Project List
IIB Projects 2013

1 Carbon-dioxide storage: numerical simulations

Silvana Cardoso (assisting Parama Ghoshal)

computational

Carbon Capture and Storage (CCS) is a high-impact technology to reduce carbon-dioxide emissions into the atmosphere. Carbon dioxide is stored in geological reservoirs, such as saline aquifers. The less dense, supercritical CO_2 accumulates at the top of the aquifer above the dense salty water, and slowly dissolves into it. This project involves conducting new computer simulations of a simple analogue to mimic the storage of CO_2 in the aqueous phase (solubility trapping) and in the solid mineral phase (mineral trapping).
The numerical simulation of CO_2 flow in an aquifer has been developed by the Fluids and Environment Group in a CFD software called FASTFLO. We would like a pair of students to adapt the code and investigate the patterns of flow in the simple analogue.
The project suits students who are interested in fluid dynamics, numerical simulations, reactor theory and geology.

2 Carbon-dioxide storage: experiments

Silvana Cardoso (assisting Ilia Cherezov)

experimental

Carbon Capture and Storage (CCS) is a high-impact technology to reduce carbon-dioxide emissions into the atmosphere. Carbon dioxide is stored in geological reservoirs, such as saline aquifers. The less dense, supercritical CO_2 accumulates at the top of the aquifer above the dense salty water, and slowly dissolves into it. This project involves conducting new laboratory experiments using a simple analogue to mimic the storage of CO_2 in the aqueous phase (solubility trapping) and in the solid mineral phase (mineral trapping).
The analogue experiment has been developed by Ilia Cherezov in the Fluids and Environment Group. We would like a pair of students to use this rig to investigate the patterns of flow and storage in the aquifer.
The project suits students who are interested in fluid dynamics, experiments, image processing, reactor theory and geology

3 The fundamentals of pharmaceutical spheronisation

Sarah Rough and Ian Wilson (assisting Matthew Bryan)

experimental

Many pharmaceutical dosage forms are based on being able to manufacture spherical granules, since little balls behave so much better than any other shape in filling machines, tabletting, storage etc. One of the main techniques used in pharmaceutical granulation is extrusion-spheronisation, where the solids are combined with a small amount of liquid to give an extrudable paste (like plasticine) which is then broken up and rounded into little balls in a spheroniser (a rotating friction plate). There was surprisingly little known about the fundamentals of the spheronisation process so Shirley Lau and Lindsay Yu's project (IIB 2012-3) did some very simple and elegant experiments tracing the steps taken as a cylindrical extrudates becomes a spheroidal pellet. They studied a simple paste consisting of microcrystalline cellulose (MCC, a common pharmaceutical excipient) and water and constructed a roadmap for spheronisation. This project will consider more complex pastes where we add a third component which represents the active pharmaceutical ingredient (API aka the drug) and identify how the presence of the API modifies the rheology of the paste mass and the extrusion behaviour. The project is primarily experimental and requires a pair of students. It is ideal for those interested in working in the pharmaceutical sector.

4 The effect of mixing conditions on pharmaceutical spheronisation

Sarah Rough and Ian Wilson (assisting Matthew Bryan)

experimental

Many pharmaceutical dosage forms are based on being able to manufacture spherical granules, since little balls behave so much better than any other shape in filling machines, tabletting, storage etc. One of the main techniques used in pharmaceutical granulation is extrusion-spheronisation, where the solids are combined with a small amount of liquid to give an extrudable paste (like plasticine) which is then broken up and rounded into little balls in a spheroniser (a rotating friction plate). Microcrystalline cellulose (MCC) is a commonly-used excipient for extrusion-spheronisation. What makes MCC so successful as an excipient is its ability to combine with relatively large amounts of water to form a workable paste. However, the method by which the powder and water are combined during the initial mixing stage has been shown to markedly influence the processing properties of the subsequent pastes generated. The effect of mixing conditions was investigated by Jane Lin and Qing Li (2012-13) using different mixing machines and they showed that the plasticity of the paste is related to its strain history. This project will follow their work and establish how the plasticity affects the spheronisation behaviour. The project is primarily experimental – you get to make thousands of little spheroids – with numerical analyses of pellet size and shape. The project requires a pair of students and is ideal for those interested in working in the pharmaceutical sector.

5 Testing the “obesity paradox” in psychiatric disorders

Sabine Bahn (assisting Paul Guest / Jason Cooper)

computational

Despite the known association of obesity with chronic diseases and mortality, an "obesity paradox" has been reported which suggests that overweight patients have a better prognosis compared to those with normal or low body weights. This paradox has been described for various disorders such as diabetes and heart disease, and has even been linked with recovery times of patients post surgery. However, no studies have been carried out thus far to test whether the hypothesis is true for patients with psychiatric disorders. The proposed project aims to prove or disprove the hypothesis using large in-house datasets of patients with schizophrenia and major depressive disorder. Specifically, we will test whether patient bodyweights are linked to severity of symptoms and/or responses to treatment. The results of the study will be submitted for publication and will include the students as authors. The project is ideal as publication will occur no matter whether the hypothesis is proved or disproved.

6 Heart-Healthy Bacteria

Nigel Slater (assisting Duncan Sharp / Krishnaa Mahbubani)

experimental

It has long been assumed that the link between eating red meat and cardiovascular disease (CVD) was due to its high saturated fat content. However, recent evidence has suggested that the dominant causal link between eating meat and CVD, may be its L-carnitine content. A trimethylamine, L-carnitine is metabolised to trimethylamine-N-oxide (TMAO) by certain

bacterial species present in the human intestine. Interestingly, these L-carnitine converting bacteria have a higher population density in the intestinal tract of regular meat-eaters as compared to vegetarians.
The study has also identified species of bacteria, which are associated with reducing levels of the damaging compound TMAO in humans (*e.g. Lachnospira*). If ingested, the balance of gut flora could potentially be altered to reduce the risk of CVD resulting from eating meat.
The aim of the project would be to assess the feasibility of bacterial species such as *Lachnospira* in out-competing the L-carnitine converting bacteria and their subsequent delivery to the gut. This delivery could potentially involve the novel Bile Adsorbing Resins system developed in the Bioscience Engineering Group.
This exciting program would involve microbiological laboratory work, which while intensive, would if successful, yield not only a publication but potentially a product with significant commercial value.

7 Membrane permeabilisation of mammalian cells

Nigel Slater (assisting Sergio Mercado)

experimental

Cryopreservation techniques are essential for long-term maintenance of cell properties in medical applications, such as fertility treatments, cancer therapies or immune disorders. However, the current state of art in cryopreservation relies on the usage of dimethyl sulfoxide and other toxic cryoprotectants that have several disadvantages.
In spite of this, previous studies developed by different groups have shown the non-toxic role of disaccharides, especially of trehalose, in improving the survival of cryopreserved mammalian cells when used along with amphipathic pH-responsive biopolymers that permeate plasma membranes. Experiments on trehalose loading, polymer incubation time, serum concentration, viability and differentiation assays will be developed to optimise cryopreservation of mammalian cells.
This exciting program of intensive lab work would yield in publications if successful with significant value in scientific and medical research.

8 Applications of controllable microstructure in novel single and multi-fibre capillary membranes

Nigel Slater (assisting Radu Lazar)

experimental

Chromatography has widespread applications in industries ranging from bioprocessing and pharmaceuticals to forensics science.
In particular, liquid chromatography is instrumental in protein analysis and purification due to its ability to separate complex mixtures while maintaining high speed, good resolution and high reproducibility. Packed bed columns are commonly used for size exclusion chromatography (SEC), ion-exchange chromatography, and affinity chromatography. Despite their popularity, these columns have significant drawbacks when used in downstream processing of biopharmaceuticals in terms of material cost, low flow rates and low mass transfer rates.
To address some of these challenges, a novel ethylene-vinyl alcohol (EVOH) micro-capillary film based column has been developed in lab. The highly porous, interconnected and macrovoid-free microstructure of the membranes lends itself well to chromatographic purposes, as well as to other novel applications.
The aim of this project is to take advantage of this variable porous microstructure to optimize anion and cation exchange chromatography systems based on these membranes. Changes in porosity based on polymer extrusion protocol will be monitored via scanning electron microscopy (SEM) and porosimetry studies, and protein binding capacity experiments will be used to optimize column and membrane design. In addition, applications involving co-extrusion with other molecules of interest (possible catalysts) may also be explored.

This project offers an opportunity to work in polymer chemistry and bioprocessing on research with high commercial relevance. Successful completion may lead to publication and to additional future applications of the novel micro-porous matrix.

9 Investigating the release of therapeutics into milk from a novel drug delivery device for infants

Nigel Slater (assisting Krishnaa Mahbubani / Radu Lazar / Stephen Gerrard)

Experimental

New drug delivery systems for the treatment of pediatric diseases are urgently needed, especially in developing countries. Each year more than 9 million children under five die worldwide from diseases that
many could be avoided if they had access to appropriate forms of simple, affordable medicines.
Students will work on the development of experimental research needed to guide the design of a recently proposed novel drug and nutrient delivery system for breastfeeding infants developed in this department - a nipple shield delivery system (NSDS) (see Justmilk.org). This thin device adapted from existing nipple shield breastfeeding aids is placed over the mother's breast during infant feeding, milk passes through the device and it releases the agent to be delivered to infant in the milk.
Students will continue development of a novel laboratory-based drug delivery simulation device for the NSDS. This will involve design and programming on an apparatus mimicking the physiological conditions of breastfeeding and modeling release patterns of drugs from the device. They will be able to compare their designed assays for drug release with industry standard methods using atomic absorption spectroscopy.
There will be various opportunities to develop and optimize novel protocols for colorimetric assays to determine release rates of the active agent and on the optimization of the NSDS feeding apparatus. Promising work will likely lead to publishable results.

10 High Lift Wing

Markus Kraft, Prof John Davidson (assisting Sebastian Mosbach/Jethro Akroyd)

computational

The idea of boundary layer suction on an aerofoil is being developed. The scheme is to suck off the air from the boundary layer near the aerofoil and thus defer or prevent separation of the airflow at the rear of the aerofoil. This significantly reduces the drag coefficient and gives a high lift coefficient. Recently, manufacturing techniques have been developed (in Delft) using laser cutting and jet abrasion that make it possible to have many small holes for suction. The presence of dust, rain or ice makes the porous or perforated wing impracticable for conventional aircraft. These hazards are not present for very high altitude flights.Approximate calculations give a prediction of how much suction is needed to keep the laminar boundary layer laminar. The project would be to use computational fluid dynamics (CFD) to answer the following questions
How much suction is needed to preserve a laminar, non turbulent, boundary layer?
How much suction is needed to prevent reverse flow – leading to separation – in the boundary layer for different adverse pressure gradients?
With boundary layer suction, what is the drag coefficient for a given aerofoil? Such predictions from CFD, could be compared with published data for aerofoils with boundary layer suction.
Low drag lifting devices could help to support balloon tethers needed to assist placement of small particles in the stratosphere to mitigate global warming.
This project requires a student with mathematical abilities.

11 NMR studies of SCR catalysts

Mick Mantle (assisting Carmine D'Agostino)

experimental

Selective Catalytic Reduction (SCR) of nitric oxides (NOx) is an important reaction for the removal of NOx from various exhausts. This reaction is usually carried out using a base oxide/metal catalyst in the presence of reducing agents. In most cases the reducing agent is a hydrocarbon, such as alkanes or sometimes alkenes; however, other reducing agents can be used such as urea, ammonia and oxygenated compounds such as alcohols. The nature of the reducing agents may significantly influence the catalytic activity especially in terms of water tolerance of the catalyst. This project will use NMR relaxometry and diffusometry, (and possibly other techniques) to investigate how molecular interactions within the catalyst change with different reducing agents and see what effect water has on such interactions. The goal of the project is to understand to what extent these interactions are responsible for the catalytic performances reported in the literature and ultimately give some guidelines to facilitate the selection process of reducing agents used in the SCR reaction.

12 Can Bayesian sphere sizing by useful to industrial R&D?

Mick Mantle and Andy Sederman (assisting Kostas Ziovas)

computational

We have recently shown that Bayesian probabilistic methods can be used to obtain bubble size distribution in two phase bubbly flow. The technique is generally applicable to bubble and particle sizing and as such is of interest in several industrial applications including enhanced oil recovery, pharmaceuticals and food products. One of the underlying assumptions of the model is that the bubbles (or particles) are spherical in shape which is not necessarily the case for real world applications. This project aims to assess the general applicability of the Bayesian sphere sizing method to non-spherical systems and in addition to develop the model to incorporate non-spherical particle sizing. In this project the students will initially use the MATLAB code that has been developed within the group to generate random distributions of both analytical and numerical shape functions that will then be tested against the purely analytical Bayesian result for spheres. Once this relationship has been explored, the Bayesian model will be developed, using numerical methods, to incorporate other shapes of industrial interest.

13 Swelling of biopolymer films and release of nutraceuticals

Ian Wilson (assisting VSV)

computational

Nutraceuticals are nutritionally beneficial components which are taken in small doses for health benefits. They are often administered in the form of controlled release products which are designed to release the compound when the product enters the gut rather than the mouth or stomach. They often feature a coating which dissolves away when exposed to the pH and ionic strength of the gut, and the same conditions trigger the swelling of the product matrix to allow the supplement to diffuse out. The time taken for the matrix to swell, and the structure of the matrix dictate the dissusion rate for the supplement. It would be nice to be able to predict this. Reliable measurements of the matrix swelling behaviour are needed and this is complicated by them being soft solids immersed in liquid. Such materials are, however, readily measured using the scanning fluid dynamic gauging technique developed in our group. This project follows on from that of Ed Blake and Shufan Jiang (2012-3) who studied the release of nutritional supplement compounds from gelatin matrices. This project will focus on developing a mathematical model of the process which incorporates the chemistry, diffusion and mechanical response of the gel. The work will be primarily numerical and is suitable for a single student or a pair (the pair may do more experiments). This work is part of a collaboration with the Indian Institute of Food Research.

14 Impinging jet cleaning

Ian Wilson and John Davidson (assisting Tao Wang)

experimental

This project follows on from that of Peter Atkinson and Kat Suddaby (2012/2013). We are interested in the way that a liquid jet spreads out and flows downwards when it impinges on a vertical (or near vertical) wall. This is a fluid flow problem that underpins the use of water jets and spray balls for cleaning the internals of many storage tanks and reactor vessels. You may be familiar with a vertical impinging jet striking a horizontal surface in the sink, where a hydraulic jump is formed: vertical surfaces are more complicated. Previous projects have provided us with an understanding of the flow patterns of the jets on surfaces with different wetting characteristics, and in this project we will extend it to surfaces with changing wetting behaviour, such as occur in the cleaning of fouling layers. The original fouling layer nature will change as it absorbs water, and once it is removed the substrate can have a different characteristic. This project will involve measuring the characteristics of the substrate and the soil, and looking at the removal of layers by impinging jets. A good grasp of fluid mechanics is needed but we will not be solving the underlying equations. This is a two-person project and a willingness to get (each other) wet is required.

15 Very sticky natural liquids

Ian Wilson, Bart Hallmark and Geoff Moggridge (assisting Loly Torres-Perez/ Ulrike Bauer)

experimental

Pitcher plants grow in tropical regions such as Borneo and are an example of a ‘carnivorous plant’. They grow in areas with limited nutrient supply and obtain proteins by trapping insects in their pitchers which large bowls containing a sticky liquid. The insects are in time digested to provide nutrients. The liquid is an aqueous solution of a biopolymer unique to the pitcher plant, but which is suspected to vary between genera. The few studies of pitcher plant fluid have demonstrated that it is characterized by a high extensional viscosity.
The devices used to measure extensional viscosities are not compatible with field work but, equally, the liquids do not travel well. Dr Ulrike Bauer is a research fellow in Plant Sciences working on pitcher plants and she would like to be able to test different genera in the field: this project will aim to develop a simple device for measuring extensional rheology over the range of values relevant to these fascinating plants. Familiarity with concepts in rheology is highly desirable but not essential. Interest in constructing a tool is.

16 Fluid dynamic gauging of biofilms

Ian Wilson (assisting Akin Ali)

experimental

Many aqueous micro-organisms prefer to exist as colonies on surfaces and form biofilms. Many biofilms are beneficial, as in waste water treatment systems, but others are detrimental, such as when they grow on heat transfer surfaces. Biofilms exhibit complex microstructures and are almost universally very soft: they deform if touched and slump if removed from their native aqueous environment. One method for measuring the thickness and strength of biofilms in situ and in real time is the technique of fluid dynamic gauging (FDG), which was invented in this Department. Previous MPhil ACE research projects (Baptiste Salley, 2011; Chen Lou, 2012) have demonstrated the capacity of FDG to study biofilms in situ and in real time. Recent work in our research group has prompted the development of a new mode of

FDG operation, which allows FDG to operate under hygienic conditions. This project will extend the FDG technique to look at biofilms under dynamic conditions, where the substrate is moving. The project features collaboration with the group of Prof. Manuel Simoes at the University of Porto: a new FDG device will be constructed that will be compatible with their biofilm reactors. The project is primarily experimental and will suit a pair of students who would enjoy the challenge of designing, constructing and commissioning experimental apparatus.

17 Characterising interactions between spore coat proteins

Graham Christie (assisting David Bailey/Julia Manetsberger)

experimental

Bacteria of the genera *Bacillus* and *Clostridium* form environmentally resistant spores upon nutrient starvation. The spore coat is a multi-lamellar structure comprising of ~100 different proteins, which is assembled during sporulation to form an extremely durable protective shell around the spore. The Christie lab is studying the composition, architecture and assembly of the spore coat with a view to developing novel oral vaccines, drug delivery systems, and improved strategies for spore decontamination. The objective of the proposed project is to identify and characterise protein-protein interactions that drive the assembly of the spore coat and underpin its properties of resistance at the molecular level. Protein interactions will be assessed using the bimolecular fluorescence complementation (BiFC) technique, as a result of which students can expect to be trained and acquire skills in molecular- and microbiology and fluorescence microscopy techniques.

18 Software Advances for Single Molecule Imaging

Eric Rees

computational

The Laser Analytics group develops advanced optical imaging microscopes, which support original research into Biology and Materials Science. One such system is our Localisation Microscope, which employs the principle of detecting individual fluorescent molecule positions at high precision, followed by computational reconstruction of the specimen at a high resolution corresponding to the precision of the individual molecule localizations.

This project involves developing and validating some upgrades to the MATLAB image analysis and visualization tools that we have developed so far. Planned advances include:

1. Drift correction techniques based on fiducial marker tracking, and image correlation methods. The aim is to minimize or eliminate motion blur that tends to affect experimental images on the 10 nm scale.
2. Three-dimensional visualization methods. This may be done by combining our MATLAB imaging software with established (and MATLAB compatible) 3D tools such as Vaa3D.
3. Diffusion and velocity imaging, so that single molecule microscopy can be used for particle tracking microrheology: bridging the gap between typical biological microscopy techniques and methods in Materials Science.

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[2] J. Am. Chem. Soc., 133 (33), pp 12902–12905, (2011), DOI: 10.1021/ja201651w

19 Non-linear Magnetic Resonance Imaging

Daniel Holland (assisting Martin Benning)

computational

Many applications involve the solution of non-linear inverse problems, as for instance phase-encoded velocity imaging, or simultaneous MRI and auto-calibration of magnetic field inhomogeneities. However, many challenges arise when solving non-linear instead of linear inverse problems. In most cases reconstruction algorithms cannot be guaranteed to find a unique, optimal solution. Therefore, analysing the impact of different initial values on the solution is crucial. Further, non-linear problems can be linearised in numerous different ways, leading to different algorithmic strategies with various different properties. Comparing these approaches is necessary to find a suitable strategy in order to tackle a specific application. This project will explore non-linear reconstruction problems in MRI. The project will primarily use simulations of the non-linear problem, but will also use experimental MRI measurements that were obtained as part of a recent post-doctoral research project.

20 Characterisation of the hydrodynamics in a circulating fluidized bed

Daniel Holland (assisting Xuesong Lu)

experimental

Circulating fluidized beds (CFBs) are widely used in the process industries, particularly in power generation. CFBs are particularly useful for many of the next generation carbon capture technologies that could achieve carbon capture with only negligible loss in terms of the efficiency of power generation, e.g. chemical looping combustion. However, for these techniques to be used successfully it is essential that the particle flow and re-circulation patterns are well characterized. This project will explore the use of electrical capacitance tomography to study flow patterns in the riser of a circulating fluidized bed. The results will be compared with both phenomenological and detailed numerical models of the flow in the riser that will be performed by the PhD student who is mentoring the project.

21 Image reconstruction in Electrical Capacitance Tomography

Daniel Holland (assisting Yi Li)

experimental

Electrical capacitance tomography (ECT) is a powerful technique for non-invasively measuring the distribution of material in industrial processes. Key applications of ECT include monitoring of oil, water and solid flows in oil pipelines, measurements of hydrodynamics and drying in fluidized beds, and the characterization of flames. ECT works by measuring the capacitance between multiple pairs of electrodes located around the outside of a process. The capacitance is related to the permittivity, which is a property of materials, within the process vessel. If the permittivity distribution can be reconstructed it permits the characterization of the distribution of material within the process vessel. However, the problem of obtaining the permittivity distribution from the capacitance measurements is severely ill-posed and requires very accurate measurements of the capacitance. For these reasons ECT is very sensitive to drift. In a current Part IIB project we have developed a novel calibration procedure that apparently eliminates instrumental drift, significantly improving the quality of images that can be reconstructed. This project will test the new calibration procedure on a variety of complex phantoms.

22 Nanoporous metal-organic frameworks for drug delivery

David Fairen-Jimenez (assisting Tian Tian)

experimental

Metal-organic frameworks (MOFs) are a relatively new family of nanoporous materials composed of metal clusters linked by organic ligands. The most striking advantages of MOFs over classical porous materials is the possibility to tune the host / guest interaction by

choosing the appropriate building blocks allowing us to design them for any specific application. Owing to their flexible composition, tunable pore size, functionalities and high porosity, MOFs have attracted great interest as drug carriers for cancer therapy.
This project focuses on the adsorption and release of different model drugs (*e.g.* ibuprofen, caffeine) on highly promising MOF structures. You will test *in vitro* selected materials to study the following key questions:
What are the loading capacities of MOFs on different drugs?
What is the release kinetics of MOFs with different drugs?
What is the effect of pore size on drug adsorption and release?
- Can we enhance the host / guest interactions by including amino groups in the MOF structures to tune the drug adsorption and release?
This research project will give you the opportunity to build your knowledge in porous materials and drug delivery process. You will be able to learn laboratory techniques for the identification of optimal pore structures, the role of host / guest interactions and the characterisation of crystalline porous materials.

23 Synthesis of nanoporous materials for carbon capture

David Fairen-Jimenez (assisting Jose de Jesus Velazquez-Garcia)

Experimental

In the last few years, metal-organic frameworks (MOFs) have emerged a class of new porous materials showing promise in several industrial applications. The potential uses of these materials include separation of fuel-related gases, energy production or carbon capture. MOFs are formed by metal clusters linked together by a variety of organic ligands which results in tailored nanoporous host materials. The most striking advantages of MOFs over classical porous materials such as zeolites or activated carbons is the possibility to tune the host/guest interaction by choosing the appropriate building blocks allowing us to design tailored porous materials. Although there has been much research on MOFs, there is still uncertainty about how their properties can be improved for specific applications such as carbon capture.
Regarding carbon capture, competitive water adsorption has been recently identified as the single greatest technical obstacle for the utilisation of MOFs. Indeed, MOFs with high affinity with CO_2 generally present higher interaction with water. In this project, you will explore the use of highly promising MOFs for carbon capture, together with the use of water-impermeable MOF coatings for these materials. The optimization of the synthesis of these MOFs in environmentally-friendly conditions will allow the scale-up production of these materials for further analysis.
Participants will be asked to test and modify, under rational basis, the actual common synthesis methods for different MOFs. You will also characterise and measure the adsorption properties of the materials, comparing and choosing the best methods according to efficiency, safety, environmentally-friendly, adsorption capacities and cost issues.

24 Investigation of protein self-assembly reactions with Atomic Force Microscopy (AFM).

Clemens Kaminski (assisting Dorothea Pinotsi)

experimental

Proteins are the fundamental building blocks of living systems. They are synthesized as linear polymer chains but attain their functionality by 'folding' into their correct three-dimensional shapes. When proteins fail to fold correctly, they can propagate from a soluble state to a non-soluble highly ordered linear aggregate structure. Major diseases such as Alzheimer's and Parkinson's diseases, among the most challenging problems facing modern society, are characterised by the formation of such insoluble deposits in neuronal cells, which are called amyloid fibrils. In this project we aim to understand what leads to the formation of these

structures and to characterise their
kinetic and mechanical properties. We also aim to elucidate the aggregation pathways. A better understanding of these processes will lead to advances in the search for therapeutic intervention. In this project we will study amyloid formation reactions using two different microscopy techniques in parallel: the Atomic Force Microscopy (AFM) system that is available in the Chemical Engineering department and Fluorescence Microscopy techniques.
The project student will:
i) obtain knowledge of state of the art molecular imaging techniques.
ii) Apply chemical engineering intuition on a problem of great
societal relevance.
ii) Get ''hands-on'' experience in working with AFM an advanced high resolution imaging and characterisation technique.
The project is experimental in character and will involve the writing of computer code in Matlab. All necessary training and supervision will be given, but "hands-on" skills and enthusiasm for
interdisciplinary science are beneficial!

25 Optimizing a sensor for extracellular matrix elasticity

Chris Lowe and Dr. William Bains (assisting Rhian Grainger)

experimental

The extracellular matrix (ECM), the protein matrix inbetween cells in animals, gradually stiffens with age, degrading its function and reducing the ability of the cells in it to grow, repair wounds etc.. This is a significant cause of morbidity in old age. The stiffening is caused primarily by chemical cross-linking between the proteins of the ECM. Our overall project is to find a way to reverse this. A central component of this is to find a way to measure the degradation of ECM function that can be related to processed ECM samples, so that chemically defined levels of cross-links can be directly linked to degradation of mechanical function, and so that treatments of the ECM that (might) break cross-links can be shown to be effective at a macroscopic as well as a chemical level. This project will support the development of an acoustic sensor for the elastic properties of the ECM. The IoB has substantial expertise in using acoustic sensors to characterize biological material. We are starting to apply these to characterizing ECM material. The project will extend this work, to show that sensor outputs can (or cannot!) be used as a fast, simple method for analyzing the stiffness of the ECM on a range of spatial and temporal scales, correlating this with endogenous cross-links or with cross-links we form in the ECM. As well as data analysis of the output, the project will include aspects of the electronics and hardware development of the sensor system, and developing methods for the best way to use samples in the system. The project may also include preparation of ECM samples, and their analysis using immunoassays currently being developed by the group.. Please note that this project involves handling animal tissue, but not live animals.

26 Algae dewatering

Bart Hallmark and Bob Skelton

experimental

There are a number of problems with the production of bio-fuels from algae:

1. Growth of algae with a reasonable lipid content
2. Harvesting and dewatering
3. Extraction of lipids
4. Esterification/ trans esterification
5. Phosphorous content

Previous projects have tried to investigate all of the above in a single project which has resulted on too many variables and dilution of effort. This project will concentrate on stage 2 using commercial dried algae but it is hoped to be able to grow fresh material later in the

project. It will take up from a project last year and will look at both cross flow filtration and froth floatation. For cross flow filtration an attempt will be made to model the performance and improve efficiency based on work done last year.
It is hoped to use a Raspberry PI computer to control the flow/pressure and the project should involve some development/programming work on the PI

27 Hydration of Tablets

Bart Hallmark (assisting K. Mahbubani)

experimenta and computational

Oral vaccines are a form of targeted therapeutics, where the active component is delivered to the small intestine via the mouth. A key challenge with this form of medication is that the active component has to be protected from the toxic environment in the digestive system prior to delivery. One method by which this can be achieved is to compound the active component with a binding material that acts to immobilise and neutralise bile salts, hence providing a protective layer around the active pharmaceutical. Of key importance with this approach is the correct understanding of the mass transfer and binding kinetics of the acids and bile salts with the tablet substrate such that a sufficient amount of the active pharmaceutical will be delivered to its eventual target.
This project will initially involve experimental measurement of the mass transfer characteristics of a coloured bile-salt mimic into the tablet substrate. This will be achieved by taking a series of time-sequenced photographs of dye penetration for a number of tablets that will be made to have different porosities. Results from the experimental analysis will then be used to tune a mathematical model, written in MATLAB, which will enable determination of mass transfer parameters.
The successful project pair will gain direct experience of tablet fabrication and of planning and executing sets of carefully-design mass transfer experiments. Additionally, the project pair will also gain experience of using MATLAB (no prior experience required) to solve mass transport problems.

28 Novel areas of application for the Timmins Process

Bart Hallmark

computational

This project concerns the process flowsheeting of an application for a novel carbon dioxide removal system called the Timmins Process. Previous projects have examined and optimized this flowsheet for carbon capture from integrated gasifier combined cycle power plants and from the ammonia flowsheet. The Timmins Process consists of a novel configuration of unit operations that has been proven to have lower energy requirements compared with competing flowsheets. This project will continue from two MPhil projects and one CET IIB project and will be carried out in conjunction with Timmins CCS Ltd and Jacobs Engineering Ltd.
This project is ideally suited to a project pair or a single person who wishes to extend their expertise and knowledge in process simulation and would like more exposure to front end engineering design. The project will consist of simulating and optimizing the process or processes, paying particular attention to thermodynamic accuracy, and energy minimization.

29 Heat pipe investigation

Bart Hallmark (assisting Bob Skelton)

experimental

Heat pipes are an efficient way to transfer heat between a source and a sink or to distribute heat across large areas from a concentrated source using phase change materials. In collaboration with an SME, Thermacore Europe (http://www.thermacore-europe.com/), this project will examine the experimental characterization of novel forms of heat pipe using a newly-acquired test unit. There will also be the opportunity for a small amount of modelling work. This project is ideally suited to pairs of students who would enjoy practical work in the heat transfer arena, and who would like to work on a research project that has potential industrial application.

30 Terahertz spectroscopy of disordered materials

Axel Zeitler (assisting Juraj Sibik)

experimental

The project will focus on understanding the thermal behavior of amorphous materials on an inter-molecular level, both in terms of fundamental research and the potential industrial applications for such materials. The fundamental challenge is to contribute to the understanding of the physical mechanism of molecular relaxation below the glass transition temperature in a range of hydrogen-bonded amorphous systems. This follows on from the results of a PhD research project as well last year's IIB project. The applied challenge is to explore as to whether there is a correlation between this thermal behavior and the long-term stability of glassy form of drugs, or indeed any inter-molecular hydrogen bonded disordered structure. The research is expected to result in a high-impact publication.

31 Terahertz Studies of Diffusion Controlled Processes

Axel Zeitler (assisting Samy Yassin)

experimental

The investigation of diffusion controlled processes using terahertz pulsed imaging (TPI), comprising of sample preparation, data analysis, spectrometry and imaging. Experiments will be carried out in the context of pharmaceutical products (tablets, controlled release agents…etc). Using terahertz sensing it is possible to understand the physical phenomena occurring within these samples in greater detail. By incorporating concepts such as porosity and microstructure into the analytical approach we aim to gain a complete understanding of the processes occurring. A set of design parameters can be obtained for the construction of these tablets by assessing the effects of different environmental conditions, structural defects and the addition of different active pharmaceutical ingredients (API) as well as excipients. This then gives manufacturers the opportunity to set up metrics for the design of these tablets, which ultimately makes it easier for optimization of the processes occurring within them.

32 Applications of 2D inverse Laplace transforms to heterogeneous catalysts

Andy Sederman, Lynn Gladden and Mick Mantle (assisting Tom Blythe)

computational

Research within our group has recently shown that the analysis of magnetic resonance relaxometry experiments of molecules within heterogeneous hydrogenation catalysts can be correlated with catalytic activity and selectivity. This promises to be an extremely valuable tool in the catalyst screening process. However, the use of the 2D inverse Laplace transform that is used for the analysis of the magnetic resonance relaxometry data attracts significant interest for the academic community. This project will involve creating simulated relaxation data that incorporates different types of noise and artifact as well as physico-chemical interactions. Once the simulated data has been generated, a sensitivity analysis of results from the 2D inverse Laplace transform of this data will be required. This will ultimately enable us to quantify errors in the analysis and lead to a greater understanding of heterogeneous catalyst mechanisms.

33 Modeling of reactors based on nanostructured catalysts and structured supports

Alexei Lapkin (assisting Xiaolei Fan)

Theoretical

Our group is developing kinetic, process, fluid flow and heat transfer models for several reaction case studies within an EU project FREECATS: www.freecats.eu
In this project an aspect of one of case studies will be separated out into a student project. The specific element would depend on the status of the project. This may be one of the following: (i) detailed kinetic modeling of a catalytic reaction with the focus on parameter estimation and structural model identifiability, (ii) fluid flow with chemical reaction in a structured reactor (using either a CFD method or a Lattice Boltzmann approach), (iii) combination of heat transfer with fluid flow and kinetics into a single model. The study will utilize data from other partners in the EU project.

34 Life Cycle Assessment for evaluation of novel catalytic processes

Alexei Lapkin (assisting Polina Yaseneva)

Theoretical

Life Cycle Assessment is being increasing used as part of decision making in developing new chemical processes. Within large integrated European project SYNFLOW our group is working on a case study of LCA of a process for manufacture of a pharmaceutical ingredient based on a new catalyst and process. The project will contribute to developing the overall LCA model. Specifically the project will take one of model's gate-to-gate components to develop full material and energy inventory and evaluate the LCA for this component. This will require an element of design project, sensitivity analysis and environmental impacts evaluation.

35 Renewable feedstocks conversion: process modeling

Alexei Lapkin (assisting TBA)

Theoretical

In this project short-cut process models will be set up in ASPEN, based on reaction kinetics and basic process data to simulate potential process scenarios. This will help to speed-up development of novel processes in the area of conversion of bio-feedstocks into higher-value chemicals. Specifically, we'll be looking at conversion of terpenes into aromatic building blocks as precursors to polymers and drug molecules. The research question of the project is in the minimum critical amount of information sufficient to develop a robust process model to evaluate several process options. The project will also aim to develop a generic tool for multi-scale process development based on system theory' 'system operator' and a description of a reaction 'context'.

36 Real-time monitoring of emulsion polymerization

Alexei Lapkin (assisting Claudia Houben)

experimental

Emulsion polymerization is a complex multiphase reaction performed industrially as a recipe-driven process. In order to improve its efficiency it is necessary to establish a way to monitor the state of the reaction in real time using advanced spectroscopic measurements, as well as robust process sensors. In this project a number of sensor approaches will be used. The primary aim will be to develop good understanding of the evolution of emulsion particles on the basis of Raman spectroscopic signal and potentially of acoustic surface wave sensor (if it will be already available). The project will combine experiments with developing spectroscopic model and linking the results with first principles theory of emulsion polymerization and light scattering.

37 Random structure in cement

Alex Routh (assisting Merlin Etzold)

Computational

This project looks at the structure of cement and its influence on the transport properties of concrete. Even though concrete structures can be on the kilometre scale, the strength of the material is given by structures with features of interest between 1 to 1000 nanometres. Surprisingly, the cement community has not come to an agreement about the structure of cement at this length scale. Advance in this direction is of high interest, because understanding the structure on such a fundamental level allows new strategies for optimising and tuning the properties of cementitious materials. The motivation for studying transport in such structures is given by the need for durability modeling, which is crucial for the introduction of new materials.

In this project, 3D model structures will be generated computationally following suggestions from the cement literature. Different methods to generate such structures will be investigated and the properties of the resulting structures will be studied. For this purpose, small angle scattering (SAS) curves are simulated with direct Fourier transform and the transport equations are solved within the pore space using a lattice Boltzmann method.

This broad approach allows developing a project tailored to the interest of the student. As an example project, the following list of items to complete is suggested. (1) & (2) would are to be coded by the student:

Generate random sequential addition (RSA) structures using different geometric base units.

Introduce multidimensionality by staged RSA, e. g., sequentially adding base units of different size

Characterise the resulting structures, e. g., which specific volume fractions can be reached for different particles, etc.

Simulate the scattering pattern

Compute transport properties (permeability and diffusivity) within the pore space.

Interested students are expected to bring an interest in computers, programing beyond Matlab(C/C++/Java) and geometry. It is advised to contact the mentor or supervisor of this project before applying.

38 Patterns in Drying Sand Beds

Alex Routh and Kam Yunus

experimental

When beds of sand dry a number of patterns are observed, such as those seen when flying over river beds. We wish to understand the different patterns that can form and explain their appearance. Experimentally we will drain water from sand beds, in different configurations. We will then photograph the resulting sand profiles and possibly measure the height using profilometry. We will model the fluid mechanics of the drainage process and hopefully explain our observations.

39 Are we getting older or just sicker?

William Bains

other

The life expectancy at birth has been rising in the Western world for over 200 years. The number of people over 60,70, 80 has been going up exponentially in the West for the last half century. But how much of this is because we simply do not die young any more, how much because we are keeping the terminally ill alive longer, and how much because we are genuinely increasing 'healthspan', the length of time we have on Earth to be happy and productive? The popular media has it that all modern medicine does is keep sick old people alive longer – healthspan is not increasing. This literature project seeks to provide evidence that we are genuinely increasing healthspan. Previous work has suggested that, by looking at historical records of those who have always lived well-fed, dry, warm, interesting lives, we can show that life expectancy has increased over that expected by the abolition of the diseases of childhood and poverty. Initial data suggest that healthspan has also increased. This study will extend this work, showing that for several classes of people both their lifespan and their healthspan has increased over the last half century in a way unprecedented in history. The project will trawl written resources (initially the Oxford Companion books on music and literature) and web resources for data. An extension will be researching the history of English foxhunting. The student will have to be willing to read way outside chemical engineering, and be quite creative about how we find data and validate hypotheses using unstructured, written history. You will learn no lab skills at all in this project, but it would be a good showcase for someone wanting to move into consultancy, policy or politics!

40 Chemical kinetic estimate of the maximum temperature for life

William Bains

computational

We know that terrestrial life can live at 120^{o}C. Could terrestrial biochemistry grow at higher temperatures, and could non-terrestrial biochemistry survive at higher temperatures? One limit on the survival temperature for life is the thermal stability of biochemicals to hydrolysis. DNA starts to break down at 100^{o}C. Some metabolites have half-lives of seconds above 110^{o}C. How does life survive? This project will expand a model for the survival of life at elevated temperature that I have started to build. The student will compile kinetic data from the literature (mostly already identified) on the hydrolysis of a wide range of biological macromolecules, metabolites and model compounds. The project will get the raw kinetic data from the papers, and re-analyse to extract Arrhenius kinetic parameters and their uncertainties, using standard formulae in Excel. We will develop a way of extrapolating from these to the possible stability of molecules whose hydrolysis have not been measured, and compile the result into a model of whether an organism could survive at a given temperature. If there is time, this will be modified to see whether an organism with (for example) quaternary ammonium-based genetic material rather than DNA could survive at a higher temperature. This will primarily be a project about reading papers and compiling numbers, with some opportunity for molecular structure analysis if the student is interested in writing code. Familiarity with basic chemical kinetic concepts and excel is required. No bench work. This is part of the supervisor's programme in astrobiology (http://www.williambains.co.uk/astrobiology/index.html)

41 Developing an LED based Phase-Shift Cavity Ring-Down Spectroscopy

Clemens Kaminski (assisting Zhechao Qu)

Experimental

Cavity ring-down spectroscopy (CRDS) is a technique in which an absorbing sample is placed within a stable optical resonator (two mirrors arranged to form an optical cavity). Light is injected into the cavity and passes back and forth through the sample hundreds or even thousands of times, greatly enhancing the absorption path length and thus sensitivity over conventional (commercial) absorption spectrometers. In CRDS a short pulse of light is injected into the cavity and on each round trip of the pulse through the cavity, a little bit of light leaks through the end mirrors. The light intensity in the cavity thus decays exponentially in time, and this so called ‘ringdown’ time can be measured with a fast photo-detector. If an absorbing sample is now placed in the resonator, the ringdown time shortens and this decrease in time turns out to be directly proportional to analyte concentration. The downside of this techniques is that, to be useful, short pulse laser sources have to be used, which need to are widely tunable to match the absorption spectrum of chemicals of interest, and very expensive detectors are required. These factors make the technique very expensive (>GBP200k) limiting its use to a few specialized research laboratories worldwide and preventing wide spread use for applications in the field. In the present project we will build on developments from two generations of highly successful part 2B projects with the overall aim to replicate the merits of laser based absorption techniques with much simpler but equally sensitive technology. Here we propose to use a high power white light emitting diode (LED) - similar to what you might use at night when cycling back from the pub – to replace the laser and build a high sensitivity CRDS spectrometer that will cost on the order of GBP 1k to make. How will we be able to get short pulses from an LED? We won’t! Instead we will develop a technique called phase-shift CRDS (PS-CRDS) in which we will modulate the LED at high frequency (100 kHz to 1 MHz). The light coming out of the cavity will be phase shifted and demodulated with respect to the input light. On absorption the light escaping the cavity picks up an extra phase shift and we will use a so called lock-in amplifier to measure this precisely. We will finally deploy this system in a chemical reaction called the Griess assay, with which it is possible to analyse nitrate content in soil samples or biological systems. You will learn how to develop a low-cost lock-in amplifier circuit and build up an optical system to design specifications. The project is experimental in nature, uses state-of-the-art instrumentation (apart from bicycle lights!) and includes analysis and modeling in Matlab. The students should be enthusiastic for experimental work and should be interested in collaborative research. The work will be closely supervised by practicing experts in the field and no prior optics knowledge is required, although ‘physics intuition’ is beneficial.

The project student will:
i) Obtain knowledge of state of the optical sensing techniques.
ii) Develop expertise in advanced spectroscopy techniques.