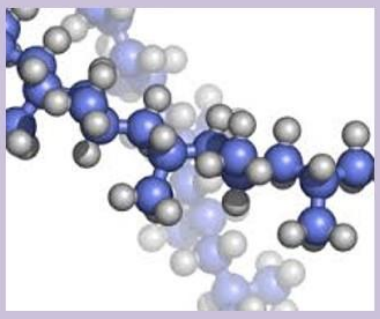
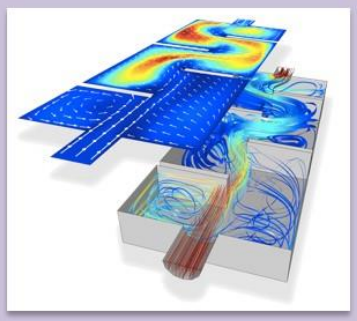
Graduate Conference 2017
April 24th & 25th

Spanning all of the major research themes:
Healthcare, Processes, Materials, Metrology and Modelling





The conference includes both talks by third year PhD students and a poster session by second year PhD students.

Hosted in the West Cambridge site of the Department of Chemical Engineering and Biotechnology from 9-5pm both days.

UNIVERSITY OF CAMBRIDGE
Chemical Engineering and Biotechnology

GRADUATE RESEARCHERS' SOCIETY

3rd Year Talks Overview – Monday 24th April 2017

Room	Time	Talk
LT1	09:30 – 10:00	***A novel tool to characterize surface acidity in zeolites using NMR relaxation methods*** Pierre Bräuer
	10:00 – 10:30	***Highly Porous Metal-organic Frameworks for Drug and Gene Delivery*** Michelle Teplensky
LT2	09:30 – 10:00	***Towards the design of a growth-adapting mitral valve prothesis*** Romilde Kotze
	10:00 – 10:30	***Stabilisation of metal nanoparticles using curved supports*** Tamsin Bell
Tea room	10:30 – 11:00	**Tea Break**
LT1	11:00 – 11:30	***Exploring Catalyst Surfaces with Nuclear Magnetic Resonance*** Neil Robinson
	11:30 – 12:00	***Evidence for microglial involvement in schizophrenia*** Geertje van Rees
	12:00 – 12:30	***Electricity Production using Bioelectrochemical Systems*** Aazraa Oumayyah Pankan
LT2	11:00 – 11:30	***High-throughput computational screening of MOFs for CO/N2 separation*** Andi Tao
	11:30 – 12:00	***A high-dimensional, mechanistic model for twin-screw granulation*** Andrew D. McGuire
	12:00 – 12:30	***Non-affine lattice dynamics of disordered systems*** Rico Milkus
Tea room	12:30 – 13:30	**Lunch**

LT1	13:30 – 14:00	***Design of Oxygen Carriers for Chemical Looping Selective Oxidations*** Martin Chan
	14:00 – 14:30	***Flow pattern created by impinging liquid jets; Application to cleaning*** Rajesh Kumar Bhagat
	14:30 – 15:00	***Principles of design of flow processes for C-H activation-type reactions*** Jacek Zakrzewski
LT2	13:30 – 14:00	***The engineering and applications of biocompatible polymers for intracellular delivery*** Alexandra Chen
	14:00 – 14:30	***Investigation of a process for the liquid-phase selective oxidation of C5-alkane*** Sam Aworinde
	14:30 – 15:00	***Fluid Phases in Catalyst Nanopores – How do they affect our reactions?*** Jacob Brown
Tea room	15:00 – 15:30	**Tea Break**

2nd Year Poster Session – Monday 24th April 2017
15:30 (Tea Room)

Gas-phase MRI measurements of inertial contributions to DPF pressure drop Jonathan Cooper
Capillary suspensions with 'non wetting' secondary liquids Jennifer Holian
Drug Delivery during Breastfeeding: in-vitro feasibility and clinical potential Theresa Maier
Tuning the endocytosis mechanism of Zr-based MOFs through linker functionalisation Sam Haddad
Secondary particle emission from diesel particulate filters Chung Ting Lao
dSTORM Superresolution Imaging to Study the Role of Endogenous α-Synuclein Florian Ströhl
Graphene Micro-Electrodes so Study the Effect of Amyloid Proteins on Neuronal Function Philippa Hooper
Experimental evidence of velocity profile inversion in developing laminar flow using MRI Andi Reci
Oscillatory and explosive behaviours of precipitation reactions in micro-flows Yang Ding

3rd Year Talk Abstracts – Monday 24th April 2017

Sam Aworinde	**Investigation of a process for the liquid-phase selective oxidation of C5-alkane**
n-Pentane is a major component of the naphtha stream from petroleum refining, however it is currently not particularly well utilised in the petrochemical industry. Stricter government regulations to control the Reid Vapor Pressure (RVP) of gasoline by reducing the light end components has also increased the availability of n-pentane. Thus, there is considerable interest from industry in a process for the upgrading and conversion of this low-cost, low-value hydrocarbon feedstock into products of higher commercial value. The direct liquid-phase oxidation of light alkanes with molecular oxygen is extremely challenging because of their low reactivity as well as poor selectivity to alcohols due to over-oxidation into ketones and carboxylic acids. The development of catalysts that are both active for conversion of the alkane and selective for alcohols has so far been largely unsuccessful. The present work focuses on the investigation of a process route for the synthesis of sec-pentanols by the liquid-phase oxidation of n-pentane. In particular, we are concerned with the study of the feasibility of controlling the conversion of n-pentane and sec-pentanol selectivity by carrying out the oxidation in the presence of a free radical initiator and a Lewis acid alcohol-scavenging specie. The influence of key process parameters (temperature, total pressure, concentration, residence time) on the rate of oxidation as well as selectivity and yield to sec-pentanols were studied to determine the optimum operating conditions.	
Tamsin Bell	**Stabilisation of metal nanoparticles using curved supports**
Metal nanoparticles exhibit unprecedented catalytic activity compared with their bulk counterpart. However, they also possess high surface energy and are thus unstable. The surface energy is reduced by the particles agglomerating into larger particles in a process called sintering. For catalysis application sintering results in catalyst deactivation because the catalytic activity is a function of the particle size. Solid supports can be used to improve the stability and my PhD research aims to determine if curved surfaces can offer enhanced stabilisation compared to conventional flat surfaces. So far during my PhD I have developed a simple hydrothermal method for the synthesis of γ-Al2O3 with morphological control, facilitating the preparation of conventional flat 2D surfaces and 1D curved supports. Subsequently, I have incorporated metal nanoparticles onto the supports and tested the resulting catalysts in a model reaction (ammonia decomposition) to assess the effect of support morphology on the nanoparticle stability. My presentation at the graduate conference will be comprised of 2 sections: 1) synthesis of the supports and 2) catalyst characterisation, activity and stability.	
Rajesh Kumar Bhagat	**Flow pattern created by impinging liquid jets; Application to cleaning**
When a coherent liquid jet impinges on a vertical wall it forms a thin film, spreading radially away from the point of impingement, until a point where the outward momentum is	

balanced by surface tension. At this point, the liquid film changes its thickness abruptly giving a jump. A model for the jump location, based on Nusselt's film theory, was presented by Wilson et al. (Chem. Eng. Sci, 2012, 68, 449-460). In this study, the flow field created by a turbulent liquid jet and the location of the film jump are studied and a new model is presented. The liquid film passes through three zones, namely the laminar boundary layer, the laminar film and the turbulent film zone. The location of the laminar to turbulent transition is described theoretically. In addition, the analysis explains why the location of film jump is observed to be insensitive to the nature of the substrate at high flow rates. The model is compared with existing as well as previously reported data for the film jump location and film thickness when a jet impinges perpendicularly and at an oblique angle. The average velocity of the liquid was estimated from the initial growth of the film. Good agreement is obtained between the measurements and the model, which has no adjustable parameters.

Pierre Bräuer	**A novel tool to characterise surface acidity in zeolites using NMR relaxation methods**

Characterisation of surface interactions in porous materials is of crucial importance in order to understand the performances of such materials in many applications, such as separation processes and heterogeneous catalysis.
Microporous solids such as zeolites represent an important class of materials with applications in many chemical processes, including cracking, alkylation, and the dehydration of alcohols and polyols. A crucial aspect to understand in these materials is that of surface acidity as the acid strength of zeolites is one of the main factors in determining the catalytic performances.
The objective of this work is to establish Nuclear Magnetic Resonance (NMR) relaxation methods as a valid tool for the characterisation of acidity in zeolites and, hence, expand commonly used zeolite characterisation techniques such as infrared (IR) and temperature-programmed desorption (TPD) experiments. NMR relaxation methods have been used to characterise mesoporous materials. However, this is the first time that NMR relaxation methods are shown to be applicable to characterise microporous materials.
NMR relaxation time studies are used to investigate acidity and understand the effect of the silica:alumina ratio (SAR) in ZSM-5 zeolites. NMR relaxation measurements are shown to be sensitive to the adsorption strength, which is mainly affected by the adsorption sites consisting of Brønsted acid sites. We propose this method as a novel non-invasive protocol for characterising adsorption in this class of materials with a simple indicator, that is, the T1/T2 ratio.
The NMR method is rather simple to implement, it reduces significantly the experimental time (the experimental time can be down to a few minutes per sample as opposed to several hours of TPD for example) and it non-invasive and non-destructive. We suggest the use of this methodology as a complementary technique to the current methods used to characterise acidity in microporous materials.

Jacob Brown	**Fluid Phases in Catalyst Nanopores – How do they affect our reactions?**

When molecules are confined in a molecule-sized pore, how do they behave? At such conditions, is a gas truly a gas? Is a liquid truly a liquid? Furthermore, how does the adsorption of such molecules onto solid surfaces affect the nature of the fluid being confined? New measurements conducted at the MRRC indicate that fluids operate differently at such reaction-like conditions, and that the effects of these on catalysis could be significant.

Industrial reactions are often facilitated by a process known as heterogeneous catalysis, in which reactant molecules (often gases or liquids) are made to contact catalytically active species in another phase state (often solids). In order to maximise surface areas available for reaction, such heterogeneous catalyst materials therefore often contain pores in the same size range as the molecules they contain. In these materials, fluid molecules do not behave as they normally do and we lack a sufficient understanding of the thermodynamics and transport properties of these new phases that are formed.

Within our experiments, novel phenomena have been observed within nanoporous materials using NMR diffusometry, relaxometry, and spectroscopy. In particular, we believe we have directly observed the diffusion of a surface phase in a gas adsorption system. In addition, it would also seem that we have been able to measure significant differences between the feed gas composition and the composition of the gases within the porous material being studied. The results so far obtained are highly interesting and future work on more industrially relevant systems is planned for the near future.

Martin Chan	**Design of Oxygen Carriers for Chemical Looping Selective Oxidations**

Chemical looping combustion (CLC) presents a novel method of combusting carbonaceous fuels. The technology has advantages, namely inherent separation between the reducing and oxidising streams with minimal energy penalty. This prompts its application to selective oxidations, which usually occurs at low to intermediate temperatures (200 – 700°C). This application requires the development of oxygen carriers that can donate their lattice oxygen selectively, are cyclically stable, and have a sufficient oxygen-carrying capacity. Previous commercial attempts at selective oxidations via chemical looping have been beset by insufficient oxygen-carrying capacities; this talk presents some novel methods which may be applicable in enhancing the capacities of selective oxygen carriers. Some preliminary results on chemical looping with silver, with a nominal oxygen-carrying capacity of zero, are also presented.

Romilde Kotze	**Towards the design of a growth-adapting mitral valve prosthesis**

Of the four mammalian heart valves, replacements for the mitral valve carry the highest morbidity and mortality risk. This risk is further compounded by the general unavailability and unsuitability of prostheses for the paediatric cohort, partly because of their inability to grow. Reducing this growth related patient-prosthesis mismatch would significantly improve patient welfare. Therefore, we propose a mitral valve concept which mimics the native valve, complete with saddle d-shaped annulus and sub-valvular apparatus, and adapts to cardiac growth. This growth-adapting mitral valve prosthesis is designed based on a theory of maintaining structural proportions between valvular components; leaflets, annulus, chordae and papillary muscles. Valve geometry is assessed using finite element analysis and

evaluated in a pulse duplicator demonstrating physiologically similar mitral valve closure and opening. This validated geometric design based on structural proportions can now be incorporated into the design and development of a paediatric growth-adapting mitral prosthesis.

Arthur Kouyoumdjian	**Micro-capillary membranes for protein chromatography**

The downstream purification of biomolecules is a complex and costly multi-step process. Looking at the purification of Immunoglobulin G (IgG), four main steps are needed: cell harvesting and removal of solids, direct capture of IgG (usually by affinity chromatography) and, viral inactivation and polishing (typically with cation and anion exchangers).
The research presented here looks at the potential application of porous micro-capillary film membranes (MMCFs) to simplify downstream processing of antibodies. To do this, we developed both cation and anion exchangers capable of separating molecules of similar charge and removing DNA contamination. Furthermore, the possibility of direct capture of IgG from unfiltered Chinese hamster ovary (CHO) lysate with MMCFs was demonstrated by cation exchange without column fouling. Finally, protein A mimics were coupled to MMCFs to be used as low cost single-use IgG capture technology.

Andrew D. McGuire	**A high-dimensional, mechanistic model for twin-screw granulation**

Granulation (also known as agglomeration, pelletisation or balling) is a common method of particle manufacture. The formation of granules is a key process in the food industry, in formation of tablets within the pharmaceutical industry and in the production of fertilisers. Twin-screw granulation is a relatively new method of continuous granule production and is currently subject to a high degree of research as viable alternative to batch granulation. In this work, we present a novel high-dimensional, stochastic population balance model for twin-screw granulation. The model uses a compartmental framework to reflect changes in mechanistic rates between different screw elements geometries. This allows us to capture the evolution of the material along the length of the equipment. The predictive power of the model is assessed across a range of liquid-solid mass flow ratios through comparison with experimental particle size distributions. The model results show a qualitative agreement with experimental trends; however, they also highlight the need to capture some of the more subtle processes that exist within the twin- screw. The stochastic treatment of the model allows the particle description to be readily extended to track more complex particle properties and their transformations.

Rico Milcus	**Non-affine lattice dynamics of disordered systems**

Despite decades of research in the field of soft matter there is still no unifying theory for glasses. One of the main differences between crystalline and glassy systems on a microscopic level is the deviation from mechanical equilibrium during affine deformations. This leads to a secondary non-affine displacement of the particles, which softens the system

and gives rise to non-trivial phenomena such as frequency dependent elastic moduli and a non-affine part of the elastic moduli. In my work I have analysed different toy models to find relations between the microscopic structure and the macroscopic quantities. One of the key features is the breaking of inversion symmetry, which governs the strength of the non-affine relaxation even for microscopically different systems. Another part of my work is an extension of non-affine lattice dynamics from central force systems to ones that include angular and dihedral forces. These latter contributions are important for modelling of polymer systems. In order to describe the behaviour of the system, I have analysed the relation between chain length and features of the vibrational spectrum as well as the influence of internal stresses on the frequency dependent elastic moduli of these systems.

Aazraa Oumayyah Pankan	**Electricity Production using Bioelectrochemical Systems**

There is a growing demand for the development of renewable energy sources for a sustainable landscape. Bioelectrochemical systems (BES) have contributed largely as an emerging sustainable technology over the past decade. BES are unique platforms, which can convert solar energy or chemical energy into electrical energy as well as other high-value products with microorganisms acting as catalysts. Two types of BES, namely the biophotovoltaic (BPV) and the microbial fuel cell (MFC) are investigated. In a BPV, photosynthetic microorganisms harness solar energy for power generation. Anode materials are being investigated to improve its efficiency. In the MFC, purple non-sulphur bacteria capture light energy for the concurrent production of electricity and hydrogen, whereby the hydrogen is further converted into electricity.

Neil Robinson	**Exploring Catalyst Surfaces with Nuclear Magnetic Resonance**

In this talk we will explore how surface sensitive nuclear magnetic resonance (NMR) techniques may be used to probe the dynamics of molecular adsorbates at surfaces relevant to heterogeneous catalysis. In particular, we will discuss how, in combination with more traditional surface science techniques, NMR may be used to investigate the adsorption, rotation and diffusion of liquid-phase molecules within porous solids of importance to green chemical processes.

Andi Tao	**High-throughput computational screening of MOFs for CO/N2 separation**

Carbon monoxide (CO) is an important reducing agent in the chemical industry as well as a valuable raw material for the synthesis of variety of chemicals . However, the number of studies on CO/N2 separation remains strikingly very limited, due to CO's toxicity and to the inherent challenge of separating molecules with similar physical properties and molecular weights. MOFs have generated an ever-increasing interest from the research community. Owing to their record-high porosity, high tunability of the pore textural as well as coordinatively unsaturated metal, MOFs have shown great potential for separating components in mixtures. To date, an outstanding number of MOFs are catalogued in the Cambridge structural database. As a result, it is infeasible to assess all of them

experimentally to identify the best structure for a particular application. High-throughput screening techniques apply grand canonical Monte Carlo (GCMC) simulations to rapidly screen in silico the adsorption properties of selected MOF library. This allow us to screen interesting and existing structures, providing important structure-property relationships as well as by guiding the synthesis of novel MOFs as industrially interesting adsorbents.

Michelle Teplensky	**Highly Porous Metal-organic Frameworks for Drug and Gene Delivery**

Metal-organic frameworks (MOFs) are a class of porous materials that recently have been applied to drug and gene delivery due to their highly modifiable surface properties and functionalities, and ability to encapsulate active molecules. The application of MOFs lowers the required amount of active pharmaceutical ingredient and provides a more efficacious therapy while decreasing potential for untargeted and undesired effects. We have incorporated recent techniques in super resolution microscopy, including structured-illumination microscopy (SIM) to better understand the release of material from the MOF and uptake of MOF inside the cell. Using novel MOFs that exhibit desirable slow-release properties, large pore volumes, and minimal cytotoxicity, we are able to load the system with siRNA and quantify upwards of 25% signal knockdown of cell fluorescence in an in vitro system. We load the siRNA inside the MOF with a variety of additional payloads to determine the best mechanism for evading endosomal retention and ensure siRNA efficacy. We are also able to visualize the effectiveness of siRNA gene knockdown using the SIM system. Through this work, we show how the efficacy and efficiency of gene therapy will be improved with implementation of these highly porous and biodegradable materials.

Geertje van Rees	**Evidence for microglial involvement in schizophrenia**

Microglia, the brain's immune cells, are widely implicated to be abnormally activated in the pathogenesis of schizophrenia. As current treatment does not cover the full spectrum of symptoms and is only effective in 40-60% of the patients, there clearly is an unmet need for new treatment. Despite evidence that immunomodulatory proteins and microglia activation could be decisive in understanding disease pathogenesis, the causative link between them has not been explored. That is were this research project has been focussing on. Furthermore, using these cells as a potential new drug target, we might bring the patients a step closer to a better quality of life.

Jacek Zakrzewski	**Principles of design of flow processes for C–H activation-type reactions.**

Despite their synthetic versatility and applicability to late stage functionalizations, C–H activation reactions are still considered as not scalable and not suitable for continuous manufacturing. This is mostly due to their inherent complexity and poor mechanistic understanding. Here, we present an approach to development of generic principles of designing continuous-flow processes based on a group of C–H activation reactions of

secondary amines. This group of transformations is of the utmost importance since a large number of biologically active molecules is based on an amine scaffold, and advantages in possible late stage functionalizations of API's are of a great interest for both industry and academia.

2nd Year Poster Abstracts – Monday 24th April 2017

Jonathan Cooper	**Gas-phase MRI measurements of inertial contributions to DPF pressure drop**

Particulate Filters, especially those designed for diesel engine exhausts (so-called Diesel Particulate Filters, or DPFs), have become ubiquitous in recent years due to restrictions on the particulate matter (PM) emissions of engines. These filters operate through the physical trapping of PM inside a porous monolith.

Minimising the pressure drop across the filter is essential to reduce engine backpressure, which can increase fuel consumption and pollutant production. The pressure drop is formed from four key contributions: Darcy effects, friction effects, and compression and expansion as flow enters and exits the filter. The former two are better understood and can be controlled through optimised design and operation. The entrance and exit effects, are not well understood and are significant contributors to the pressure drop at high flow rates and low soot loading.

Gas-phase magnetic resonance imaging (MRI) offers a powerful way to investigate flow inside filters as it can image opaque samples at high spatial resolution. MRI has already been applied to study gas flow in DPFs. In this project, gas phase MRI has been extended to achieve fast 3D velocimetric and diffusometric images, subsequently applied to the inlet and exit regions of a DPF sample to observe turbulent flow effects.

Yang Ding	**Oscillatory and explosive behaviours of precipitation reactions in micro-flows**

Far from the thermodynamic equilibrium, many precipitation reactions can create complex structures with fascinating features caused by the unique chemical physical origin. Chemical gardens, a typical example of reaction–precipitation system, are of great research interests nowadays owing to their vital role in understanding the origin of life. Here, we report on a greatly simplified experiment of growing chemical gardens in a micro-fluidic device where an inorganic membrane and multiple precipitation fingers are formed simultaneously. Various patterns of precipitation reactions are observed when the concentrations of reactants are altered. Pressure measurement reveals oscillatory and explosive behaviours of the micro-flows. We show that such harmonic pressure changes of the reaction–precipitation system exhibit characteristics of the Lotka–Volterra model, with non-dimensionalized pressure acting as prey and concentration of products as predator. Five regimes are identified in the time-dependent solutions: (i) non-oscillatory explosion (ii) oscillatory explosion (iii) constant-amplitude oscillations (iv) oscillatory stable and (v) non-oscillatory stable. The manifestation of predator-prey behaviour in reaction–precipitation micro-flows allows understanding of these complex self-organizing systems.

Sam Haddad	Tuning the endocytosis mechanism of Zr-based MOFs through linker functionalisation
A critical bottleneck for the use of metal-organic frameworks (MOFs) as drug delivery systems has been allowing them to reach their intracellular targets without being degraded in the acidic environment of the lysosomes. Cells take up particles by endocytosis through multiple biochemical pathways, and the fate of these particles depends on these routes of entry. Here, we show the effect of functional group incorporation into a series of Zr-based MOFs on their endocytosis mechanisms, allowing us to design an efficient drug delivery system. In particular, naphthalene-2,6-dicarboxylic acid and 4,4'-biphenyldicarboxylic acid ligands promote entry through the caveolin-pathway, allowing the particles to avoid lysosomal degradation and be delivered into the cytosol.	
Jennifer Holian	**Capillary suspensions with 'non wetting' secondary liquids**
It is known that adding a small amount of a secondary fluid (that is immiscible in the bulk phase) can increase the mechanical properties of a suspension. This increase in strength is assumed to occur as a result of the capillary force in liquid bridges formed between the particles. This poster investigates if this could this be the reason why adding a small amount of glycerol to chocolate leads to a heat stable form of chocolate. A heat stable chocolate is a form of chocolate that remains stiff at high temperatures.	
Philippa Hooper	**Graphene Micro-Electrodes to Study the Effect of Amyloid Proteins on Neuronal Function**
The physiological functions of neurons can be probed by making electrical recordings of action potentials associated with neuronal firing. Protein aggregates, of about ~10 nm in size occur in neurodegenerative diseases and can be imaged by super-resolution microscopy. To understand the effect of protein aggregation and propagation through connecting neurons on neuronal firing, it is desirable to take simultaneous recordings of electrical activity and super-resolution images. These techniques can be combined using optically transparent, electrically conductive and biocompatible micro-electrode arrays. Graphene is ideally suited to this application. In this work, nanofabrication techniques have been developed to fabricate large area, chemical vapour deposited graphene electrodes arrays on glass coverslips suitable for inverted super-resolution microscopy. The impedance properties of the electrodes are compared to conventional gold and ITO (indium tin oxide) micro-electrodes and action potential from cultured iPSC cardiomyocytes are recorded using the graphene electrodes.	
Chung Ting Lao	**Secondary particle emission from diesel particulate filters**
Diesel particulate filter (DPF) is the state-of-the-art after-treatment technology for particle emission control from diesel engines. Numerical models have been developed	

in the literature which can model how DPF filters soot particles from engine exhaust accurately. Trapped soot particles need to be oxidised to avoid excessive pressure drop across the DPF. This process is called regeneration. It is common to assume that all products of regeneration are gaseous species.
The European Union introduced a particle number (PN) emission limit for diesel engines in addition to the previously mass based limit in 2011. Experimental studies have shown that significant amount of nanoparticles (around 10nm) can be produced during regeneration, which is can be significant in terms of PN limit.
It is suggested that these nanoparticles may be the product of fragmentation of soot oxidation. There are numerical models in the literature which describe the fragmentation in diffusion flame. This project attempts to combine the classic DPF filtration model with soot fragmentation model for flame reactors to describe the emission of secondary particle emission from diesel particulate filters.

Theresa Maier	**Drug Delivery during Breastfeeding: in-vitro feasibility and clinical potential**

Current methods of oral infant drug delivery are limited, and confront parents with numerous challenges. Drug delivery during breastfeeding by means of a Therapeutic Nipple Shield (TNS) is believed to provide an alternative measure to dosing spoons and oral syringes for infant drug delivery. This comprises a nipple shield device containing a therapeutic that can be delivered to infants during breastfeeding. The poster displays both feasibility of zinc delivery from non-woven fibres into human breastmilk, and the investigated clinical potential of a TNS by means of semi-structured interviews at Addenbrooke's Hospital. The latter illustrates the attitude of parents and healthcare professionals (n=30) towards the concept of a TNS in a high-resource environment. Participants described both physical and emotional challenges using commonly available infant oral drug delivery devices. They responded positively to the concept of a TNS, believed that a TNS could address some of these challenges, and would be acceptable to both parents and staff. In-vitro studies explored the feasibility of zinc delivery from non-woven fibres, a potential dosage form of the TNS. Fibre-based zinc delivery was identified to be superior to the delivery from tablets manufactured by direct compression.

Andi Reci	**Experimental evidence of velocity profile inversion in developing laminar flow using MRI**

A discrepancy exists between the predictions of analytical and numerical methods about the development of laminar flow at the entrance of circular pipes. Analytical methods predict the velocity profile to have a maximum at the centre of the pipe at all times. Some numerical methods have suggested that the location of the velocity profile maximum moves from the wall to the centre of the pipe in a short distance from the entrance, after which it remains at the centre. This study shows, to the best of our knowledge, the first experimental evidence of the moving velocity maximum. A monolith was used to obtain a uniform velocity profile. Magnetic Resonance Imaging (MRI) was then used to acquire the velocity profile at a short distance from the outlet

of the monolith. The experimentally observed variation of the position and size of the velocity maximum with the Reynolds number is in good agreement with the predictions of numerical methods.

Florian Ströhl	**dSTORM Superresolution Imaging to Study the Role of Endogenous α-Synuclein**

Alpha-synuclein is the key protein in Parkinson's disease, however its physiological function remains elusive. Using superresolution microscopy we aim to analyse the spatial distribution of alpha-synuclein within the presynaptic terminal upon neuronal stimulation. Conventional microscopy is limited by light diffraction and thereby a maximum resolution of 200 nm can be achieved. Superresolution microscopy permits a resolution of around 10-20 nm and thus detailed insights into 500 nm small synapses. To study synaptic molecules we prepared synaptosomes – 'pinched-off and resealed nerve endings' - from adult rat brain. Alpha-synuclein and specific synaptic proteins were stained and imaged by direct stochastic optical reconstruction microscopy (dSTORM). Interestingly, we observed a highly specific localization of alpha-synuclein at the active zone of the presynaptic terminal upon treatment of synaptosomes with KCl and Ca2+, whereas synaptobrevin positive vesicles were localized throughout the synaptosomes, even upon stimulation. Alpha-synuclein was never found across the whole population of synaptic vesicles, unlike synaptotagmin and synaptobrevin, even in the absence of KCl and Ca2+ stimulation. This study shows that alpha-synuclein is not uniformly distributed within the
presynaptic terminal. Thus, its co-localization with the active zone may emphasize its possible role in fusion and reuptake of synaptic vesicles.

3rd Year Talks Overview – Tuesday 25th April 2017

Room	Time	Talk
LT1	09:00 – 09:30	***Innovating dairy: Investigating the performance of fluoropolymer anti-fouling coatings in bovine milk pasteurization*** Ole Mathis Magnes
	09:30 – 10:00	***Large Amplitude Fourier Transform Voltammetry Investigations of Electrochemical Mechanisms*** Luweng Meng
	10:00 – 10:30	***Elastic correlations in central-force spring networks*** Johannes Krausser
LT2	09:30 – 10:00	***Aqueous core colloidosomes with a metal shell*** Qian Sun
	10:00 – 10:30	***Carbon Microsphere Supported Molybdenum Sulfide for Hydrogen Sulfide Decomposion*** Feng Zheng
Tea room	10:30 – 11:00	**Tea Break**
LT1	11:00 – 11:30	***Chemical Looping Combustion: A Multi-Scale Analysis*** Matthias Schnellmann
	11:30 – 12:00	***Investigation of multiphase reactor hydrodynamics using MRI*** Nicholas Paul Rice
	12:00 – 12:30	***An Optimal Control Approach to Scheduling Maintenance Problems*** Riham Al Ismaili
LT2	11:00 – 11:30	***NMR Studies of Enhances Oil Recovery*** Isabelle Bush
	11:30 – 12:00	***Fouling in Heat Exchangers*** Petar Besevic
	12:00 – 12:30	***Particle-modified SPR Biosensor*** Yao Du
Tea room	12:30 – 13:30	**Lunch**

LT1	13:30 – 14:00	***Mechanism of wax anti-settling additives and their role within wax crystallisation*** Joanna Starkie
	14:00 – 14:30	***Rheology of an aerated elasto-viscoplastic fluid*** Douglas Gibson
	14:30 – 15:00	***Application of Magnetic Resonance Imaging in characterizing the rheology of suspensions*** Rittick Batua
LT2	13:30 – 14:00	***Micro-capillary membranes for protein chromatography*** Arthur Kouyoumdjian
	14:00 – 14:30	***Light-sheet microscopy combined with Magnetic Tweezers can probe the deep tissue mechano-biology of developing zebrafish embroys*** Craig Russel
	14:30 – 15:00	***Exploring gas fermentation of biomass to gasoline replacements*** Paul Hodgson
Tea room	15:00 – 15:30	**Tea Break**

2nd Year Poster Session – Tuesday 25th April 2017 15:30 (Tea Room)

Portable sample preparation for nucleic acid diagnostics for low resource settings Cassi Henderson
Adsorption and extraction of bisphenols from water using ZIF-8 metal-organic framework Diana Vulpe
Understanding transport phenomena in complex fluids using nuclear magnetic resonance Daniel Hurst
Developing NMR techniques for general reaction and bioreactor systems Adeline Klotz
First Person Bioimage: share and manipulate 3D volumetric data on the web Marcus Fantham
Optimized Protocol for Manufacturing an Integrated Microfluidic Device for Neuronal Studies Jhalique Jane Fojas
Upconversion Nanoparticle-Antraquinone Sensors for measrung pH Evaline Tsai
Protein fibril electrode Ziyan Zhao
Nuclear Magnetic Resonance Studies of Gas-to-Liquids and Fischer-Tropsch Synthesis Leonard van Thiel
Investigating Oncolytic Spores Manja Neumann
Elliposoid localization microscopy infers the size and order of protein layers in Bacillus spore coats James Manton

3rd Year Talk Abstracts – Tuesday 25th April 2017

Riham Al Ismaili	**An Optimal Control Approach to Scheduling Maintenance Problems**
Fouling in heat exchangers is a major industry-wide problem. Fouling results in the loss of efficiency in heat exchangers which in turn impacts process economics. The cleaning scheduling problem is a multiperiod decision making problem, it consists of binary decision variables and hence it is combinatorial in nature. Generally it is a mixed integer nonlinear programming problem which is non-convex, making it difficult to find the global optimum. Current solution methods for the cleaning scheduling problem are computationally expensive and sometimes fail to converge. This problem is in actuality an optimal control problem dealing with the determination of control trajectories and state trajectories for a dynamic system over a period of time to minimise a performance index. The present research is focused on making novel contributions to the multiperiod optimisation of the scheduling of heat exchanger network cleaning problems and other discrete decision making based multiperiod maintenance scheduling problems arising in chemical engineering processes.	

Rittick Barua	**Application of Magnetic Resonance Imaging in characterising the rheology of suspensions**
Rheology of suspensions has been the focus of various research simply because of their ubiquitousness and importance in many industrial processes. Complex suspensions are of particular interest to the oil and gas industry, specifically, in the well drilling and cementing operations.Nuclear Magnetic resonance imaging and velocimetry (rheo-NMR) technique have been utilised extensively to characterise the rheology and particle migration of such suspensions. Rheo-NMR has the critical ability to provide quantitative information regarding the particle concentration along with direct visualisation of flow field under shear. However, most studies primarily utilises round particles and with narrow size distribution. In contrast, the particle shapes and sizes in industrial systems such as drilling mud or oil well cement differs vastly from this ideal system. In this talk we will explore the rheology of suspensions and migration of rough edged particles at various size range in a density matched Newtonian fluid. Model for the particle migration of suspensions in Newtonian medium is well established. A comparison between the experimental data acquired and simulations at various size ranges and concentration is presented.	

Petar Besevic	**Fouling in Heat Exchangers**
Heat exchangers are devices which transfer heat energy from source of heat to a cold fluid and are used extensively in industrial plants and domestic appliances. A familiar example of a heat exchanger to students in Cambridge is the kettle. In Cambridge it is common to see a build-up of limescale on the inside of kettles due to the local, hard water. One of the problems associated with the build-up of unwanted material, a phenomenon known as fouling, is the reduction in heat transfer performance. Using the kettle as an example, as limescale forms, it takes longer and requires more energy to boil your water. My project	

focuses on the effect of fouling on heat transfer of more complex hard water systems, including water which contains silica, and also the effect of fouling on more complicated heat exchanger geometries, such as those used in heating, ventilation and air conditioning (HVAC) applications. Two experimental cells have been designed and commissioned to study fouling. Results from batch experiments using solutions containing calcium and/or silicon hardness are presented, including imaging using electron microscopy, diffraction techniques for structural analysis and spectroscopic techniques for compositional analysis. These results will be reconciled with theory regarding solution chemistry and heat transfer.

Isabelle Bush	**NMR Studies of Enhanced Oil Recovery**

Laboratory-scale core flooding experiments in which, typically, one fluid displaces another from the pore space of a rock core plug, are widely used in petroleum research for oilfield evaluation and screening of fluids for Enhanced Oil Recovery (EOR) processes. Magnetic resonance methods offer the opportunity to provide significantly greater insight into these displacement processes, such that a scientific understanding of fluid displacement mechanisms and how these are influenced by factors such as surface chemistry, pore structure and fluid properties can be obtained.
In this talk, the applications of spatially resolved nuclear magnetic resonance (NMR) relaxation time (T1-T2) analysis to monitoring continuous flooding processes in rock core plugs will be discussed. Results will be shown from a primary drainage injection of dodecane into a brine-saturated Bentheimer sandstone rock core plug. Spatially resolved T1-T2 (z-T1-T2) correlation maps, provide localised quantitative saturations of each of the hydrocarbon and water phases, as well as qualitative trends in surface wetting and pore filling mechanisms within the rock. Simultaneous monitoring of injection pressures with the z-T1-T2 correlation maps, facilitate correlating localised pore-filling behaviours to the global capillary pressure response.
It is experimentally shown that upon approaching irreducible water saturation, synonymous to the onset of rapid capillary pressure rise and when no further water is displaced from the plug, a continuous water-wetting film is established throughout the pore space of the plug. This is consistent with the theoretically expected behaviour for the injection of non-wetting hydrocarbon phases into a water-wet rock.

Alexander Chen	**The engineering and applications of biocompatible polymers for intracellular delivery**

The recent advancement in material synthesis and the understanding of biological science have made synthetic polymer an ideal candidate for drug delivery applications. A variety of polymer have been developed specifically for intracellular delivery, which is to facilitate the transportation of membrane impermeable material into the cellular cytosol. The most extensively used material is the positively charged polymer, poly ethylenimine (PEI) for mammalian cell transfection of plasmid DNA. PEI is, however, toxic to cells and only effective to cells with high endocytosis activity. Poly lysine iso-phthalamide (PLP) is a polymer inspired by a viral protein of influenza virus crucial for the intracellular delivery of viral materials.PLP was shown to be a pH responsive polymer that is well tolerated and

effective intracellular delivery agent. By grafting hydrophobic amino acid onto the polymer, the delivery efficiency could be increased two-fold in vitro. To further increase the effectiveness of the PLP-based polymers, the structure and mechanism of the polymer and its derivatives would have to be thoroughly characterised. By using different enantiomers of lysine and phenylalnine to synthesise the polymers, the chirality of the overall polymer becomes different. By using CD and neutron diffraction to study the structural difference of the polymer variants, the structure and mechanism of intracellular delivery could be better understood. Modifications with biological active molecules can also be tailored towards specific application to maximize the effectiveness of the polymer to improve current biological processes. For example, by grafting vitamin E to the PLP backbone, a more effective intracellular delivery agent with antioxidative characteristic could be created. The polymer was applied to develop a new cryopreservation protocol that is as effective as the currently standard.

Yao Du	**Particle-modified SPR Biosensor**

Biosensors based on the principle of surface plasmon resonance (SPR) poses many advantages over other sensors. Thanks to being intrinsically highly sensitive, versatile, label free and real-time, SPR biosensors have been a hot area of research for the past two decades. However, SPR biosensors are only sensitive at the surface only a few hundred nanometres into the sample and this poses challenges for capture ligand immobilisation and selective detection of biomolecules of low concentration.
This project aims to utilise particles as carriers for capture ligands instead of having them immobilised on the sensor surface. By having silica particles mechanically pressed onto a SPR sensor with a micro channel, the sensor is spared from tedious modification process before ligand immobilisation. Results shows such immobilisation technique allows the biosensor to detect binding events of immunoglobulins although at a lower sensitivity. Furthermore, if particles are pack in the channel, the entire sensor becomes a chromatography column with integrated refractive index detector. Although the sensitivity of the integrated chromatography SPR is less than traditional SPR sensors, it is desirable as it greatly simplify the functionalisation of the sensor and it provides additional functionality such as in situ sample separation and serial spatial multiplexing.

Douglas Gibson	**Rheology of an aerated elasto-viscoplastic fluid**

Bubbly liquids are found in many different products including foodstuffs, cosmetics and construction materials. Foamed cement, as used in well cementing operations, is an example of such a material where gas bubbles are dispersed in the viscoplastic cement slurry. The bubbles are part of the microstructure of the liquid and play an important role in determining its rheology and thus its flow behaviour during well cementing. Very little research has been conducted concerning the rheology of bubbly liquids with a non-Newtonian continuous phase, such as the foamed cement slurry, and so this field takes the focus of the PhD project.

ClearGlide is a carbopol and is used commercially as a lubricant. It exhibits similar rheological behaviour to that of a foamed cement slurry and is thus used as a test material. Experiments have been performed to investigate the relationship between the rheology of the aerated ClearGlide and that of its continuous phase. The results obtained will be presented with the influence of factors such as the bubble volume fraction considered.

Paul Hodgson	**Exploring gas fermentation of biomass to gasoline replacements**

Biofuels are a direct replacement for liquid transport fuels derived from fossil resources, and present at least a partial solution to issues surrounding the use of fossil resources (CO2 emissions, fuel security, etc.). This project has investigated gas fermentation to biofuels, a route from lignocellulosic feedstocks to direct drop-in replacements for gasoline, mainly butanol. Butanol has fuel properties clearly superior to those of bioethanol, a biofuel produced extensively in Brazil and USA, as well as being a valuable chemical feedstock.

Gas fermentation consists of gasification of non-crop based biomass to crude syngas, which is fermented to liquid products using acetogenic organisms. This route is relatively immature compared to methods such as direct biochemical fermentation and thermochemical gas-to-liquid routes, e.g. gasification followed by Fischer-Tropsch. The route can be broadly split into three sections: upstream gasification and gas clean-up; syngas fermentation; and product separation from the fermentation. Each of these sections present different problems, as well as opportunities for efficient integration. This project has characterised these bottle-necks by modelling theoretical flowsheets, and has devised a number of novel solutions, including efficient gas clean-up, increased mass transfer and reduced power consumption of syngas fermentation, and a low energy separation method from aqueous media.

Johannes Krausser	**Elastic correlations in central-force spring networks**

The mechanical, thermal and vibrational properties of defective crystals have been studied extensively in the past in different contexts, from metallurgy and solid-state physics to, more recently, soft matter and colloidal physics. We study two different models of disordered fcc crystal lattices, with randomly- removed bonds and with vacancies, respectively, within the framework of non-affine lattice dynamics. We find that both systems feature the same scaling of the shear modulus with the newly defined inversion-symmetry breaking (ISB) order parameter, which shows that local inversion-symmetry breaking around defects is the universal root source of the non-affine softening of the shear modulus. This finding allows us to derive analytical relations for the non-affine (zero-frequency) shear modulus as a function of vacancy concentration in excellent agreement with numerical simulations. Nevertheless, due to the different microstructural disorder, the spatial fluctuations of the local ISB order parameter are different in the vacancy and bond-depleted case. The vacancy fcc exhibits comparatively a more heterogenous microstructural disorder (due to the broader distribution of coordination number Z), which is reflected in a different scaling relation between boson peak frequency in the DOS and the average Z.

Ole Mathis Magens	**Innovating dairy: Investigating the performance of fluoropolymer anti-fouling coatings in bovine milk pasteurisation**

Fouling of pasteurisation units processing raw milk causes energy and production capacity losses and gives rise to daily heat exchanger cleaning. The associated extra operating cost and environment impact are substantial. Although a range of anti-fouling coatings has been proposed by researchers and industry, the problem still persists in practice.
Testing antifouling coatings can require significant resources. A further consideration is that raw milk contains microbially active species, so it is advantageous to identify promising coatings early in an experimental stage-to-stage approach. Micro- and bench-scale heat exchanger systems were constructed to study fouling under surface temperatures and wall shear stress conditions representative of sections on a high temperature short time (HTST) pasteuriser. The apparatuses operate with flow rates ranging from 12 ml/min (laminar regime) to 13 l/min (turbulent regime) which enables fouling studies to be carried out with batches from 1 to 20 l raw milk. The fouling resistance and pressure drop across the units is monitored over time and the deposition process is analysed in-situ with confocal laser scanning microscopy. Tests were conducted on stainless steel and fluropolymer coated stainless steel heat transfer surfaces. Effects of the surface free energy, roughness and coating material on the amount and type of deposit formed are discussed.

Luwen Meng	**Large Amplitude Fourier Transform Voltammetry Investigations of Electrochemical Mechanisms**

Large amplitude Fourier transform (FT) voltammetry contains a dc waveform overlapped with the sinusoidally varying potential. Compared with traditional CV methods, these large amplitude sinusoidal voltammetry methods are more sensitive because they enable the separation of the Faradaic current more accurately and this benefits the quantitative electrochemical analysis.
In this work, large amplitude AC strategies were employed to study a well-known redox reaction and then extended to investigate and detect the presence of sulfide-like (L-Cysteine) species via an electrocatalytic (EC') process. Various parameters including flow rates and concentrations of substances were tested in both stagnant and microfluidic systems. Furthermore, the oscillation voltammetry was studied via this technique as well. The result showed that from harmonics extracted from AC voltammograms contain a wealth of kinetic information, especially the higher harmonics when large amplitude was applied.

Nicholas Paul Rice	**Investigation of multiphase reactor hydrodynamics using MRI**

This talk concerns the use of magnetic resonance techniques to quantitatively characterise multiphase flow in fixed and fluidised beds. Pulsed field gradient methods are used to acquire spatially-resolved velocity maps in gas-liquid trickle bed reactors in order to assess the slip and shear behaviour at the gas-liquid interface. Additionally, a novel pulsing flow approach is employed in gas-solid fluidised beds to study the flow of both phases around an isolated fluidised bed bubble. This is done in order to corroborate early analytical models by

Davidson (1961) for fluidised bed bubble flow, and to look to modifications which may aid numerical simulation of fluidised beds for improved industrial design. Compressed sensing methods are used across both sets of data in order to shorten signal acquisition times. Interesting behaviour unique to multiphase flow in porous media is shown by the fixed bed images, whilst the fluidised bed images represent the first full quantitative characterisation of flow surrounding a 3D fluidised bed bubble. The fixed bed data indicate that more sophisticated methods of experimentation are required to assess the interfacial behaviour, and the fluidised bed data show significant similarities with the Davidson model.

Matthias Schnellmann	**Chemical Looping Combustion: A Multi-Scale Analysis**

Chemical looping combustion (CLC) allows fossil fuels to be burnt with inherent separation of carbon dioxide. It is based on the redox cycling of an oxygen carrier and is generally carried out in two interconnected fluidised beds. The oxygen carrier is fed to the fuel reactor in its oxidised form, where the lattice oxygen in the solid reacts with the fuel. The gaseous product, after removal of water, is pure carbon dioxide, suitable for sequestration. The reduced carrier is re-oxidised with air in the air reactor.

To better understand the CLC process, a model has been developed consisting of two, coupled fluidised bed reactors with steady circulation of particles between them. Models from the single particle scale are integrated to account for the behaviour of the oxygen carrier material. The simulation has been used to investigate the effect of different particle kinetics, residence time distributions and particle size distributions and is being expanded to account for particle deactivation and attrition.

On the larger scale, the potential role of CLC in future electricity systems was investigated by including it in an electricity system model. The results were promising and indicate that CLC is more favourable than current carbon capture technologies.

Joanna Starkie	**Mechanism of wax anti-settling additives and their role within wax crystallisation**

Wax anti-settling additives (WASA) are used to mitigate against the problems caused by the settling of n-alkane wax crystals, which crystallise from petroleum diesel. This can result in the blocking of fuel filters and hence vehicle failure. However, the mode of action for such additives is not currently known and two mechanisms have been proposed: they reduce the wax crystal size to such an extent that they settle very slowly or that they induce a repulsion in the wax crystal suspension, causing gelation. This project aims to locate the WASA within the diesel system to better understand its action. Techniques used include differential scanning calorimetry, infra-red spectroscopy, electrophoresis and small angle neutron scattering.

Qian Sun	**Aqueous core colloidosomes with a metal shell**

Colloidosomes have attracted interest in recent years because of their capability for storage and delivery of useful materials. Traditional polymer capsules fail to encapsulate small molecular weight materials for long times, since they are porous and the encapsulated material diffuses through the polymer shells. Therefore, our works focus on the formation of aqueous core colloidosomes with a silver or gold shell, which are impermeable.
Metal coated colloidosomes are prepared by taking aqueous core polymer shell capsules and adding $AgNO_3$ with L-ascorbic acid for silver shells or $HAuCl_4$ with L-ascorbic acid for gold shells. The resulting capsules are triggered using ultrasound. In addition, we used these metal coated colloidosomes to encapsulate cargos such as doxorubicin, an anticancer drug, for cell viability tests.
The polymer shells are fully covered with silver or gold particles sealing the core. The diameter of the water core is between 0.7 μm and 2 μm. The silver shells have a low cytotoxicity, but after triggering, the doxorubicin and broken silver fragments kill cells. This shows the possibility of using these capsules in targeted cancer treatment. The results demonstrate a new type of metal shell microcapsules with non-permeability and ultrasound sensitivity for potential medical applications.

Feng Zheng	**Carbon Microsphere Supported Molybdenum Sulfide for Hydrogen Sulfide Decomposition**

It has been widely aware of the hazards of sulfide in its hydrogen sulfide (H_2S) form. One of the methods to eliminate H_2S is the decomposition of H_2S into valuable product hydrogen and sulfur. It has been realised the catalytic activity of molybdenum sulfide for the decomposition of H_2S. In this work, we report the preparation of MoS_2 embedded carbon microspheres. Highly dispersed molybdenum dioxide crystals are synthesized from a hydrothermal route. This solid precursor then undergoes another hydrothermal synthesis with the addition of thioacetamide. During the reaction, oxygen is substituted by sulfur to generate molybdenum sulfide. Different preparation methods for the material were also conducted, including doping of other metal compounds. Various characterisation of the material has been done and a high specific surface area has been found. The MoS_2 embedded carbon microspheres indicate high catalytic activity toward the decomposition of H_2S under a range of temperature.

2nd Year Poster Abstracts – Tuesday 25th April 2017

Marcus Fantham	**First Person Bioimage: share and manipulate 3D volumetric data on the web**
Modern microscopes (e.g. SIM, 3D-STORM, SPIM) produce stunning 3D volumetric data. Sharing and publishing this data effectively is a difficult challenge. Furthermore, visualising 3D data interactively requires specialist software packages and expert skills. Here we present First Person Bioimage, an online tool to address both of these problems.	
Jhalique Jane Fojas	**Optimized Protocol for Manufacturing an Integrated Microfluidic Device for Neuronal Studies**
In this project, a microfluidic platform was developed as a brain-on-a-chip tool which allows the control of the ordering and connectivity of single neurons as well as its environmental conditions. The design was optimized for advanced optical techniques, such as multi-parametric imaging and super-resolution microscopy, fluorescence lifetime imaging and single molecule localization microscopy which are ideal for imaging live synaptic activity and tracking protein transport in the cells.	
Cassi Henderson	**A portable nucleic acid test for resource-poor settings**
Early detection of infectious disease in low resource settings necessitates portable nucleic acid diagnostics that can detect pathogens in a fingerprick of blood. To achieve this aim, the functions of sample preparation, nucleic acid amplification, and detection should be combined into a small-scale system suitable for point-of-care use. This work explores these functions with respect their potential for integration in a small-scale device. Results to date demonstrate sonication as a promising lysis method for small volumes, capillary fill structures enabled by particles as platforms for amplification, and first steps towards a colorimetric detection method.	
Daniel Hurst	**Understanding transport phenomena in complex fluids using nuclear magnetic resonance**
Rheological Nuclear Magnetic Resonance (rheo-NMR) is a non-invasive alternative to conventional rheometry of complex fluids that allows spatially resolved visualisation of flow field inhomogeneity. Effects such as wall slip, shear-banding and particle migration can therefore be captured. Rheo-NMR has traditionally been used to study time-invariant systems, with conventional two-dimensional (2D) methods measuring over a timescale of the order of half an hour. However, many systems, such as suspensions, can demonstrate time-dependent rheology at considerably shorter timescales. In order to study such behaviour the timescale accessible to rheo-NMR must be reduced. This project is developing fast quantitative acquisition techniques that reduce the acquisition timescale to as low as 100 ms. These include: one-dimensional (1D), fast 2D and fast 1D acquisitions. In particular, a method has been developed that is capable of capturing flow fields in a fast rotating Couette geometry, a	

scenario where previously published methods fail. The developed methods have been successfully applied to demonstrate the effect of xanthan gum concentration on solution rheology; the next step will be to apply them to a high weight-fraction suspension where the rheology is time-dependent. These results will be used to inform technique development on a low-cost, low-field instrument, for online rheological characterisation.

Adeline Klotz	**Developing NMR techniques for general reaction and bioreactor systems**

In this study, two 2D spectroscopy techniques, COSY and HECTOR, have been validated, velocity imaging has been optimized for a high shearing system and a model reaction has been selected based on preliminary reaction mixture studies. In porous media, HETCOR was proven to be superior, allowing chemical shift identification due to less peak spread in the C13 dimension. This technique was demonstrated to have a sufficient resolution for different compounds in a bulk mixture, not including isomers. The velocity imaging technique was modified from the standard spin-warp technique to remove high shearing artefacts, adding velocity compensation and introducing a reduced flow contrast time. It quantitatively obtained images of porous media until a superficial velocity of 15.8 mm/s, whereas without modifications, quantitative results were only obtained until 11.7 mm/s. Preliminary testing of an aldol-reaction mixture was performed at a range of temperatures and pressures (180 - 220 °C, 3 - 12 bar) over porous silica, proving its initial applicability as a model reaction to initially apply the developed NMR techniques to. These techniques will be crucial in understanding the relationship between hydrodynamics and spatially resolved conversion for application to a lignocellulosic reaction system in the future.

James Manton	**triSPIM: light sheet microscopy with isotropic super-resolution**

We propose a three-objective light sheet microscopy geometry capable of isotropic super-resolution imaging in mesoscopic samples. An inverted geometry using 0.8 NA objectives ensures that this system is compatible with imaging samples mounted conventionally on cover slips, while providing high innate resolution. We first describe an excitation scheme, Maximally ORthogonal Detection Excitation Nanoscopy in Thin Sheets (MORDENTS), in which skewed lattice light sheet excitation through multiple objectives is used in combination with computational image fusion to produce volumes with ~240 nm isotropic resolution in EGFP imaging. We then describe a second excitation scheme, Twinned-MORDENTS Requiring Interfering Lattice Light Sheets (TRILLS), in which simultaneous coherent excitation through two objectives is used to further substantially increase resolution, providing an isotropic lateral resolution of ~120 nm combined with ~190 nm axial resolution for EGFP imaging.

Manja Neumann	**Investigating Oncolytic Spores**

Some bacterial species from the genus Clostridia show significant oncolytic properties - particularly promising species include Clostridium sporogenes and Clostridium novyi-NT. These bacteria selectively target hypoxic/necrotic cancer tissue for germination and growth, and subsequently destroy adjacent tumour cells. Although the approach of using Clostridia in

cancer treatment has been recognised and widely investigated for several years, surprisingly little information is available regarding the immune response to Clostridium species.
In this work, the innate immune response to Clostridium sporogenes was studied by exposing the human cell line THP-1 and murine bone marrow derived macrophages to bacterial spores and vegetative cells. Transcriptomics, proteomics and several immunoassays were used to analyse the induced innate immune response.
The present study represents a significant step towards the understanding of the innate immune response to Clostridium sporogenes.

Evaline Tsai	**Upconversion Nanoparticle-Anthraquinone Sensors for Measuring pH**

The development of optical pH sensors for measuring intracellular pH is highly useful to studies of cellular biology as well as applications in diagnostics and therapeutics. However, currently available pH-sensitive nanoprobes suffer from photobleaching and autofluorescence background in biological samples. We designed a pH nanosensor that avoids these problems by taking advantage of near-infrared excitation with the use of upconversion nanoparticles (UCNPs) that emit visible light when excited with a 980 nm laser. This nanosensor is based on fluorescence resonance energy transfer between UCNPs and pH-dependent anthraquinone dyes. Due to the advantages of upconversion photoluminescence, the nanosensor has the potential to be used for detection of pH in in vitro and in vivo applications.

Leonard van Thiel	**Nuclear Magnetic Resonance Studies of Gas-to-Liquids and Fischer-Tropsch Synthesis**

The aim of this project is to understand the behaviour of liquid mixtures and vapour-liquid-equilibria (VLE) inside porous media, relevant to Fischer-Tropsch (FT). Understanding phase behaviour has significant implications for catalyst design, reactor performance and more importantly Gas-to-Liquids (GTL) as a whole. There have been two themes to the project.

First, a method has been developed to identify droplet formation within hydrocarbon/water mixtures in these porous catalysts using Pulsed Field Gradient (PFG) NMR experiments. Various dodecane-in-water emulsions imbibed in porous alumina were studied. It was found that emulsions were formed and that the droplets sizes were significantly larger than the average pore size.

Second, a FT pilot plant has been built and commissioned at the MRRC, for operation inside the NMR magnet. Training in running FT experiments has been undertaken at the Shell Technology Centre in Amsterdam (STCA) in preparation for operating this new pilot plant. Initial studies at the MRRC have been completed. In particular, an in situ NMR study of the reduction of a packed bed of catalyst extrudates has been completed in the FT reactor.

Diana Vulpe	**Adsorption and extraction of bisphenols from water using ZIF-8 metal-organic framework**

For almost two decades, considerable efforts in the field of porous materials have build a structured and well-integrated knowledge of a class of materials with exceptional promise,

metal-organic frameworks (MOFs). MOFs express previously unobserved high surface areas and porosity as well as finely tuneable physico-chemical characteristics. Up to date, MOFs have gained considerable interests in a vast array of fields, perhaps the most well know being that of gas adsorption and storage. MOFs, however, offer an attractive solution to current water treatment technologies due to their ability to adsorb targeted chemical species. This thus circumvents the problematic removal of potentially hazardous side-products formed as a result of catalytic degradation of micro-pollutants.
In this project, zeolitic imidazolate framework (ZIF-8) MOF is tested for the purpose of bisphenol B (BPB) removal from water. The key factors being taken into account are ZIF-8 configuration (powder versus porous and non-porous monoliths) as well as varying concentrations of BPB in the ppm range. Lastly, adsorbent recovery and re-use in subsequent cycles is briefly presented.

Ziyan Zhao	**Protein fibril electrode**

The immobilisation of redox protein is a key research interest in developing an enzyme-based electrochemical biosensor, for which good communication between the enzyme with the electrode material is an ultimate aim. A method of producing redox-active conducting protein fibres as a novel electrode material is being investigated. This method combines a traditional protein self-assembly approach at an air-water interface, with the protein engineering technique to facilitate the formation of the redox-protein fibre construct. The conductivity of the fibre is further enhanced through two methods: incorporation of a carbon fibre core and fusion with carbon nanotube. The performance of the redox-protein fibre electrode will be examined electrochemically in its corresponding substrate environment. A promising enzyme-integrated electrochemical biosensor will thus be achieved with high sensitivity and selectivity.

Graduate Conference 2017

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