2), is a beneficial technique to increase the spreading stability of the NPs in different aqueous medias. However, interjoining forces such as the wettability alteration and disjoining pressure, will be studied and investigated as the main mechanisms and effective parameters in EOR. Consequently, have a straight impact on the oil recovery, which will be evaluated as a result of a core flooding performance.

Keywords:

Enhanced Oil Recovery, Nanotechnology, Functional groups, Functionalized NPs, Wettability alteration

2.14: Microfluidic Synthesis in an Advanced Flow Reactor: A Case Study of Silver Nanoparticles

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Abstract

Noble metal nanoparticles (NPs) with size/morphology-dependent properties present exciting opportunities in the fields of sensing, heterogeneous catalysis as well as cancer therapy. Therefore, morphology size and control of noble metal NPs are essential to achieve accurate adjustment of their physicochemical properties and performances. However, it is usually difficult to synthesize noble metal NPs with narrow particle size distribution (PSD), particularly on a large scale via a conventional batch method due to the inferior transport performance, scale-up effect and batch-to-batch variation.

In this work, we developed a microfluidic-based approach using Corning Advanced-Flow Reactor (AFR) for the continuous synthesis of metal NPs with a tunable particle size and narrow particle size distribution, taking silver NPs as a case. AFR was composed of three highly engineered fluidic modules, including a reaction module sandwiched with two heat transfer modules. The design of the reaction module introduced a series of heart-shape connected cells, which yielded excellent micromixing and mass/heat transfer performance. In addition, the large-scale production could be easily achieved by parallelly increasing the number of the reaction module.

It has been widely reported that the average particle size and PSD of noble metal NPs were closely related to the micromixing performance of a microreactor. Therefore, it was of vital importance to demonstrate the relationship between the average particle size and PSD of Ag NPs, and the micromixing performance of AFR to guide the continuous synthesis of noble metal NPs. The micromixing performance of AFR was investigated by Villermaux-Dushman protocol, and the effect of the micromixing performance on the particle size and PSD of Ag NPs was studied systematically. The segregation index (X_S) was defined to quantify the micromixing efficiency. X_S equaled to 0 for ideal mixing, while X_S equaled to 1 for total segregation. As the total flow rate increased from 1 to 3 mL/min, X_S significantly decreased, indicating the micromixing performance became much better. When the total flow rate further increased from 3 to 9 mL/min, X_S slowly decreased. Correspondingly, Ag NPs synthesized at the total flow rate of 1mL/min showed the widest PSD. The flow rate ratio was found to be another key factor affecting the micromixing performance, and thus the PSD of Ag NPs. This could be attributed to the different thicknesses of the reactant layers and strength of interfacial turbulence at different flow rate ratios. In addition, the effects of molar ratio of $NaBH_4$ to $AgNO_3$ and synthetic temperature were also studied.

Keywords: *Continuous Synthesis, Silver Nanoparticles, Corning Advanced-Flow Reactor.*

2.15: Nanoparticle Modified Polyacrylamide for Enhanced Oil Recovery at Harsh Conditions

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Abstract

Silicon dioxide (SiO_2) nanoparticles (NPs) have been recently proposed to boost the performance of polyacrylamide (PAM) for enhanced oil recovery (EOR) applications. However, SiO_2/PAM nanocomposites tend to agglomerate or even sediment under harsh conditions such as high temperature-high salinity (HT-HS), which greatly decreases the potential for future field applications. In this work, SiO_2 NPs were modified using (3-aminopropyl) triethoxysilane (M_SiO_2) to create positively charged active groups that enhanced a stronger interaction with PAM functional groups, leading to high dispersion stability. Three samples including M_SiO_2/PAM, SiO_2/PAM and NP-free PAM were synthesised *in-situ* via free radical polymerisation, and their thermal stability, rheological properties and the effect of aging time were studied. It was found that M_SiO_2 could inhibit thermal degradation of the polymer and safeguard its backbone to prevent the polymer molecule from rupture. As a result, M_SiO_2/PAM exhibited much better thermal stability in harsh environments. After 90 days of aging, SiO_2/PAM and NP-free PAM had 45 and 78% viscosity reduction; whereas only 10% reduction was observed in the case of M_SiO_2/PAM. Additionally, core-flooding experiments showed that M_SiO_2/PAM solutions produced more oil recovery than those from SiO_2/PAM and NP-free PAM solutions at HT-HS condition.

Keywords: *Enhanced oil recovery; Polymer flooding, Polyacrylamide; Silicon dioxide nanoparticles; High temperature and high salinity; Stability.*

2.16: TiO_2 based Nanocomposite Hydrogel for Solar Disinfection

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Abstract

Sol-gel chemistry was adeptly exploited to fabricate nanocomposite gels for solar disinfection to render clean drinking water, especially in the developing countries. The present research is a novel approach to acquire potable water by improving the adsorption or catalysis through exploiting the synergistic effect of three different notions; the high surface area and controlled porosity of xerogels, immobilization of photocatalytic Titanium dioxide (TiO_2) nanoparticles and red shift of absorption edge alongside high electron transport properties of carbon. The characterization and analysis through UV-Vis spectroscopic studies concluded the reduction in the bandgap (from 3.2 eV to 2.9 eV) of TiO_2, hence, these nanocomposites possess light absorption ability in the visible region of the electromagnetic spectrum. Moreover, the morphology examined through FESEM and EDX confirmed the predicted the structure and property profiles. Finally, the S_{BET} for surface area analysis and the reduction in dye concentration over time validated that these nanocomposites are potential disinfectants for the antimicrobial activity due to large surface area for maximum absorption of organic pollutants. Noteworthy advantage of these nanocomposites is the green synthesis approach and disinfectant was proved efficient after being sequentially used for a several number of cycles.

***Keywords*:** Photocatalytic degradation of dyes; Water; Disinfection; Porous gels; TiO_2 Nanocomposites; Green synthesis

2.17: Application of Nano materials for the treatment of Produced water

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Abstract

Water pollution is an acute problem in recent days, thus making wastewater treatment an important component towards sustainability. Regarding oil and gas wastewater treatment, several environmental problems have nowadays arisen, associated with an increase in oil and gas production activities and coupled with improper management of produced water and lack of compliance with environmental safety standards. All these have resulted to high levels of toxicity near oil and gas fields. The application of hybrid nanomaterials for the treatment of toxic compounds has not been effectively studied. Conventional methods of treatment i.e., physical, chemical and biological treatment designed to eliminate toxic contaminants from produced water leading to the generation of secondary pollution from one phase to another. Several studies on the application of nanostructured catalytic materials have made considerable progress, and it is fundamental to enhance the catalytic activity of these materials. Nano-crystalline titanium dioxide finds extensive applications in photocatalytic degradation of harmful organic compounds pollutants in and water. Here the effect of an environmentally friendly and thermally stable iron oxides when doped with titanium dioxide for the treatment of toxic organic compounds was investigated. The prepared nanoparticles were characterized using XRD, FTIR, SEM, and EDS which provided information about the catalysts' structure, chemical composition, purity, and morphology. The catalytic and photocatalytic activities of $CuFe_2O_4$ samples were tested and evaluated for the degradation of phenol using HPLC. CuFe2O4 nanoparticles shows a higher catalytic activity compared with TiO2 nanoparticles

Keywords: *Produced Water, photocatalysis, Nano-materials, Synthesis, hydroxyl radicals*

2.19: Investigating the Intermediate Regime of Granular Materials

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Abstract

Granular materials represent a large percentage of the materials handled and produced in the chemical and process industries. Such materials are widely used in powder-based unit operations such as granulation, drying and fluid catalytic processes [1]. The flow behaviour of those materials falls generally in three regimes: the quasi-static, the inertial and the intermediate regimes. The quasi-static (slow) regime, where the particle's stress is independent of the applied shear rate, is characterised by the formation, rotation and breakage of particles force chains. The inertial (rapid) regime is characterised by instantaneous and binary collisions between particles. The intermediate regime, which develops between the slow and rapid regimes, has recently become the subject of a number of numerical and experimental studies. In this regime the particle's shear stress is shear rate dependent and it has been observed in aerated bed configurations [3], where the gas velocity is lower than the minimum fluidisation velocity, Umf.

The work reported investigates the intermediate regime in an aerated virtual Couette rheometer that was previously developed in our lab [4]. This device is made of the FT4 Freeman aeration kit combined with a new 3D printed cylindrical bladed cell (6 blades) designed for this study. The 3D printed cell is 70 mm in height and 36 mm in diameter. The experimental procedure is as follows: the cell moves downward through the material placed in the FT4 cup until it reaches a fixed position. The cell is then rotated at different rotational speeds, and the torque, needed to move the aerated powder placed in the cup, is evaluated. The shear stress, τ, and shear rate, $\dot{\gamma}$, are computed from the recorded torque and the rotational speed, respectively. This new configuration was calibrated without aeration using a Newtonian fluid with a known viscosity [4]. It was also tested with aerated and non-aerated glass bead powders in the quasi-static regime [4]. The results previously obtained [4] are extended to higher U/Umf to investigate the intermediate regime. Experiments were performed on the aerated glass bead powder with a particle diameter of 0.08 mm and an aeration ratio ranging from 0 to 0.8 (below the minimum fluidisation limit); the shear rate was increased from 5 to 42 s-1.

Results showed that, for an aeration ratio lower than 0.6, the shear stress is independent of the shear rate over the studied range of shear rates, indicating that the powder is in the quasi static regime. For U/Umf higher than 0.6, the shear stress was found to be independent of the shear rate for shear rates lower than 25 s-1. For higher values of the shear rate, the shear stress was found to increase proportionally with the increasing shear rate, which indicates that the studied sample is no longer in the quasi-static regime. These first observations confirm the existence of the intermediate regime in aerated beds. Further measurements, including different particle diameters, will be performed to confirm and expand the first measurements and observations.

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Keywords: Granular material, Aerated bed, intermediate regime, particle's stress.

2.20: Influence of screw configuration on granule size distribution produced using twin screw granulator

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Abstract

Twin screw granulation (TSG) has been introduced over the last decade as a continuous process in granulation technology. This has the advantages of short and efficient processing times (energy efficiency), flexibility in operation and ease of change of screw configuration. Use of TSG as the means of continuous manufacturing is rapidly gaining grounds in the food and pharmaceutical industries.

The aim of this study was to assess the influence of screw configuration of the final size distribution of granules. This work involves the use of three different screw elements; conveying, kneading and chaotic to understand the formation of granules, under varying operational and formulation conditions namely; temperature and screw speed, binder percentage and blend ratio respectively. Calcium carbonate ($CaCO_3$) was used as the feed powder and polyethylene glycol (PEG) of molecular weight 4000 as the binder in percentages of 5%, 10% and 15%, under set temperatures of 60°C, 65°C and 70°C and screw speeds of 50rpm, 100rpm and 150rpm.

The samples were subject to characterization of physical and mechanical properties such as strength, size distribution, shape, etc. It was found that a screw configuration comprising 2 kneading elements produced the highest percentage (over 70%) of desired size range of granules followed by 4 chaotic elements and 2 chaotic elements. The narrowest and widest size distributions were obtained under chaotic screw configuration of 2 mixing elements and 4 mixing elements respectively, as will be discussed in the presentation. This work is ongoing to further explore the impact of screw configuration on the strength and internal structure of granules.

Keywords: *wet granulation, twin screw granulation, granule size distribution,*

2.21: Hydrodynamic Flow Focusing for Fouling-Free Production of Iron Oxide Nanoparticles

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Abstract

Micro/millimetre scale processes are increasingly utilized for the synthesis of micro/nanoscale materials with tailored properties, due to the excellent control of hydrodynamics, and enhanced heat and mass transfer. This work aims to utilize these properties of microfluidic devices for the production of monodisperse magnetic iron oxide nanoparticles (IONPs) while simultaneously avoiding fouling, which is one of the main problems when handling particles at these scales. For this purpose, a dual 3d-flow focusing microfluidic device was designed, manufactured and used for IONP synthesis via co-precipitation of Fe (II) and Fe(III) in an aqueous solution with a strong base. 3D flow focusing was achieved by using channels of different heights in the lateral streams. A separation stream between the reactant streams was employed to prevent fouling near the reactor entrance, which is a usual occurrence in microfluidic devices. The device design was driven by CFD simulations, in a model setup in COMSOL Multiphysics. The geometric parameters under scrutiny were the relative channel heights in a cross-shaped flow focusing junction. The simulations aided in identifying appropriate geometric parameters that would enable multiple steps of 3D flow focusing in a single device and result in a double co-axial flow: Iron salts solution flowing engulfed in a layer of water (separating stream) and another layer of the base solution. The device was manufactured from PMMA via milling. It was demonstrated to operate continuously for a long period without evidence of fouling, while without the intermediate stream fouling was almost immediate. A minimum flowrate of the separation stream was found necessary to achieve fouling-free operation. The flow pattern in the device (thickness of the focusing stream) was found to affect the produced nanoparticles by altering the transverse concentration gradients and resulted in a decrease of yield of magnetic iron oxide phases (magnetite and maghemite) in favour of non-magnetic ones. The effect of the separation stream in the particle synthesis was expected to be mitigated by reducing its flowrate. For that, an optimized 3D geometry was designed, modelled and manufactured via 3D printing. Current work aims to improve the understanding of the concentration gradient effect in particle synthesis, and improve the reactor performance.

Keywords: nanoparticles, microfluidics, CFD, flow focusing

2.22: Case Study: Packing and Filling of Powders at Pilot Scale

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Abstract

With packing and filling being the final stage of manufacturing before shipping to consumers, it is essential that the product contents are consistent and delivered according to marked weight. An understanding of product characteristics must also be carried out to ensure that no time loss occurs from equipment breakdown caused by poor material handling.

This presentation will tackle the work within the powders area at CPI's National Formulation Centre in a packing and filling line. This includes different modes of filling such as gravimetric and volumetric and examining their impact from batch to continuous operation. It will discuss process optimization to achieve consistent and accurate packing weight in line with regulations. Other areas to be presented include integration of process analytical technology (PAT) within the process to determine powder characteristics. Moreover, the future of the capabilities will be discussed such as work with other types of packaging to reduce use of plastics.

Keywords: *powders, pack and fill, characteristics, gravimetric, volumetric, weight*

3.1: Understanding Cleaning using Chemical Engineering

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Abstract

Cleaning is an essential step in many processes, whether to prevent the carryover of residual product between batches or to remove fouling deposits. Cleaning consumes large quantities of chemical agents, energy and solvents – particularly fresh water in the food and FMCG sectors – and is an exemplar of the food-water-energy nexus. Improving the sustainability of cleaning operations requires knowledge of how cleaning happens, which in many cases means understanding how a cleaning *solution* acts on a *soiling* layer formed on a *substrate*.

In the food and fast moving consumer goods sectors this is often a challenge as the soil layers are soft solids and are hard to measure in situ reliably and cheaply. This has led to the development of tools measuring various aspects of soil behaviour in real time, affordably, based on chemical engineering principles. This presentation will introduce these tools in the context of studying the cleaning of baked food deposits which are known to cause problems in domestic and commercial dishwashing machines. The deposits are generated from mixtures of starch, fats, carbohydrates and sugars, and take the form of a complex porous matrix.

The soils swell rapidly on contact with aqueous solutions. Measuring this swelling in an opaque environment can be achieved using fluid dynamic gauging, which is based on a technique developed for making heat transfer measurements. New variants of fluid dynamic gauging can capture the initial hydration and longer term swelling behaviour, as well as determine changes in the strength of the soil, aseptically, with accuracies better than ±10 μm. The effect of temperature, pH and flow of cleaning solution on the cleaning of the baked food deposits has been investigated and provides valuable insights into the cleaning mechanisms involved.

Surfactants are often used and the question to be answered is whether these agents act on the bulk structure of the soil, affecting cohesion, or at the soil-substrate interface, influencing adhesion. This was investigated using a controlled strain 'millimanipulation' device which allows the contribution from the two regions to be assessed. The results can also be used, with swelling measurements, to estimate the rheology (and changes therein) of the soil matrix on contact with cleaning solution, using computational fluid dynamics solutions.

Combining these 'physical' measurements with 'chemical' ones is essential to understand how the different components interact. The release of mobile oils from the soil matrix was quantified by imaging droplets which formed and grew on the soil-solution interface, using techniques familiar to those studying two phase flows. This fusion of results from chemical engineering approaches provides new insights into these complex, real problems.

Keywords: *Cleaning, Fluid mechanics, Mechanisms, Surfactant, Swelling, Tools.*

3.2: Waste Stream Recycling within Drug Substance Manufacturing to Improve Sustainability in the Pharmaceutical Industry

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Abstract

Sustainability and, more specifically, environmental protection has become increasingly important within the pharmaceutical industry over the last decade due to the climate crisis. AstraZeneca's environmental protection strategy aims to manage the environmental impact across all products and activities. It focuses on five main areas: product environmental stewardship, waste management, greenhouse gas reduction, pharmaceuticals in the environment and water stewardship. In 2020, AstraZeneca made the commitment to have a carbon negative value chain by 2030. Due to these ambitious targets, AstraZeneca is implementing novel processes to improve our products sustainability. One approach we are taking to this is the implementation of a Waste Stream Assessment (WSA) across all drug substance projects approaching commercial launch. The WSA fits into the waste management and greenhouse gas reduction categories for the environmental protection strategy. It is aiming to reduce the carbon footprint and process mass intensity (PMI) of drug substance development, two metrics for sustainability in the pharmaceutical industry. The WSA helps to increase understanding of waste streams and prioritises which waste streams could recover valuable product or where carbon emissions could be significantly reduced. This abstract presents the implementation and methodology of the WSA. It also presents a number of case studies to showcase how process modelling and lab work can be used to make solvent and product recovery a reality.

Keywords: *Sustainability, Pharmaceuticals, waste recycling*

3.3: CO_2 mineralisation of brines with regenerative hydrotalcites in a cyclical process

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Abstract

CO_2 mineralisation is a process that can store the CO_2 as a solid mineral permanently. Brines rich in alkaline earth metals present an opportunity to trap CO_2 in the form of insoluble carbonates. Moreover, this can be accomplished in this work, using flue gas concentrations of CO_2 and at near-ambient temperatures, eliminating the energy-intensive CO_2 capture step.

Alkali or pH-buffering substances to neutralise the acidification of brines caused by CO_2 dissolution is one of the primary costs that limits the technology deployment. Hence, we herein developed a process to remove chloride anions from brines by ion-exchange, namely hydrotalcites (HT), while avoiding the addition of alkali. These layered double hydroxides release hydroxyl groups in exchange for chloride, sufficiently raising the pH of brines by dechlorination to enable the precipitation of carbonates during CO_2 mineralisation. Moreover, the HT is recyclable for multiple usage by taking advantage of the 'memory effect' property.

Gaseous CO_2 and Na_2CO_3 solution were tested as the recharging agents, to replace the chloride anions from the spent HT interlayers and intercalate with HCO_3^- or CO_3^{2-}, followed by a calcination process to produce the reusable calcined-HT; the approach of gaseous CO_2 regeneration is newly proposed. It was found that the chloride removal efficiency remains over 70% after multiple cycles, and calcium utilisation efficiency of the brine carbonation process can surpass 90%. This unique cyclical closed-loop HT process presents a potentially more cost- and energy-effective approach to brine carbonation than our previous studies. In addition, the precipitated calcium carbonates are of sufficient quality for a variety of applications that can reduce the process cost and accelerate the progress of CO_2 capture, utilisation and sequestration.

Keywords: *Layered double hydroxide; carbon capture utilisation and sequestration; regenerative additive; dechlorination; alkaline brines; precipitated calcium carbonate.*

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3.4: Energy efficient recycling of thermosets

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Abstract

Thermoset materials are inherently difficult to recycle because their thermal stability and crosslink structure leads to difficulties with reprocessing. Thermoset elastomers are a flexible type of polymer produced by vulcanization. This process forms crosslinks between the polymer chains using either a sulphur or peroxide cure system. Most rubber products are made from these thermoset materials, containing a 3D chain network that cannot be easily recycled. In many countries waste tyres and other rubber products are burned for energy recovery, however this process is estimated to be only 37% efficient [1].

One key problem preventing the efficient recycling of sulphur-cured rubber is the difficulty in discriminating between the flexible C-S linkages that form the crosslinked network and the C-C bonds that makeup the polymer backbone. Therefore, when grinding and mechanically devulcanizing the 3D crosslinked network, the main chain C-C bonds are often damaged. Devulcanization of rubber can be achieved using either mechanical or chemical processes. Mechanical devulcanization processes such as solid-state shear milling (S3M) may transform waste rubber into a useable powder form with a reduced crosslink density [2,3]. This devulcanized powder can then be processed either as a filler material, a matrix material or as an elastomer phase of a thermoplastic vulcanizate [2,4–6].

This work investigates waste natural rubber products as well as waste cable shielding. Since these end-of-life materials were obtained from a recycling plant, they contain some impurities. In order to quantify these impurities as well as batch variance, SEM-EDX was used to analyse the elemental composition. By understanding the nature of the bulk waste material, we may seek to optimise the processing parameters for an energy efficient conversion to a value-added product. Producing the best possible mechanical properties with the minimum process energy is a key goal.

In order to understand how the S3M process affects the chemical crosslinks and main chain bonds, electron spin resonance (ESR) was used to investigate the radicals present in the devulcanized powders. Evaluating how chemical bonds are broken by the S3M process may allow us to optimise the devulcanization process. Additional work will consider statistical modelling of the flow of the waste material through the pan mill.

A more readily recyclable product can be produced by combining the natural rubber waste with a thermoplastic waste. The devulcanized thermoset can be converted to a thermoplastic vulcanizate by blending with a thermoplastic and dynamically vulcanizing [7,8]. Thermoplastic vulcanizates (TPVs) are the fastest growing elastomers to replace traditional thermoset rubbers [8]. They offer a significant advantage over thermosets in that they can be easily reprocessed by melt mixing.

Recycled materials were prepared using either a two-roll mill or by extrusion and their mechanical properties measured by tensile testing. Raman spectroscopy, SEM and rheology were used to characterise the final product. Our initial work focuses on improving the processing parameters to allow efficient revulcanization. Future work will consider the cure package used for revulcanization.

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Keywords: *Recycling, Elastomer, Thermoset rubber, Devulcanization*

3.5: Optimisation of cesium and strontium removal by ion-exchange column using natural clinoptilolite

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Abstract

Low grade natural clinoptilolite has been investigated for the recovery decontaminated water from nuclear waste effluents, especially for removal of cesium and strontium, by optimising elution in ion-exchange columns. The results found that 200 ppm concentrations of cesium could be removed for significantly longer times compared to strontium, where breakthrough for cesium and strontium was 600 and 50 times bed volumes, respectively. By reducing the concentration to 100 ppm, the strontium breakthrough was found to be 350 bed volumes, or around 7 times higher than for 200 ppm strontium. However, reducing column residence time from 30 minutes to 15 minutes resulted in a decrease of the breakthrough to only 50 bed volumes. The Thomas and Modified Dose Response (MDR) models were used in order to fit the breakthrough data and to estimate the maximum adsorption capacity (q_e). It was also found, as expected, that the q_e for cesium was higher compared to strontium for a 200 ppm dose, at 170.437 and 16.667 mg/g, respectively. Moreover, the q_e for 100 ppm strontium was estimated at 48.205 mg/g, which was almost 3 times higher than at a 200 ppm concentration. In contrast, reducing the residence time decreased the strontium q_e, to 14.644 mg/g. Both models displayed a good fit to all the breakthrough data with $R^2 > 0.9$, where MDR models tended to fit closer to most breakthrough data compared to Thomas model.

Keywords: *adsorption, adsorption capacity, cesium, clinoptilolite, ion-exchange column, strontium*

3.6: Modification of Bio-based PLLA to Improve Properties

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Abstract

Polylactic acid (PLA) is a bio-based biopolymer which is regarded as one of a number of promising candidates to replace oil based polymers in a range of commodity applications due to having properties comparable to oil-based polymers such as polyethylene terephthalate (PET). It can be synthesised from sugars derived from starch using plant-based sources such as corn, sugar beet or potatoes. There are however a number of challenges which currently limit the uptake of PLA as a commodity polymer, such as its low impact strength and low heat deflection temperature.

In this study, attempts were made to improve the properties of commercially available PLA using three routes; blending with other biopolymers, increasing crystallinity and by formation of a stereocomplex structure. For the blending route, a commercially available grade of PLA was melt blended with two biodegradable polymers in an attempt to modify its properties and processability. Binary and ternary blends of a PLA matrix with polybutylene succinate (PBS) and polycaprolactone (PCL) were produced with up to 30wt% loading. Mechanical (tensile, impact and flexural), thermal and rheological characterisation were used to quantify properties of the different blend formulations. Phase separation and miscibility were also investigated using scanning electron microscopy. Results showed that addition of both PBS and PCL caused a reduction in melt viscosity, elastic modulus and tensile strength, whilst causing an increase in impact strength. Analysis of morphology suggested that immiscibility was apparent, particularly at higher PCL and PBS loadings. Results indicated that optimum properties and miscibility was obtained when both of the additives at low loadings were blended with PLA.

Attempts to improve crystallisation rate were made by blending up to 15wt% of the D enantiomer PDLA to PLLA. Crystallisation was controlled by injection moulding samples into a heated mould and by annealing samples after moulding at a controlled temperature. Results showed that the addition of PDLA increased crystallisation rate, heat deflection temperature and elastic modulus of the polymer. A stereocomplex structure was also formed by melt blending a 50/50 mixture of PLLA and PDLA at optimised extrusion conditions. The resultant polymer was found to have a melting temperature significantly higher than conventional PLLA and heat deflection temperature also increase from around 65 to 130°C. Moulded samples were stiffer but had lower impact toughness than PLLA. These results demonstrate that a number of routes are available to improve the properties of PLLA through tailoring of blend structure and morphology.

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Keywords: *PLA, biopolymer, stereocomplex, crystallization*

3.7: Avoidance of the operational problem of Bed Agglomeration during Gasification of Barley Straw in Fluidized bed energy generation technologies.

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Abstract

Problematic lignocellulosic waste such as straw (around 5%wt of ash and low bulk density causing problems during reactors' feeding) cause defluidisation in fluidized bed energy generation systems. Such waste contain much higher amount of alkali and alkali earth metals (especially K). Potassium (K) for example interacts with the cheap and easy to find bed material (silica sand), leading to bed agglomeration operational problems which in turn results in pressure drop increase and loss of fluidisation due to eutectic mixtures creation. Leaching (water washing) the problematic inorganic constitutes from such type of waste reduces the tendency towards bed agglomeration of FB technologies commonly used in wasteto-energy plants. Untreated barley straw was fed to the fluidized bed reactor at temperatures ranging from 750 to 950oC and bed agglomerated. The de-fluidization operational problem became more prominent as the bed temperature increased. On the other hand, pre-treated barley straw didn't lead to any bed agglomeration during continuous operation and lowered gaseous emissions compared to raw barley straw. Leaching reduced also both K and chlorine (Cl) by almost 90% after leaching in the water as well as improved feeding of feedstock into the gasification system. SEM/EDX characterization of the bed material before and after de-fluidization indicated the nature of bed agglomeration phenomena and actual composition of the ash decoration on the surface of the bed material. The raw straw coating composition presented a high K content (50%wt) with low content of Si (15%wt). However, the SEM/EDX results of the bed material after gasifiying the leached straw didn't show any agglomeration by eutectic mixtures of very low concentration of K (< 2%wt) and Si (~70%wt). The latter enabled avoidance of the FB agglomeration operational problem and decreased the chances of forming eutectic mixtures.

Acknowledgments: Authors would like to thank the BRISK2 Project (Horizon 2020 Research and Innovation programme, grant: 731101) and EPSRC for co-funding parts of this project (EPSRC New Investigator Grant (former First Grant), grant number EP/P034667/1).

Keywords: Lignocellulosic biomass waste, Bed agglomeration, Leaching, Fluidized bed, Continuous process

3.8: Optimal electric vehicle charging schedule considering user travel behaviour and distributed energy resource availability

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Abstract

The devastating effects of climate change, and the role greenhouse gas (GHG) emissions play, have been widely acknowledged across the globe. In the United Kingdom, targets have been set to achieve a net-zero GHG emission by 2050 (Committee on Climate Change, 2019). With transport being the largest contributor to GHG in 2017, one of the scenarios outlined towards achieving this goal involves ‘extensive electrification, particularly of transportation and heating’ (Committee on Climate Change, 2019; Küfeoğlu & Khah Kok Hong, 2020). This directly involves a transition to electric-powered surface transport vehicles. At present, Electric Vehicles (EVs) benefit from capital subsidies and lower fuel and vehicle taxation. This, combined with other factors such as its increasing cost-competitiveness compared with traditional internal combustion engine-type vehicles, has led to a growing adoption of EVs. This EV growth has its impact on the power grid. Unregulated connections of EVs to the power grid can result in a substantial increase in aggregate demand, reduction in power quality, or an outright destabilization of the grid (Ahmadian et al., 2020; Xiong et al., 2017). There are, however, benefits. EVs act as additional energy storage devices as well as energy sources through vehicle-to-home (V2H) and/or vehicle-to-grid (V2G) services. This allows for peak load shaving, reduction in household energy costs and backup power supply during outages. It then becomes important that an optimal scheduling strategy be proposed to leverage these benefits whilst minimising the negative impacts to the grid.

This work thus proposes an optimal EV charging schedule for households considering the availability of EVs, stationary battery energy storage systems and/or solar power generation. Given a number of EV types and properties providing V2H services, as well as a number of different classes of EV user travel behaviour, the proposed optimisation model obtains the dayto-day charging schedule with the minimum cost based on available electricity tariffs and household energy demand data. Using real-world cases, the most cost-effective electricity tariff can be selected, with its associated charging schedule, for a particular household and/or EV user type based on the aforementioned considerations.

Keywords: Electric vehicles; Optimisation; Scheduling; Battery Energy Storage Systems; Renewable Energy

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3.9: Biogas Upgrade using biomass based physical Activated carbons

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Abstract

The problem of global warming and increasing energy demand can be addressed by the use of biogas but the high concentration of CO_2 in its composition decreases the heating value of the biogas, which hinders its use. Hence, in this work, we have attempted to upgrade biogas to bio methane by removing CO_2 using optimized physical (CO_2) activated carbons. Four different precursors including three biomass based (Spruce Sawdust, Miscanthus straw and wheat straw) and one municipal waste (Sewage sludge) based char samples were used to get efficient activated carbons having high CO_2 capture capacity and CO_2/CH_4 selectivity. The activated samples were denoted as ACXY (a-b-c) where AC: activated carbon, XY: precursor name (MS-Miscanthus straw, WS-wheat straw, SS-sewage sludge and SD-spruce sawdust), a: activation temperature in ^{o}C, b: heating rate ^{o}C/min and c: activation time in minutes. The selection of the optimum activated carbons was based on chemical (CHN analysis and FTIR spectra) and textural characterization (N_2 and CO_2 adsorption isotherms at 77 and 273 K, respectively) and performance testing of the sorbents for CO_2 and CH_4 capture capacity and selectivity. Chemical characterization showed the presence of nitrogen and O-H based functional groups in the samples, which usually helps for CO_2 capture. Textural characterization revealed that activation of the char samples increased the porosity and surface area with a dominant narrow micro pore and ultra-micro pore volume. More than 70% of the pore volume distribution of the narrow micro pores was in pore size < 0.7 nm and there was no distribution of pores above 1 nm. Performance testing of the activated carbons showed that ACMS and ACSD had the best CO_2 capture capacity. The capture capacity was linearly correlated with textural properties (BET surface area, total pore volume, micro pore volume from N_2 isotherms and narrow micro pore volume from CO_2 adsorption isotherms) and a poor correlation was established between capacity and CO_2/CH_4 selectivity. Instead, CO_2/CH_4 selectivity showed a good linear correlation with pore volume for pore size 0.52-0.54 nm. This pore range was found to be critical for CO_2 uptake at 298 K but CO_2 uptake at 273 K was having much broader range of critical pore size (< 0.8 nm). Hence testing and characterization of all activated carbons revealed that ACSD (860-10-30), ACMS (900-10-30) and ACWS (805-10-90) were the optimum ACs with CO_2 uptake and selectivity of 2.42, 2.23 and 1.84 mmol/g and 3.36, 3.17 and 3.17 respectively at 298 K and atmospheric pressure. Capture capacity of the Activated Carbons produced in this was higher than many commercial activated carbons and meets the upper limit of 2.3-2.5 mmol/g of good physical activated carbons [1-3]. CO_2/CH_4 selectivity usually lies in between 2-3 but values higher than three make them suitable for pressure adsorption[4], also values obtained in this work was close to the highest values reported in literature[5, 6].

Keywords: *Activated Carbon, Biogas, Bio Methane, Carbon Capture, Narrow Micropore, Selectivity.*

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3.10: Analysis of flexible operation of CO2 capture plants: Predicting solvent emissions from conventional and advanced amine systems

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Abstract

Due to the penetration of renewable intermittent energy in most energy systems, it is foreseen that CO2 capture plants will need to operate flexibly; in particular, to adapt to changes in flue gas load and stream conditions in order to efficiently abate CO2 emissions from power plants. The flexible operation can impose additional operational constraints on the plant, such as emissions permit limits, that cannot been addressed during the design stage. Accurate models to predict the emission of volatile components like mono-ethanolamine (MEA) and ammonia, which are linked to solvent evaporation and degradation, are of great importance. There is currently a lack of data and understanding of volatile emissions, which may lead to overdesign the capture plant and inherently large investments in mitigation technologies, which can probably be avoided with process optimisation.

This study helps to accelerate the process and development of a second generation solvent CESAR-1 (a mixture of 2-Amino-2-Methyl-1-Propanol (AMP) and Piperazine (Pz)) by providing missing experimental data and accurate models on volatile emissions during flexible operation. The AMP/Pz mixture is investigated and proposed as a new benchmark for carbon capture applications as it requires much lower regeneration energy and amount of solvent (in comparison to the well-studied MEA solvent), which may lead to lower solvent emissions and solvent degradation (Kvamsdal et al., 2011; Mangalapally and Hasse, 2011). The experimental data of the AMP/Pz/H2O (CESAR-1) are obtained during the transient operation of the RWE capture pilot facility at Niederaussem. The experimental data resulted from a parametric study based on single step perturbations of the most relevant plant variables that have an impact on solvent emissions. A mathematical model developed in Aspen Plus is used to predict the capture plant performance, including solvent emissions, at steady states of the transient scenarios. In addition to the steady state predictions, second order response functions are used to evaluate the dynamic response of solvent emissions during single step changes of plant parameters (Moser et al., 2020). The following step response function (Ogunnaike, 1994) is used to evaluate the dynamic response of solvent emissions

$$y(t) = y_0 + KM\ [1 - (\tau_1 - \xi\ /\tau_1 - \tau_2)e^{-(t-\vartheta)/\ \tau 1} - (\ \tau_2 - \xi\ \tau_2 - \tau_1\ )e^{-\ (t-\vartheta)/\ \tau 2}\ ],$$

where where y_0 represents the initial value of the response function $y(t)$, K is the steady-state gain ($K = \Delta y/\Delta u$), M denotes the magnitude of the input function $u(t)$, τ is the time constant, ϑ is the time delay, ξ refers to the lead-time constant, and t is the time.

Future work aims to develop a dynamic mathematical model to predict capture performance in transient scenarios considering mass and heat transfer in the absorption and stripping columns in the AMP/Pz/CO2/water system. The mass transfer will be described by the two-film theory and rigorous rate-based approach (Gáspár et al., 2011; Kvamsdal et al., 2009). The performance of the proposed model will be evaluated using the obtained experimental data and the results obtained for the step response functions. This model will provide measurable improvements in the environmental performance of post-combustion capture plants and the integration of costeffective amine emissions control systems. Such models are also essential for eliminating the uncertainty in the scaling-up design of a capture plant.

Keywords: *CO2 capture; flexible operation; solvent emissions; predicting emissions; pilot plant data; dynamic testing.*
Acknowledgement:The authors would like to thank ACT ALIGN-CCUS Project (No 271501) for funding this study. ACT ALIGN-CCUS project has received funding from RVO (NL), FZJ/PtJ (DE), Gassnova (NO), UEFISCDI (RO), BEIS (UK) and is co-funded by the European Commission under the Horizon 2020 programme ACT, Grant Agreement No 691712; www.alignccus.eu.

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3.11: Kinetic evaluation of CO_2 adsorption over micro and mesoporous activated carbons produced from low-value coal tar distillation products

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Abstract

Adsorption-based carbon capture processes are considered as one of the most promising technologies to reduce CO_2 emissions. Amongst the different solids that are considered Activated Carbons (ACs) have shown low regeneration costs, high surface area and micropore volume and a good CO_2 capture capacity. Moreover, in previous studies, new ACs (synthesized from low-value coal tar distillation products) have been tested for CO_2 capture under specific postcombustion conditions [1]. These new ACs were divided in different families based on their textural properties; i.e.: micropore carbon gels and ordered mesoporous carbons. Those findings highlighted the possibility to use those materials as the obtained carbon capacity values under realistic conditions overpassed those values reached by commercial ACs. However, for scaling up the process, further research is needed to establish the dynamic behavior of the material and the kinetic mechanism that is followed in the adsorption process.

In this work, a deep kinetic model evaluation of CO_2 adsorption was done, considering the micropore activated carbon gels and ordered mesoporous carbons, synthesized from low-value products, that show the highest CO_2 capture capacities. To carry out this study six temperatures, between 25 and 150 ^oC, were consider Furthermore, six different kinetic models were evaluated: first, second and n-order, Langmuir, LK1 and LK3.

It was determined that in all cases, the kinetic model was irreversible, independently of the type of porous structure that the material presents. Also, it was determined that in most of the cases the adsorption follows a n-order model, being close to a first order. This finding implies, conversely to previously reported models, that the adsorption of the CO_2 molecules on the AC materials is heterogeneous, taking place over one and two active sites, with more influence the adsorption over one site. Furthermore, it was concluded that in some cases (mainly in the high microporous AC gels) the CO_2 adsorption process follows a two first order step process, being the first step a transit state before the real adsorption one. In all cases, the calculated activation energy (Ea) for the process corroborated that the CO_2 capture (irrespective of the model) is a physisorption process, as Ea < 30-40 kJ/mol [2].

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Acknowledgments

Financial support from the European Commission under the “Research Fund for Coal and Steel (RFCS)” Programme (Project No 709741) is gratefully acknowledged.

Keywords: *Adsorption/Desorption, Activated carbons, coal-tar distillation, Kinetic models, ordered porous structure.*

3.12: Dynamic behaviour of a single polypropylene particle in bubbling fluidised bed reactors

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Abstract

Thermochemical conversion in fluidised bed reactors shows a long record of successes on both laboratory and industrial scales. Despite the favourable mixing features of fluidised bed reactors, segregation and self-segregation of fuel particles can take place. At high temperatures the volatile content is released in form of bubbles which generally exert a “lift” effect on the particle itself, by dragging it up to the bed surface. Such phenomenon leads to high release of volatile matter into the freeboard and limited mass and heat transfer with catalyst particles in the bed inventory. This issue is particularly relevant during thermochemical conversions of material with a high content of volatile matter, such as biomass, plastics and RDF (Refused Derived Fuel).

The aim of this work is to investigate the behaviour of a single reacting polypropylene sphere in a hot fluidised bed reactor by means of advanced X-ray imaging techniques. The analysis was undertaken at different operating conditions and sample densities to closely mirror industrial applications. Furthermore, with the help of an online gas analyser, it was possible to measure the rate of the gas produced in the temperature range of 500-700 °C at both combustion and pyrolysis conditions. Pieces of lead were inserted into the polypropylene particles to make them visible upon the x-ray irradiation and to vary the sample density. The X-ray technology allows a better understanding of the segregation in fluidised bed reactors by characterising the fuel particle motion with high precision. Information regarding the fuel particle location within the fluidised bed reactor can represent a starting point for the development and validation of mathematical models, which describe the segregation behaviour of solid fuels during the thermochemical conversions. These predictions are of prime importance for the design of industrial scale reactors.

The results from the X-ray imaging showed that this phenomenon was hindered for high particle densities. As a consequence, heavier plastic particles (e.g. PVC) tend to have a longer residence time in the bed, with potential advantages gained from more efficient mass and heat transfer with the fluidised bed. Moreover, experiments have shown that the segregation of the polypropylene particle to the bed surface is limited under pyrolysis, and more pronounced during combustion condition. It was observed that when pure nitrogen is used as fluidising medium, plastic particles are more likely to reside in the bed until complete conversion into gas. On the contrary, when the same flowrate of air is used, the oxygen present in the emulsion phase greatly enhances the generation of gas species by reacting with the volatile material released from the plastic polymer. This results in more vigorous bubbling and potential entrainment of fines and char in the gas products, which limit conversion efficiencies.

The same process can be adapted and engineered for the conversion of non-recyclable plastic waste usually present in RDF, as well as the biodegradable fraction.

Keywords: *Fluidised bed; segregation; devolatilization; thermochemical conversion; plastic waste; X-Ray.*

3.13: Upcycling of Elastomeric Waste Residues into Valuable Acoustic & Thermal Insulation Materials

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Abstract

The research described in this presentation demonstrate how elastomeric waste particulates (remnant from the reprocessing of tyres and automotive elastomeric bumpers, upholstery, etc.) can be transformed in porous structures than insulate against noise (open pores structures) and/or reduce heat loss (close pores structures). The transformation uses binders that react chemically with water to produce CO2 which then foam the mix binder-particulates. By controlling the reaction kinetics open or close pores can be formed. The talk will also describe the structural (porosity, pore distribution, tortuosity, elasticity) and functional (noise absorption and thermal conductivity) properties measurement method. In addition, we will present models used to underpin the measurements.

3.14: Development of an Automated Gas Phase Catalytic Microreactor Platform for Kinetic Studies

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Abstract

Flow microreactors have been proven as an effective experimental tool due to superior mass and heat transfer, improved safety and low material consumption. As such, they enable isothermal kinetic studies with minimal material resources. Ease of automation and integration with online analysis allows a large amount of experimental data to be generated rapidly. An automated system based on a flow micropacked bed catalytic reactor was developed in this work to conduct pre-planned experiments.

The microreactor was fabricated using photolithography and deep reactive ion etching of a silicon wafer. Anodic bonding was used for sealing the silicon to a glass cover. Isothermal operation was possible owing to the microreactor high surface to volume ratio. The main microreactor channel width was 2 mm and depth 0.42 mm. Serpentine channel between the microreactor inlet and the main channel aided the mixing of the gaseous feed. Methane combustion on Pd/Al_2O_3 catalyst was selected as reaction to test the performance of the developed automated system. The feed consisted of 5% CH_4/He, O_2 and N_2 as internal standard. Online Gas Chromatography (GC) was used to perform analysis of the outlet stream. The experimental system was monitored and controlled by LabVIEW. Computation of GC results was done by a Python script that communicated with LabVIEW through the Python integration toolkit. Safety measures with respect to temperature and pressure were included in the automated platform.

Temperature difference was found to be < 3°C at operating temperature of 350°C across the packed bed. The reproducibility of the system was ascertain with relative standard deviation of 2% at higher conversion (74-94%), and 10% at the lowest conversion (6%). Difference in carbon balance of reactant and product was < 3% within the experimental conditions investigated. Methane conversion observed at 300°C was 22.3 and 22.5% for a reaction time of 40 and 200 minutes respectively, which inferred good catalyst stability. Within each experimental campaign, the system adjusted the process variables (methane concentration, oxygen-methane ratio, temperature and total flowrate) and collect information on the experimental composition of the product stream (via GC) in a continuous mode, when running a set of factorial experiments without user intervention. The platform will be used for kinetic model identification to discriminate among possible models and estimate the set of kinetic parameters of each potential model.

Keywords: *Microreactor, automation, methane.*

3.15: New Strategies for Sustainable Synthesis of Bio-Derived Chemicals through Coupled Dehydrogenation/Hydrogenation Processes: A Fascinating Challenge

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Abstract

Sustainability is a critical problem facing the chemical sector, where the development of atom efficient continuous processes based on renewable feedstocks is key to the application of "green chemistry" principles. Hydrogenation, a core catalytic reaction in synthetic organic chemistry (30-40% processes in the fine chemical industry), is typically operated in batch mode using excess of pressurised (5-100 bar) *non*-renewable H_2 (12 kg CO_2 generated per kg H_2). We have set out the development of a technology that can replace this traditional catalytic hydrogenation route by an atom-efficient continuous-flow alternative operated at ambient pressure. The process involves coupled dehydrogenation with hydrogenation directed at the conversion of renewable bio-sourced materials over novel heterogeneous catalysts. Hydrogen generated (*in situ*) through (*non*-oxidative) alcohol dehydrogenation is utilised in the hydrogenation of an unsaturated/oxidised functionality. Two valuable products are obtained in a single-pot process with enhanced yield (*i.e.* zero waste) and improved process safety (*i.e.* absence of external pressurised H_2 supply).

Catalyst design is critical and requires two types of active sites (for hydrogen production and utilisation) that must be maintained separated but in close proximity to facilitate selective conversion and hydrogen transfer. We have adopted heterogeneous Cu/Au nano-catalysts in (i) oxide supported monometallic Cu systems with modified Cu^+/Cu^0 content, (ii) physical mixtures (of monometallic Au and Cu) and (iii) Cu-Au bimetallics. Catalyst optimisation has involved a systematic evaluation of: (i) support redox/acid-base properties and metal (ii) size and (iii) oxidation state/charge density. Active site properties have been examined using a range of surface science techniques (*i.e.* elemental analysis/AAS, BET, H_2-TPR, H_2 chemisorption, CO_2-TPD, XRD, HRTEM, HRSTEM-EDX, TGA and XPS measurements) that provide critical information in terms of bulk/surface composition, geometric/electronic properties and adsorption capacity. The sustainability of the coupling process has been quantified using the green metric environmental factor (E-factor, $kg_{waste}\ kg_{product}^{-1}$). Our results demonstrate the feasibility of innovative coupling catalytic dehydrogenation (as a source of reactive hydrogen) with hydrogenation. We prove catalytic synergy in the coupled system and the simultaneous production of a range of high value products (*e.g* 2-butanone, furfuryl alcohol, styrene). Moreover, we demonstrate orders of magnitude enhanced H_2 utilisation, elevated selective hydrogenation rate and a significantly lower E-factor relative to conventional hydrogenation. Our coupled system circumvents the use of compressed H_2 from *non*-renewable sources with important safety and long term supply implications for large scale production.

Keywords: *coupling, dehydrogenation/hydrogenation, heterogeneous catalysis, one-pot continuous process, sustainability.*

3.16: Funnelling strategy for production of a single-component chemical from lignin

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Abstract

Lignin, a main component of lignocellulosic biomass accounting for 15%-30% by weight and 40% by energy, is holding a great potential for the production of aromatic chemicals but is still not sufficiently used in biorefineries. Transformation of lignin into value-added aromatic chemicals is hampered by the complexity of monomeric products obtained from lignin depolymerisation.

The depolymerisation of lignin has been intensively investigated. Among various methods, reductive lignin depolymerisation is able to afford a much higher yield of aromatic monomers. For example, starting from birch wood, the total monomer yield reached as high as 46%, with syringyl- and guaiacyl-type phenolic compounds as the main components. Even higher yield of monomers comprising mainly guaiacyl- and syringyl-compounds with 4-ethyl and 4-propyl substitutions were achieved more recently from poplar wood lignin with a formaldehyde pretreatment step. However, because lignin is composed of three types of substituted phenolic monomers, a mixture of structural similar phenolic compounds with different substitutions is resulted from reductive lignin depolymerisation. The efficient transformation of this mixture into an easily purifiable, single-component, value-added chemical remains challenge.

This talk will discuss a few advances of applying funnelling strategy to design and optimise catalytic conversion routes for the transformation of lignin or lignin derived monomer mixtures into a single-component chemical, such as phenol[1] or terephthalic acid[2].

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2. Song, S., Zhang, J., Gözaydın, G. & Yan, N. Production of Terephthalic Acid from Corn Stover Lignin. *Angew. Chemie - Int. Ed.* **58**, (2019).

Keywords: *lignin; aromatic chemical; funneling strategy*

3.17: Microalgae technology for wastewater and waste treatment

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Abstract

Achieving Carbon Dioxide (CO_2) mitigation targets for the wastewater and waste industry will require substantial changes in delivering public services. In the UK, retrofitting existing plants with new photosynthetic biological routes could be financially more viable than changing complete infrastructures [1]. Globally, enabling sustainable wastewater treatment technologies would help reduce the 6.6 million people lacking access to adequate sanitation technologies. The cultivation of microalgae provides a photosynthetic route to reduce CO_2 emissions, increase nutrient removal and the recovery of valuable products. This presentation will summarize the innovative work published in the last two years from microalgae cultivation, to their separation and extraction of valuable biocompounds [1-6]. A simple and robust microalgae kinetic model was developed for application in the prediction and control of algae cultivations. Results demonstrated that it is possible to integrate wastewater and landfill leachate treatment with the production of microalgal biomass [2] and that a kinetic model we could accurately predict microalgae growth, wastewater nutrient removal, and changes in the culture media pH [3]. Biomass productivity of the algae culture was associated with an exponential increase in the media pH, which led to ammonia volatilisation and decreased carbon intake. It was found that the optimal pH for the microalgae culture was 8.1, at which point microalgae could achieve about 99% carbon fixation efficiency. To ensure constant pH in the microalgae growing system, immediate removal of the OH^- generated is needed, which could be facilitated by injections of 1.14 g CO_2 and 0.067 g OH^- per gram of produced algae when using NH4+ nutrient [3]. Microalgae harvesting using ozone flotation has been shown to achieve a high efficiency. Best results were obtained with a flow of 0.6 L/min achieving 88.5% efficiency, increased biomass oxidation, destabilization of microalgal cells (zeta potential 3.17 mV), highest protein release (46.7 mg/L) and, a demonstrated efficiency of proteins in reducing bubble coalescence [4]. Ozone flotation also pre-treated microalgae reducing, at least, 92% the solvent waste and 80% the extraction time [5]. Further processing the separated microalgae through hydrothermal liquefaction produced bio-crude yields 14–16%w with low nitrogen (4.55 and 3.19%) and oxygen (4.77 and 7.85%) content [6]. With this, an overall perspective in the use of microalgae for wastewater treatment is given which could help reduce CO_2 emissions and expand sustainable wastewater treatment.

Keywords: *cultivation kinetics, ozone flotation, carbon dioxide, microalgae, hydrothermal liquefaction.*

Recent Publications:

[1] **Velasquez-Orta SB**, Heidrich O, Graham DW. **Energy use and carbon emissions across a English wastewater network**. *Institute of Water Journal* 2019, **3**, 17-23.
[2] Hernandez-Garcia A, **Velasquez-Orta SB**, Novelo E, Yanez-Noguez I, Monje-Ramirez I, Orta Ledesma MT. **Wastewater-leachate treatment by microalgae: Biomass, carbohydrate and lipid production**. *Ecotoxicology and Environmental Safety* 2019, **174**, 435-444.
[3] Eze V, **Velasquez-Orta SB**, Hernandez-Garcia A, Monje-Ramirez I, Orta-Ledesma MT. **Kinetic modelling of microalgae cultivation for wastewater treatment and carbon dioxide sequestration**. *Algal Research* 2018, **32**, 131-141.
[4] Alves Oliveira G, Monje-Ramirez I, Carissimi E, Teixeira Rodrigues R, **Velasquez-Orta SB**, Chávez Mejía AC, Orta Ledesma MT. **The effect of bubble size distribution on the release of microalgae proteins by ozone-flotation**. *Separation and Purification Technology* 2019, **18**, 340-347.
[5] Gonzalez-Balderas RM, **Velasquez-Orta SB**, Valdez-Vazquez I, Orta Ledesma MT. **Intensified recovery of lipids, proteins, and carbohydrates from wastewater-grown microalgae Desmodesmus sp. by using ultrasound or ozone**. *Ultrasonics Sonochemistry* 2019, ePub ahead of print.
[6] Nava Bravo I, **Velasquez-Orta SB**, Cuevas-Garcia R, Monje-Ramirez I, Harvey A, Orta Ledesma MT. **Bio-crude oil production using catalytic hydrothermal liquefaction (HTL) from native microalgae harvested by ozone-flotation**. *Fuel* 2019, **241**, 255-263.

3.18: Development of Oil Spill Monitoring Sensors Using Polymer-based Materials

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Abstract

Detection and control of petroleum contaminants resulting from oil spillage pollution activities to the environment remain a major challenge to both developed and developing countries. Generally, the crude oil spill discharge to the environment is regulated and one of the key parameters used for compliance monitoring is the measure of oil concentration. Environmental laws require oil companies to keep oil spill total hydrocarbons concentration at 50 mg/kg soil (50 ppm). Mostly, soil analyses for oil spillages use the standard gas chromatographic methods, but these methods are expensive, require high expertise and not suitable for in-situ analysis. This study was conducted to evaluate the possibility of developing low power and inexpensive chemi-resistive material based sensors for in-situ detection of hydrocarbons in soils. Contaminated soils obtained at different depths from different oil spillage sites were extracted using Soxhlet technique and analysed by gas chromatography-flame ionization detector to determine types of hydrocarbons and their concentrations, as they are required to be detected by chemiresistors. The results recorded carbon numbers ranging from C8 – C36 with varying concentrations up to 20125 mg/kg at different sampling sites. Composites of non-conducting polymers (Poly(methyl methacrylate) (PMMA) and Polyvinyl chloride (PVC)) and conductive filler (carbon black) were prepared to make polymer-based sensors. The films were dried to evaporate the solvent and the morphology of the films was characterised using scanning electron microscopy (SEM). The impact of carbon concentration and geometry on the measured resistance of the polymer composite to hydrocarbons was determined. The optimum response was found to be with 10% w/w carbon black (CB) with 90% w/w polymer. Three sets of polymer-based sensors CB-PMMA, CBPVC and CB-PMMA+PVA were constructed by depositing thin films of a carbon black/polymer onto interdigitated electrodes and investigated. The CB-PMMA sensors showed much higher responses when exposed to range of hydrocarbons with varying sensitivities compared to the other two, however, the three sensors detected diesel range hydrocarbon concentrations up to Eicosane (C20) more than the existing devices [3]. The sensors responses to the EPA maximum concentration (50mg/kg soil) limits are large (resistance changes), fast (90% in less than 1s), reversible and selective, hence validating high adaptability of this method. The underlying mechanism of this high sensitivity of sensors might be due to the strength of the hydrophobic interactions between the polymer and the hydrocarbons.

The findings reported here expand the potential applications for inexpensive composite thin-film conducting polymer-based sensors for oil spillage monitoring.

Index Terms — Polymer, oil spill, petroleum hydrocarbons, polymer-sensor

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4.1: Hybrid tutorial- lecture-computer cluster style for engineering mathematics

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Abstract

The integration of a variety of techno-based activities improve leaning outcomes and student engagements. The application of electronic toolkit, encompassing computer lab among tutorials added a touch of modernity and ease of use on the go, with the added benefit of quantifying what students already knew about the subjects in question.

Here, shared and discussed the implementation of computer labs in teaching and learning process to assess and engage 230 undergrads at the Department of Chemical Engineering and Analytical Sciences, The University of Manchester, pertaining to Engineering mathematics.

A transferable experience in terms of teaching math in a computer-based cluster room was applied where every student involved in the gradual unfolding complexity of the course in an adapted problem-solving fashion. Calculus and statics based chemical engineering mathematics have been taught in computer labs by employing Excel to enhance student skills to find solutions for difficult problems, Excel can significantly simplify the understanding of pure calculus and statistical principles and can considerably reduce students' misunderstanding in applying calculus and statistical principles

The feedback from the students was remarkable, and these changes not only increased student engagement, but also helped me hone my teaching skills and thus further work on these learning aids will be in progress.

Keywords: Engineering mathematics, computer lab, Excel, tutorial

4.2: The use of real world problems as an educational tool in Biochemical Engineering and related disciplines

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Abstract

Due to changes in societal needs for medicine, food, technology and energy, there is a rising demand for universities to produce Biochemical and Chemical engineering graduates that are well equipped to address these issues. Future engineers will need to be leaders, able to create strategic vision, work well with other scientists and engineers, effectively communicate their findings with audiences of various expertise and implement economically and ethically viable solutions. This poses the need to develop effective teaching and learning strategies that incorporate the technical *and* professional skills required to produce such engineers.

Traditionally, the approach to learning in higher education has been teacher-centred and technical-content driven, placing the onus on the educator for the student's learning and leaving little room for the development of professional skills. Over the past two decades, the requirement for broadening of the curriculum has been highlighted by a number of stakeholders including industry, professional institutions, accreditation bodies and government. All have emphasised the need for a reform in engineering education that encompasses a whole set of transversal skills, from the ability to think critically, to working in teams, socio-economic considerations, sustainability and ethics, all built on deep technical understanding.

To address this challenge, the UCL Faculty of Engineering Science undertook a major review and revision of all its undergraduate educational programmes and after extensive consultation with various stakeholders, the Integrated Engineering Programme (IEP) was introduced across the faculty in September 2014. All students enter discipline-specific routes on the IEP but share a common framework of real world problem-based learning experiences (Scenarios) and interdisciplinary collaboration (The Challenges) that strengthens the technical understanding and threads throughout their degree.

As early as the first term of Year 1, Biochemical Engineering students work with Chemical Engineering and Biomedical Engineering students in interdisciplinary teams in order to solve a pressing global issue; the manufacture of an effective vaccine to eradicate tuberculosis in Uganda. The concepts of problem-based and design-based learning are used by the educators to guide the students through the project of creating a small-scale bioreactor, to simulate the best possible conditions for vaccine production and carry out scale-up studies. This Challenge allows for the development of technical understanding of the biological make up of a vaccine as well as the engineering theory behind bioreactor design and operation. It also allows for practical lab experience that the students use to create their small-scale bioreactors, as well as independent and collaborative research skills that the students use to facilitate their experiments. The Biomedical Engineers contribute expertise in the creation of probes for monitoring conditions in the bioreactor, while the Biochemical and Chemical engineers contribute expertise in optimising bioreactor mixing and heat transfer.

The interdisciplinary nature of The Challenges and the use of real world problems as a tool for educating our undergraduate students has proven successful in addressing the need to produce future engineers that possess transversal skills. This approach is one that we believe to be widely applicable and relevant to other IChemE accredited institutions.

Keywords: *Biochemical Engineering education, interdisciplinary learning, technical skills, professional skills, problem-based learning, design-based learning.*

4.3: How students work in project teams

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Abstract

In engineering education, teamwork is extremely common as it helps to prepare students for their future professional careers. Additionally, groups are the perfect setting where students normally have to deal with different situations; disagreements, shared responsibility and discussions that promote learning through collaboration. Despite the fact that teamwork is widely used in engineering education settings, supporting students adequately in their skills' development is difficult to achieve in practice. In some instances, there is an expectation that by the simple fact of putting students to work in teams they will develop these skills. In order to provide adequate support to students in their teamwork skill development, there is a need to understand first how students actually manage their own work in the team.

This work looks at a group of six students of the third year of chemical engineering program working in a project-based learning environment. In their project students have to manage their own team effort loosely supported by the tutor. The study uses a body of video and audio footage of project meetings while the teamwork in the completion of a conceptual design project. The transcription of the oral speech done has served as the principal corpus to carry out the analysis, and build a scheme model associated with the development of share social-regulation of learning processes. The preliminary analysis of the data identifies as key elements the way students organise the different activities and tasks, manage their time and deal with the different situations that could arise along with their meetings. The current results show that the students in this team have in-depth discussions and share knowledge with a strong tendency to seek consensus in the decision-making aspects of the project. At the same time, individuals look for social approval from team members. Also, the team prefers to have a 'Laissez *faire'* leadership as opposed to a single leader or different leaders over a period of time.

These results help us understand how students manage their team themselves in order to progress their team effort and how they develop autonomy when working without the direct supervision of a lecturer or tutor. These are beneficial in considering teaching practices that can support and foster students self-regulatory behaviour in teams.

Keywords: *Project-Based Learning, Autonomy, Self-regulation*

4.4: An investigation into the use of the Microsoft Office 365 toolkit to manage group projects in Undergraduate Chemical Engineering

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Abstract

This is a template document to guide authors in writing their extended abstracts. Abstracts are limited to a maximum of 500 words. The authors will be required to present an extended summary of their study including their findings, conclusions and outcomes.

Group projects are a key aspect of all undergraduate chemical engineering programmes, driven by a professional body requirement to mirror industrial practice. At Teesside University, this requirement is met by provision of a group project at each level of both BEng and MEng programmes. Whilst it is important to assess the technical competency of students within these group projects, the projects also allow for assessment of organisation, project management and group working skills.

The typical cohort of undergraduate chemical engineers at Teesside University is such that there are a number of students who are enrolled as Part-Time with a day-release timetable, as well as students who have significant commitments and responsibilities outside the academic environment. The diverse nature of this cohort makes group work a challenging (and often contentious) aspect of the student experience.

The IChemE under its 2024 strategy is actively promoting the increased use of digitisation and technology to enhance engineering training. It is therefore serendipitous that this drive coincides with the launch of Teesside University's Future Facing Learning initiative. As a part of this initiative, all new undergraduate students are issued an Apple iPad and access to a range of educational software applications. This work presents the authors' efforts to comply with the IChemE's strategy by taking advantage of the unique technological provision of Teesside University to improve the group-working environment.

The applications used in this study include Microsoft Teams and Microsoft OneNote. At present all students up to (and including) Year 2 have been issued both software and hardware, whereas students in Year 3 and Year 4 have full access to the software only. The perceived student-focused advantages of using this toolkit include added flexibility within the group-working environment (using the collaborative features of MS Teams and MS OneNote) and support for more inclusive practice (using the accessibility features of both the software and hardware provided). For academics, use of the toolkit promotes engagement from all students, and the generation of a virtual logbook in MS OneNote promotes increased data security without the storage concerns brought on by physical logbooks. It is also of note that MS Teams is increasingly being used in the industrial sector.

The study detailed here has been conducted in two parts: a testing phase and a trial phase. In the testing phase, volunteers from all years of the programmes have worked in simulated groups to establish the capabilities and limitations of the software on a range of devices, including desktop PCs and the university-provided Apple iPads. In the trial phase, Year 3 students on the BEng and MEng Design Projects have trialled the use of the software to manage their project teams and activities.

This work presents the findings of these initiatives, with qualitative and quantitative results from both students and academics. It is envisaged that the results of this study will be used to inform the roll out of toolkit in other group projects, both in chemical engineering and in other disciplines within the university.

Keywords: *education, group work, management, digital learning enhancement.*

4.6: Teaching with Technology: Investigation of online assessment software, WeBWork, in an introductory probability and statistics course

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Abstract

Online software systems are extensively used to give students practice on course content, especially in mathematics and physics courses. They offer instant feedback, and several of these systems are open source or very economical compared with hiring graders for traditional paper and pencil–based homework (PPH). In this article, the authors evaluate WeBWorK (WW), an online software tool, in an introductory course on probability over two semesters. WW is compared with PPH by measuring student perception, average time spent on a problem, collaborative work outside of classroom, resilience, self-efficacy, and exam performance. The authors find that except for working in groups on homework, students perform similarly on all the aforementioned aspects in both PPH and WW. The authors also suggest potential strategies to improve student understanding and learning while using WW and recommend the use of WW in mathematics-oriented courses. Keywords: Formative assessment, Online, WeBWork, Mathematics, Engineering, Self-efficacy

4.7 Kitchen Chem Eng: Teaching Equillibrium Stage Processes Using Classroom Demonstrations

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Abstract

We present a simple live classroom demonstration for illustrating the idea of an equilibrium stage process which is commonly considered one of the defining concepts that distinguishes chemical engineering from other related disciplines in science and engineering. The proper understanding of such processes is important for the design and analysis of efficient separation processes but can be intellectually very challenging for first or second year undergraduates.

McCabe-Thiele and Ponchon-Savarit are classical graphical solution techniques for calculating the number of stages required for distillation columns and similar methods exist for gas absorption and multi-stage solvent extraction. These techniques involve ‘stepping off’ between an equilibrium line and an operating line, the latter derived from a mass balance between adjacent stages.

In this presentation we use £10 electronic balance and a plastic bottle of fizzy water to demonstrate the stepping between the operating and equilibrium lines to a live audience in an interactive way. The bottle is repeatedly sealed, shaken up (to reach Henry’s Law equilibrium between gaseous and dissolved CO2) and the cap is loosened to vent the headspace and reduce its pressure back to atmospheric.

As well as presenting the method, we will also present results from its deployment for second students studying the Separation Processes module in Chemical Engineering at the University of Chester.

Keywords: *Equilibrium stage processes, future learning and teaching.*

4.8: A cross-cultural study on the perception of the use of immersive virtual reality in health and safety training for professional chemical engineers

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Abstract

The use of immersive virtual reality (IVR) has become a feasible alternative to conventional training methods. This is due to the fact that IVR provides the user with a dynamic, immersive, interactive, and safe training space where they can construct their knowledge through trial and error techniques that reflect real-life situations and events. With the rapid development of IVR tools, it is important to understand the direct determinants affecting professionals' decision towards this new technology for training purposes. Yet, little is known about the specific factors that impact the intention to use IVR in the training environment. The purpose of this study is to examine the key factors that may hinder or facilitate the adoption of IVR in health and safety training; and to provide a preliminary analysis of a framework that predicts the level of IVR technology acceptance in a cross-cultural context. To understand professionals' perceptions towards IVR, a conceptual framework was developed through adapting and modifying the Unified Theory of Acceptance and Use of Technology (UTAUT2). Data was collected using an online survey from professional chemical engineers who were either coming from developed or developing country. These were analysed using structural equation modelling based on SmartPLS 3. The findings from this study will help the stakeholders, especially company executive officers to understand the issues facing IVR adoption in different cultural settings. Moreover, the results will guide them in formulating appropriate strategies to improve the acceptance of IVR by both developed and developing countries.

Keywords: *Virtual Reality, UTAUT2, Technology adoption, Training, Culture, Health and Safety.*