EPSRC
Pioneering research and skills

EPSRC Centres for Doctoral Training
Poster Event

Wednesday 24th May 2017

13:30-15:30

University of Leeds

UNIVERSITY OF LEEDS

Contents

Welcome

Welcome to the EPSRC Centres for Doctoral Training (CDT) Poster Event. The EPSRC CDTs at Leeds bring together diverse areas of expertise in order to train researchers to address a wide range of problems in engineering and physical science.

The purpose of this cross-CDT event is to bring together students from different EPSRC CDTs at Leeds to share their research via poster presentations with students, staff and industry partners from participating CDTs and to discover research outside of their own CDT.

EPSRC CDTs taking part in this event are:

- Bioenergy
- Complex Particulate Products and Processes
- Fluid Dynamics
- Integrated Tribology
- Tissue Engineering and Regenerative Medicine – Innovation in Medical & Biological Engineering

Schedule

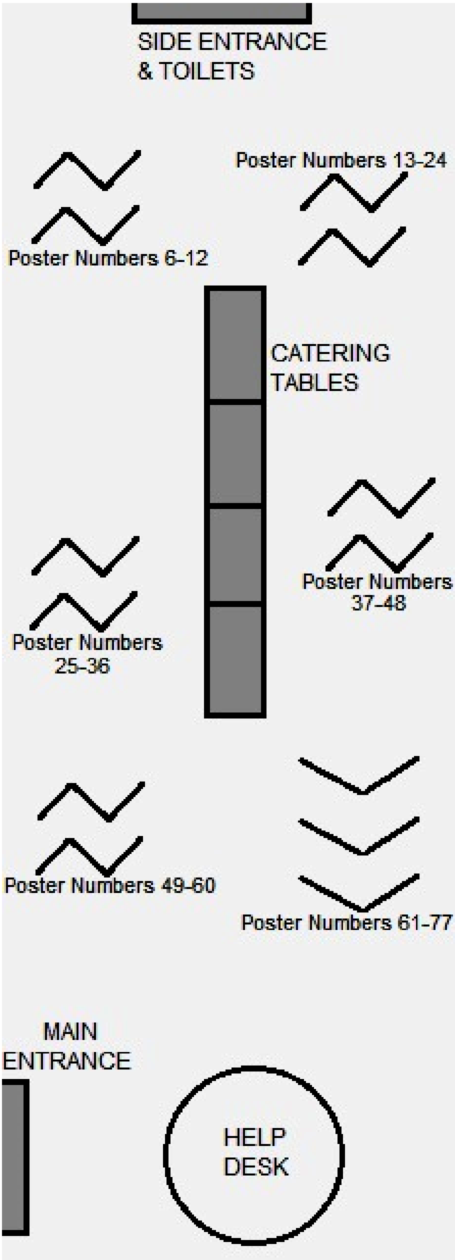
Wednesday 24th May 2017

Time	Activity	Venue
12:30-13:30	Posters available for viewing	Parkinson Court
13:30-15:15	Poster presentations and light refreshments	Parkinson Court
15:15-15:30	Prizes* announced and awarded	Parkinson Court

*Prizes to be awarded include a prize for best poster per CDT, overall best poster and the Thesis Twitter Conference winners.

Floor Plan

Venue: Parkinson Court, Parkinson Building, University of Leeds



Key	
6-23	Bioenergy
24-32	Complex Particulate Products & Processes
33-45	Fluid Dynamics
46-57	Integrated Tribology
58-77	Tissue Engineering & Regenerative Medicine — Innovation in Medical & Biological Engineering

Bioenergy 2015 Cohort

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Using additives to reduce the emissions of NOx from large scale power production

Coal still provides 41% of the world's electricity production. 8000 M tonnes of coal is produced each year, a result is large amounts of harmful emissions are released into the atmosphere from power production every day. An emission of particular concern is nitrogen oxides (NOx). A typical 600MW coal power plant with emissions control, still emits approx. 3300 tonnes of NOx each year.

To combat the emissions there are ever increasingly stringent environmental policy and regulation. The electricity production industry has to reduce the amount of emissions during combustion. The current regulations in the EU require emissions of 200mg Nm-3 and by 2020 a further reduction to 150 mg Nm-3 of NOx.

Currently there are several methods used to achieve the current limits; specialised combustion chambers, and secondary converters fitted in the exhausts to reduce the amount of NOx emitted. With the future targets ever tighter, new methods are required to reduce the emissions. This research is focused on using an industrial waste product additive to combine with the fuel to reduce the NOx emissions at source, enabling the secondary reduction techniques to make significant reductions below the required limits for 2020.

Bioenergy 2015 Cohort

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Gasification of Real Biomass with Plasma-Catalytic Tar Reduction Process to Deliver High Quality Syngas

Climate change has become one of the most important social and political issues in recent years. To tackle climate change, renewable energies are promoted in order to reduce our society's dependence of fossil-fuels. Thermal processes such as pyrolysis and gasification are an attractive way to produce energy and high-valued chemical products from biomass. The main product of biomass gasification is syngas. Syngas can be combusted for power and heat generation or used in the production of fuels and chemicals as an alternative raw material to fossil-fuels. The main drawback however for industrial implementation of this technology is the presence of tars in the syngas produced from biomass gasification. Tars can accumulate within the equipment resulting in damaged machinery. The main objective of this research is to produce a high quality syngas from biomass gasification by developing a plasma-catalytic process to reduce the presence of tars.

In this study, wood pellets were used in a two-stage pyrolysis reactor consisting of fixed-bed and plasma DBD reactors. The biomass was first pyrolyzed under nitrogen atmosphere at 600 ºC. The volatile products went directly through the plasma-catalytic system, heated externally to 250 ºC to avoid condensation. Ni based catalysts, prepared by conventional wet preparation method and calcined at 750 ºC, were used in the plasma-catalytic reactor. The gaseous and liquid products were analysed by packed column gas chromatography.

The results showed the advantage of using plasma-catalytic systems instead of catalytic reactor only. The plasma-catalytic system was partially optimised, modifying parameters such as the power.

Bioenergy 2015 Cohort

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Assessment of spontaneous combustion risk of biomass dust

The usage of biomass for power generation is increasingly more popular. North American white wood pellets are one of the biomass fuels used in larger power stations. Power generation requires the storage of large quantities of biomass fuel pellets in piles or silos. And throughout the process of storage, conveying and through to eventually burning large amount of dusts are created. This latest research focuses on the industrial handling of dust and the health and safety involved. Dust layer ignition tests (standard and non-standard) are performed to characterise the biomasses ignition risk potential in the industrial environment.

Bioenergy 2015 Cohort

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Bio-oil upgrading and why there is need for it

Upgrading is a secondary treatment of bio-oil or biomass pyrolysis vapour with the aid of different catalysts and/or co-feeds (e.g. steam, alcohol, hydrogen). But how important is this process, bearing in mind possible financial cost implications? Bio-oils produced from thermal processing of dry organic materials are considered as future renewable liquid fuels. However producing bio-oils whose physical and chemical fuel properties are consistent with conventional fossil fuels are important in marketing and commercializing the products. The aim of this poster is to show some key physical and chemical fuel properties of raw bio-oil, upgraded bio-oil and conventional transport fuels in order to highlight the significant role of producing better liquid fuels from biomass through upgrading. Heating value which is a significant fuel property can be increased up to 30% or more through upgrading. Besides, desirable lower oxygen values and others are also achievable through upgrading. For all of these fuel attributes, upgraded bio-oil figures are closer to the conventional fuels than the raw bio-oil. Bio-oil upgrading however can become increasingly expensive as facilities or material requirements produce a varied range of cost implications. But the outcome, as shown here is indispensable for product marketing and commercialisation.

Bioenergy 2015 Cohort

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Agarose gel electrophoresis of kraft lignin

Lignin is a highly diverse aromatic polymer that is a rich sustainable feedstock for high value chemicals, many of which are traditionally produced by the petroleum industry. A major source of lignin is the paper and pulp industry, where the kraft process is utilised to separate lignin from cellulose fibres. The kraft lignin produced by this process is considered as waste and is currently not utilised as a high value chemical feedstock. Determining the concentration of lignin is extremely time consuming and challenging. Equally it is difficult to characterise the structure of lignin polymers and determine information such as the molecular weight of the polymer. This severely limits studies on the chemical and biological degradation of lignin, due to challenges in assessing whether the lignin polymer has structurally altered or degraded. In this work agarose gel electrophoresis was investigated as a method of separating kraft lignin, to provide information about the molecular weight of the lignin polymers. Additionally SDS-agarose gels were utilised in order to produce a single band that increases in density according to lignin concentration. After imaging using UV light, ImageJ was utilised to produce a standard curve and this could potentially be used to determine the lignin concentration of an unknown sample. These techniques could therefore be used in order to assess lignin degradation in view of producing high value chemicals.

Bioenergy 2015 Cohort

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Effects of Iso-butanol on Spark-Ignition Engine Performance

Butanol shows promise as a potential transport fuel in spark-ignition engines; it has a higher calorific value than ethanol, is a potential octane booster and when compared to ethanol, butanol is not as hydrophilic. Butanol can also be blended to higher ratios in a conventional SI engine. Of the bio-derived butanol isomers, iso-butanol has the greatest ignition properties, as seen in work by Weber and Sung [1], giving it the greatest anti-knock properties. While some work has been concluded into the ignition characteristics of iso-butanol [1] [2] [3], very little has been done into the properties of iso-butanol and gasoline blend fuels. To operate in conventional engine technologies, flued blending is a necessity and as such, it is important to understand the impact that the blending of iso-butanol will have on the combustion properties of gasoline fuels, at engine relevant conditions. This project will focus on the fundamental combustion properties of iso-butanol and iso-butanol/gasoline blends and the effects on engine performance. This will include studies on fuel auto ignition (using the Leeds rapid compression machine) and a study of engine knock (using an optical access research engine. Chemical kinetics models will be completed using CHEMKIN software and will be validated using experimental data from the RCM. These models allow for the prediction of ignition properties as well as providing an insight into the underlying chemistry driving the ignition process.

Bioenergy 2015 Cohort

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Laser Photolysis Study of Low Temperature Biofuel Ether Combustion Kinetics

Fossil fuels need to be replaced, and biofuels offer a potentially carbon-neutral alternative to conventional petrol and diesel. Dimethyl ether (DME) and diethyl ether (DEE) are two ether biofuels of current interest, due to their high cetane ratings and reduced particulate emissions. In order for their application in novel engines to be efficient, their low temperature combustion mechanisms must be fully understood.

Laser photolysis techniques have been used to study the kinetics of the reaction between ethers and hydroxyl radical, OH. The bimolecular rate coefficients for these reactions have been determined over a temperature range of approximately 300 – 750 K, and the addition of oxygen, to simulate combustion conditions, has been explored.

The room temperature bimolecular rate coefficients for the reaction of DME and DEE with OH were measured as 2.68 × 10-12 cm3 molecule-1 s-1 and 1.23 × 10-11 cm3 molecule-1 s-1 respectively. OH recycling was shown to increase with increasing oxygen.

Bioenergy 2015 Cohort

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Influence of hydrothermal pre-treatment on biofuel production from microalgae

There is an increasing interest in the hydrothermal processing of microalgae for the production of high energy density biofuels, such as bio-coal and bio-crude. There are however, certain drawbacks to hydrothermal processing, which include problems with recovery of valuable nutrients, contamination of intermediates with inorganics, high amounts of phosphorous and nitrogen along with high levels of corrosion. Hydrothermal carbonisation as a means of pre-treatment has the ability to reduce these issues. Therefore the main aim of the research is to investigate the potential of hydrothermal carbonisation as a means of pre-treatment to improve the quality of products from hydrothermal processing of microalgae. The main objectives are to recover and recycle nutrients in the process waters and to understand the influence of nutrient removal on product quality and its impact on process operations such as grinding and pumping.

The process waters produced from the hydrothermal carbonisation of microalgae have been investigated. The potential for nutrient recovery and recycling has also been demonstrated. The methods of separation and recovery of the nutrients include physical and chemical separation along with in-situ and regenerative adsorption. Further work will investigate the use of the formulated process waters from sequential treatment, which contain soluble hydrocarbons and inorganic compounds, for the cultivation of microalgae in the recycled process waters.

This approach also has the potential for application to other high nutrient and high ash containing feedstocks such as macroalgae, sewage sludge, manure and other biomass materials.

Bioenergy 2015 Cohort

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Kinetic Studies of the Isomers of Bio-butanol under Low Temperature Combustion Conditions

Several of the isomers of butanol have recently received interest as potential biofuels, and can be made via a range of fermentation methods. The bio-butanols demonstrate several key advantages over other biofuels, such as being more energy dense and less corrosive than competitors such as bioethanol. There currently exists a large gap in the kinetic data at relevant low temperature combustion conditions for the reactions of the different isomers of butanol with OH, a key reaction in the combustion of the potential fuels in an engine.

Using the pulsed laser photolysis – laser induced fluorescence (PLP-LIF) method under pseudo-first order conditions, the rate coefficient (k) for the reaction of OH with n-butanol and i-butanol has been measured over the temperature range 298 – 673 K at 20 – 30 torr. A rate coefficient k(298 K) of (8.95 ± 0.07) x10^{-12} cm^3 $molecule^{-1}$ s^{-1} was measured for i-butanol + OH, and (7.84 ± 0.20) x10^{-12} cm^3 $molecule^{-1}$ s^{-1} for n-butanol + OH. Both temperature ranges have been compared to the rate coefficient data of Sarathy *et al.* and McGillen *et al.* across the temperature range 300 – 1000 K.

Bioenergy 2015 Cohort

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Harnessing hydrogen: advanced reforming of bio-compounds

Hydrogen is already widely used as a feedstock in industry, and it could be a low carbon, flexible fuel for the future. However, harnessing its potential in a decarbonised economy will require the development of large-scale production processes which ensure that lifecycle carbon emissions are low.

One possible route to do this is to combine advanced reforming techniques with biologically sourced feedstocks. Through process modelling, this project explores the potential for bio-compound use in steam reforming with carbon capture. Another option is sorption-enhanced chemical looping steam reforming (SECLSR), a novel process which has in-situ carbon capture.

Initial work has involved modelling an adsorption bed which purifies the product gas from the SECSLR reactor. Results suggest that combining the SECSLR with this adsorption bed can achieve H2 purity over 99%. While there is scope for further development, the foundations have been built for a rigorous whole process model, which will enable evaluation and development of a promising new low carbon hydrogen production technique.

Bioenergy 2015 Cohort

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A Comparison of Tailpipe Gaseous Emissions for RDE and WLTC using SI Passenger Cars

The drive characteristics and gaseous emissions of legislated RDE test data from 8 different spark ignition vehicles were compared to data from corresponding WLTC tests. The effect of the official RDE exclusion of cold start and idling on the RDE test, and the effect of the use of the moving averaging window (MAW) technique, were simultaneously investigated. Specific attention was paid to differences in drive characteristics of the three different driving modes and the effect this had on the distance-based CO2, CO and NOx emission factors for each. The CO2 emission appeared on average 4% lower under the RDE tests compared to the WLTC tests. The CO was 60% lower, and appeared loosely positively correlated with average acceleration and relative positive acceleration (RPA). The NOx values were 34% lower under the RDE testing, and appeared linked to the average acceleration. The exclusion of cold start and idling decreased all RDE emissions. RPA appears positively correlated with CO and CO2 distance-based emissions, but not for NOx. RPA was shown to be uncorrelated with any mass-rate emissions. The range of RPA values seen was much greater for RDE tests than WLTC tests, with individual RDE tests having variable values for each drive mode. The application of the MAW technique had minimal effect on the CO2 distance-based emission, but it appeared to decrease emissions of both CO and NOx for some drive modes, decreasing the average values by 12% and 21% respectively. The MAW also decreased the variation in emissions across different modes.

Bioenergy 2015 Cohort

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The Impact of Bioenergy on Land Use Change and the Climate

Bioenergy is expected to play a key role in reducing GHG emissions and mitigating climate change over the next century. Although there are many advantages to Bioenergy, there is ongoing discussion about how sustainable it will be in the future, with regards to both environmental and socio-economic issues. In particular, there are concerns as to its impact on land use change (LUC) that could further accelerate deforestation, biodiversity loss and ultimately increase global warming. This study explores four recently-developed future scenarios of LUC from Bioenergy production, based on the 'Middle of the Road' SSP2 scenarios: 'NoBio' – A reference scenario excluding bioenergy production from 2015-2100; 'Bio' – Includes increase in second generation bioenergy from 0EJ in 2015 to 300EJ in 2100; 'Bio-REDD' – Equivalent to Bio but including forest conservation; and 'Bio-WP' – equivalent to Bio but including water conservation. These scenarios have been thoroughly analysed with regards to forestland impingement from second generation crops, and then inputted into an Earth System Model (ESM) to determine their impact on Earth's climate over the next century. The outputs studied are biogeochemical and biogeophysical effects such as carbon flux and surface albedo.

Bioenergy 2015 Cohort

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Comparison of the growth and neutral lipid accumulation of seven strains of the microalga Chlamydomonas reinhardtii grown in synthetic wastewater

There is extensive interest in microalgae as a means by which to produce bio-oils for bioenergy production, however the low efficiency of biomass to oil and the heavy start-up and operational costs currently restrict the wide-scale use of microalgae as a sustainable fuel source. Microalgae are able to assimilate high quantities of nitrogen and phosphorus. Coupling biomass and lipid production with nutrient bioremediation for wastewater treatment removes many of the economic barriers associated with biofuels from microalgae. Here we present the growth characteristics and lipid production of seven strains of the microalga Chlamydomonas reinhardtii grown in synthetic wastewater. Algal samples were grown under continuous light at 25°C and shaken to promote aeration. Optical density and chlorophyll content were monitored and the lipid content compared by means of Nile-Red staining. With the exception of one strain (CC4267) which saw no growth over a 12 day period, all strains grew to an optical density of approximately one third that when grown on TAP media. Chlorophyll content increased in all strains initially before decreasing in line with the plateau in optical density. Strain CC4035 saw no drop in chlorophyll content. Nile red straining revealed intracellular spherical lipid droplets under red fluorescent light. Lipid quantity was largely correlated with the loss of chlorophyll content. The results presented here reveal that five of the Chlamydomonas reinhardtii strains tested are able to accumulate neutral lipids under nutrient conditions present in wastewater.

Bioenergy 2015 Cohort

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Cost benefit analysis and comparison of UK biofuel powered vs. diesel powered truck fleet

This research aims to elucidate the complex dynamics governing the attractiveness of and impetus towards use of biofuel and automation technology by UK Truck Fleet Operators (TFOs) from a whole-systems perspective.

Here both emission and cost savings attainable by UK TFOs from selective integration of biofuel and automation technology in their fleet operations are quantified to establish effective strategies for enabling such benefits. An equally important focus of the study is to unravel key synergies arising from simultaneous implementation of both technologies that could further maximize said benefits.

The findings are then applied to elucidate critical technology pathways which UK TFOs could take for achieving optimal balance between cost and fleet emission. Both PESTLE framework and VENSIM system dynamics modelling will be used as part of the analysis to ensure real-world applicability of findings, the implication of which will be significant towards enabling UK to achieve its 2020, 2030 and 2050 emission reduction goals within the road freight sector against the backdrop of anticipated increase in freight activity.

Results of this study can be i) applied to further evaluate the extent to which a virtuous cycle of “biofuel and automation technology adoption” can be achieved for various UK TFOs on a whole-systems and ROI (Return on Investment) versus emissions savings basis, and ii) further extrapolated to enable initial evaluation of benefits attainable from biofuel and automation technology implementation by TFOs across the EU.

Bioenergy 2016 Cohort

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Grass-to-Gas: Roadside Biomass for Anaerobic Digestion, Storage, Pre-Treatment and Application

An initial investigation found that road-verge grass was a suitable feedstock for anaerobic digestion (AD): having a similar theoretical methane production potential to current feedstocks, acceptably low-levels of contamination and the potential to be harvested profitably.

In light of these findings, subsequent work has been undertaken investigating the practical use of road-verge-grass as an AD feedstock for commercial applications. AD is the biological degradation process of organic substrates into biogas in an oxygen-free environment. The viability of a potential feedstock is dependent upon sufficient digestion, annual availability and uniformity of supply to the plant. Seasonal harvesting of road-verge-grass results in intermittent feedstock availability. As such, ensiling was investigated as a potential storage or pre-treatment solution. Theoretical bio-methane potential was evaluated in contrast to fresh material so as to understand potential advantageous or detrimental processes associated. Ensiling grass was found to provide a similar methane output to fresh feedstock.

So as to fully evaluate the performance of road-verge-grass, and other substrates, feedstock material was analysed for a true biomethane potential within a bench-scale anaerobic digestion reactor. Samples where processed via thermal hydrolysis prior to analysis. Results indicate verge grass generates competitive levels of bio methane compared maize. Farmers were interviewed and it was found that there is a potential market for grass to be delivered to farms. The options for the use of methane produced by AD were compared and the income, incentives, greenhouse gas reductions and potential problems of each use were compared.

Bioenergy 2016 Cohort

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High value products from waste biomass

Moving away from fossil fuels is not just a matter of producing electricity or fuels, it includes another areas. The need to manufacturer fine chemicals, drugs and materials in a sustainable way is crucial. Hence, biorefineries appear as a solution to co-produce a range of products whilst decreasing the environmental impacts. This study examines three parts of the biorefinery system as case studies: pre-treatment, conversion and whole analysis.

Three studies were completed in tandem, based around the production of high value products from biomass: degradation of polyphenols to form phloroglucinol, Au-TiO2 nanoparticle photocatalytic degradation of lignin and LCA comparison between PVP and seaweed derived alginic acid.

Each area of research had distinct objectives set out. To develop more sustainable alternatives to the synthesis of phloroglucinol, currently derived from TNT. Research a novel approach to the degradation of lignin using photocatalytic-based chemistry. Finally to establish an environmental comparison between a conventional building-block for the cosmetic industry and a seaweed alternative.

Bioenergy 2016 Cohort

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Biofuels in Engines: Isobutanol

Biofuels are fuels derived from biological resources. They can play a part in reducing the effects of global warming by minimising future greenhouse gas emissions. Isobutanol is one such biofuel with a high potential for greenhouse gas reduction. A full analysis of the potential of Isobutanol for spark ignition engines was considered, comprising a Life Cycle Analysis (LCA), Chemical Kinetics Modelling and Experimental measurements of the ignition delay within a Rapid Compression Machine. Experimental tests were undertaken at iB100 and modelled computationally at iB10 and iB100 at different air/fuel ratios using a gasoline surrogate of Toluene Reference Fuel (TRF). The gasoline surrogate is used to simulate the behaviour of gasoline since gasoline is very complicated to model. The experiments were run between 740K and 910K at stoichiometric conditions with the simulations tested between 714K and 910K under stoichiometries of 0.5, 0.8 and 1.0. The modelled simulations showed that the greatest difference in ignition delay times came about at lower temperatures, with results converging at higher temperatures. This correlates with the experimental results with poor repeatability experienced at low temperatures of 740K with stable readings noted at 910K. The LCA evaluated the potential carbon impact of UK manufactured Isobutanol using a low carbon natural gas alternative and a UK electricity mix for 2016. Recent advances in biological routes to Isobutanol were also investigated to assess the potential of upcoming developments in the industry.

Bioenergy 2016 Cohort

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Mitigation of Slagging and Fouling through the use of Additives

The aim of the poster is to show various methods used in analysing the propensity of slagging and fouling from biomass combustion. Due to the higher concentrations of potassium and calcium in biomass fuels, this causes slags to form at lower temperatures compared to some coals. If these deposits sinter they have a very high strength and density, which can only be removed during plant shutdown or unplanned outages.

Additive use is a method used to reduce the strength of the deposits. Utilising olive cake ash and fly ash deposits various analytical tests were carried out to determine the effectiveness of an alumino-silicate additive. The tests used were Ash Fusion Test (AFT), compression sinter strength tests and Scanning Electron Microscopy (SEM).

The additive had a mixed impact on the ash depending on the test. AFT data showed that the additive clearly increased the flow temperature as the percentage concentration increased on both the olive cake ash and fly ash. The sinter strength tests showed that an increased additive concentration resulted in an increase in the strength of the fly ash samples at 900 and 1000oC, and in the olive cake ash at 10000C. However, at 900oC the additive has the desired effect of reducing the compression strength. The conclusion from this is that at 1000oC the additive is liquefying and interacting with the ash increasing the compressive strength, therefore the use of alumino-sillicate additives to mitigate slagging may be ineffective at higher temperatures for some biomass.

Complex Particulate Products & Processes 2015 Cohort

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Core Level Spectroscopy of Paracetamol and its Formulations

Tailoring formulations by design would benefit from detailed fundamental understanding of the relationship between molecular level properties and the performance of API physical forms, including interfacial interactions with other formulation components (excipients). Modern core level spectroscopies such as X-ray photoelectron spectroscopy (XPS) and the variants of X-ray absorption spectroscopy (XAS, including NEXAFS, RIXS, XRS) are emerging as bulk- and surface- sensitive techniques that provide deeper structure/performance relationships relevant for manufacturing by design.
To study the solvent influence on nucleation and crystal growth NEXAFS and RIXS studies of paracetamol solutions were performed. A strong solvent influence on the chemical state of paracetamol in solution is evident from the data, with major differences arising due to the absence and presence of hydrogen bonding in protic solvents (ethanol) vs aprotic solvents (DMSO). Comparison with the spectrum of hydrogen-bonded paracetamol in the solid state underlines how sensitive core level spectroscopies are to the state of paracetamol in solution. Initial peaks corresponding to 1s→LUMO transitions were fit by comparison to Time-Dependent Density Functional Theory simulations[1]. The σ* resonances were assigned by comparison to previously published NEXAFS spectra of 4-aminobenzoic acid[2]. In addition, Laboratory XPS analysis with an AlKα photon source was performed on different crystal facets of a single crystal of paracetamol grown in methanol. These studies showed that there is variation in the atomic concentrations at different facets. Furthermore, various surfactant (poloxamer) molecules were adsorbed to the surfaces and could be quantified in terms of concentration.[3]

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Complex Particulate Products & Processes 2015 Cohort

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Monovalent salt effects on enhanced solvent relaxation and particle surface area determination via. spin-lattice NMR relaxometry

Nuclear magnetic resonance (NMR) is commonly used for the identification of unknown compounds; however, the use of proton relaxation rates also allows for surface area determination, from the enhanced relaxation of bound solvent molecules (nominally for particles of any size or shape). Relaxation NMR (relaxometry) is a rapid non-invasive and non-destructive method to study the behaviour of liquids in porous and non-porous media and offers the potential for high speed data acquisition. This research investigated the use of relaxometry to measure the specific surface area (SA) of calcite, silica and titanium dioxide at industrially relevant concentrations and in the presence of electrolytes. The method was shown to correlate well with conventional Brunner-Emmett-Teller (BET) SA measurements of dry powders when suspensions were well dispersed, with the added advantage of being able to measure dispersions wet and over significantly faster timescales. It was particularly advantageous for the measurement of colloidal silica, with good agreement between the measured NMR SA and the calculated D50 SA (assuming sphericity) where the BET measurement was not able to accurately measure the SA. The addition of high electrolyte concentration (1 M KCl) showed no change to the relaxation measurements for aggregated titanium dioxide at the isoelectric point. However, for de-stabilised suspensions of calcite and silica, a relaxation rate enhancement was observed, despite the coagulation of the dispersion (which would be assumed to reduce available SA). It is proposed that this enhancement is due to specific ion effects at the surface of these particles, which arises as a result of particle charge. This study highlights the value that NMR relaxation measurements can offer to industry for the monitoring, and formulation control of concentrated slurries, more specifically, understanding particle surface area and interfacial chemistry.

Complex Particulate Products & Processes 2015 Cohort

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A density functional study of the approach, adsorption, and integration of molecular salt species at crystal surfaces

In order to develop a better understanding of how molecular salt crystals grow and dissolve, it is important to understand what is happening at the surface of these crystals during phase transitions. This work will use density functional methods to simulate the conformational changes of ionic species as they approach surfaces, adsorb onto the surface, and as subsequent layers form over them. 4 amino(biphenyl)carboxylic acid (ABCA) has been selected as the model system, due to its relatively simple structure and its ability to form both anions and cations.

These simulations will reveal energetic pathways associated with the approach, adsorption, and integration of ABCA into a crystal structure at a specific surface and from a specific solvent. By comparing the conformer favoured in solution, with the conformer favoured in the solid states, and understanding the energetics of conversion from one to the other, a link between the chosen solvent and the polymorph which grows will be made. Extending this idea to consider how these energetics are modulated at specific crystal faces will establish a link between the conformer of the molecule in solution and the growth rate of individual faces.

Ultimately, this work will establish a method of crystallisation solvent selection based on the desired polymorph and crystal habit.

Complex Particulate Products & Processes 2015 Cohort

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Beyond Matched Molecular Pairs: Can incorporation of crystallographic information provide a useful insight into solid state behaviour of small organic molecules?

Matched molecular pair Analysis (MMPA) is method based on comparison of pairs of molecules that differ by one transformation. The corresponding change in properties across a large dataset of molecules can be used to statistically infer the effect of the particular transformation on a property of interest. This method performs efficiently on large datasets and provides chemists with useful information on potentially beneficial transformations for optimisation of a given candidate molecule. Many of the properties that are relevant to manufacturing of pharmaceuticals, such as solubility, are influenced by the molecular and the crystal structures. These properties are difficult to predict, making assessment and improvement of molecule's 'manufacturability' challenging.

The aim of the project is to expand upon the concept of MMPA by inclusion of crystallographic data. This adds a second dimension to the change that can be studied – solid state transformations. It provides a novel way to predict properties that influence 'manufacturability'. The poster presents a method for incorporation of crystallographic data from CSD (Cambridge Structural Database) into a MMP relational database and show how it can be used to study a wide range of properties within the context of material science and manufacturability of small organic molecules.

Complex Particulate Products & Processes 2015 Cohort

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The Interfacial Interactions between Faceted Crystals: An in-silico & Atomic Force Microscopy Study

The formulations of pharmaceutical products have historically been a time and resource extensive endeavour[1]. The compatibility between the active pharmaceutical ingredients (API) and the excipients (Exp) used plays a critical role in the final product performance. Gaining an understanding of the inter-particle interactions between API-Exp within solid dose formulation can impact the drug product manufacturability. The ability to pre-screen API-Exp compatibility in-silico would allow formulators to make a more informed decision on the experimental studies to be carried out thus reducing the development time and resources required to get a product to manufacturing. However, as with any computational model, this must be validated with experimental data. Atomic force microscopy (AFM) is being used to bring together two surfaces of faceted and indexed crystals of acetaminophen and a range of excipients to measure the adhesive forces at the interface. AFM studies[2] have been previously carried out using colloidal probes and coated cantilevers, however, there is a lack of fully faceted crystals adhesion data. As part of the in-silico studies, both Molecular Mechanics (MM) and Molecular Dynamics (MD) methods are deployed to examine the interface with and without the presence of solvents on specific facet interfaces. By focusing on facet-specific interactions both computationally and experimentally, energetics associated with the surface chemistry can be identified and thus surfaces could be modified to restrict certain facet-specific properties such as hydrophilicity. A ranking system can be developed thus allowing for a comparison between relative figures across the two work streams to illustrate the optimum formulation for a given product.

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Complex Particulate Products & Processes 2015 Cohort

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Dissolution of Complex Particulate Based products

In-vitro drug dissolution measurement is vital in evaluation of bioavailability, efficacy, batch to batch quality, screening of potential candidates, and as a single important quality control parameter. Therefore accurate dissolution modelling is required as a predictive tool before going into expensive experimental methods. There are many dissolution models which are currently being used to predict dissolution of particles and most of them are based on Noyes Whitney equation. This project looks into both computational and experimental aspects of dissolution to incorporate those factors into modelling, which are very important but have been ignored by models based on Noyes-Whitney equation, like surface specific dissolution based on the chemistry of different faces and the effect of hydrodynamic environment. Visualhabit, Molecular dynamics and CFD are part of the tool set being used for computational work. Visualhabit has been used to list relative dissolution rates of ibuprofen crystal faces based on binding energy loss, when slices are cut from different faces in vacuum. It was predicted that in low index faces, (110) dissolves faster than (100). Similar results were obtained when surfaces were probed by using ethanol molecule. The effect of solvent is being predicted in more detail by using MD simulation. Experimental work on single crystal will be carried out in stagnant and hydrodynamic environment to verify results of simulation.

Complex Particulate Products & Processes 2015 Cohort

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Crystal Growth Inhibition: Inhibitors for Molecular Salts

The control of crystal shape during solution crystallisation processes is a significant challenge: for example, in pharmaceutical applications, crystal shape influences both manufacturability and the product performance of solid dosage-forms. An ability to modify the relative rates of crystal growth on different crystal surfaces, due to the presence of low concentrations of additive species in the mother liquor during solution crystallisation, is an interesting challenge from both a scientific and technological perspective. Crystal habit modification is an area that has received attention. Naturally occurring impurity species, or a purposely added additive species, in a crystallising solution may preferentially bind to particular growth surfaces host crystals during the growth process, changing the structure of the solution at each interface and hence affecting the growth kinetics on a surface-specific basis. The modification of the crystal growth kinetics and resulting change in crystal morphology may enhance both the physical-chemical properties of solid forms of drugs and provide benefits during downstream processing. Due to the complexity of the crystallisation process it is often difficult to determine growth mechanisms through experimental approaches alone. Considerable progress has been made in the development of in-silico methods for modelling crystal growth processes over recent years for organic molecular systems. In the research presented here, the Amber molecular dynamics package was used to simulate the deposition of ibuprofen solute molecules onto a bulk ibuprofen crystal in the presence of two synthetic impurities closely related to ibuprofen in an aqueous environment. This work would enable greater foresight in the development of mechanistic, kinetic-models to describe crystal growth at crystal/solution interfaces for active pharmaceutical ingredients in the presence of impurity or additive species.

Complex Particulate Products & Processes 2016 Cohort

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Investigation into the effectiveness of Panadol Advance over generic paracetamol

A series of experiments was devised to examine the formulation of Panadol Advance and test the manufacturer's claim of a faster acting formulation. The claim was shown to be true with respect to an own-brand Boots paracetamol tablet. This was achieved through physical observation and by placing samples within an ultraviolet-visible spectrometer to measure dissolution. It was hypothesised that the higher rate of disintegration and therefore dissolution is achieved due to the effect of disintegrants within the Panadol Advance tablet, which are not present in the Boots own-brand equivalent. Fourier transform infrared (FTIR) spectroscopy, Scanning Electron Microscopy (SEM) with energy dispersive X-ray (EDX) analysis, thermogravimetric analysis (TGA) with differential scanning calorimetry (DSC) and X-ray powder diffraction (XRD) all showed that paracetamol was the major ingredient and in some cases dominated the test, making it difficult to distinguish other components that were in very small quantities. The presence of calcium carbonate was detected through XRD and TG analysis, as well as through the presence of Ca ions under SEM-EDX analysis. FTIR and TGA also detect the presents of starch. Whilst the mass of calcium carbonate, alginic acid, and the combined masses of paracetamol and starch were estimated using TGA, an overall composition with percentages was not established within this study.

Complex Particulate Products & Processes 2016 Cohort

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Investigation into Dulux Brilliant Matt White Paint - What is it and How does it work?

An experimental investigation was undertaken with the aim of understanding the composition and performance properties of Dulux Pure Brilliant Matt White Paint (DM), with specific attention towards its advanced ingredients and associated properties. Thermal analysis using thermogravimetric analysis (TGA) and Differential Scanning Calorimetry (DSC), allowed for organic polymers within the paint to be identified, such as the advanced copolymer, Ropaque Ultra E. XRD analysis showed numerous inorganic, crystalline material present in the paint, relating towards extender particles used in the 10 formulation and the primary pigment, titanium dioxide (TiO2). Furthermore, Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) were utilised to gain images of the rough surface of dried DM, responsible for its matt finish, and also Energy-dispersive X-ray spectroscopy (EDS) mapping, which enabled chemical elements in the paint to be identified, allowing for further compositional information, and showed DM's product advancement – Chromalock. Also, stability of the paint pre-application, relating to its shelf-life, was analysed, showing the importance of solvent content 15 in the formulation and showing DM is stable over a period of approximately two months, but not over approximately two years. Moreover, rheological properties were analysed, relating towards the paints application, arguably dictating its overall performance, as paint is no use at all if it cannot be applied to a surface. DM was found to have good rheological properties for paint, having desirable viscosity when applied, showing thixotropic behaviour and having a relatively low apparent yield stress. Finally, optical comparison between DM and its gloss finish counterpart, Dulux Pure Brilliant Gloss White Paint (DG) 20 found that the DM does have its desired matt finish.

Fluid Dynamics 2015 Cohort

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Fluid Mechanics of Printed Electronics

Using inkjet and 3D printing to produce electronic circuits used in printed electronics has experienced significant growth. New technologies have resulted from this including wearable computing, sensor and diagnostic devices and flexible and lightweight solar cells. This project is in partnership with Dupont Teijin Films (DTF) who is a primary producer of the base film substrates onto which electronic circuits are printed by several customers. In order to understand the properties of the substrate that provide long-lasting performance once printed onto them, the project studies the fluid mechanics at the microscale. The wetting and spreading of fluids on surfaces are examples of microscale properties. Lattice Boltzmann Method (LBM) is used to investigate these properties as it has been shown to to capture the molecular interactions of wetting and spreading. The project aims to understand the effect of the most common/ problematic surface defects on printing by studying droplet-wall interactions. LBM can deal with complex geometries fairly easily making it suitable for this kind of simulations. The Shan-Chen multiphase LBM model is used to model the printing process. This poster will highlight the methodology, example simulation results including printing onto a step and into a pixel, and plans for future work.

Fluid Dynamics 2015 Cohort

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Surge propagation in debris flows

Submarine debris flows are a potential geohazard to telecommunication cables, pipelines and seafloor equipment, such as well heads. They may also transform into turbidity currents (whose deposits can form hydrocarbon reservoirs). Current theory does not well capture the transitions between laminar (non-Newtonian) to turbulent (Newtonian) rheological states; further insight is required to enable more accurate hazard prediction and to maximise economic benefits.

Surges are inherent to debris flows, and may play a role in flow transformation; here they are investigated in experiments in which dyed diluted glycerol at varying concentrations was released inside a 5m long, 0.25m wide Perspex tank via the removal of two pneumatically-controlled lock gates; a phased lock release generating a laminar flow with an internal surge. Evolving flow was captured with a series of HD cameras. For certain concentrations, the pulse propagates as a bore on the upper flow surface; an abrupt transition from relatively-dense, laminar flow to turbulent dilute flow may occur as the bore reaches the flow front.

To model bore propagation, a finite-difference numerical scheme based on depth-averaged, shallow water equations in the Lagrangian frame of reference was implemented in both a single-layer and two-layer formulation and validated with the experimental data. Both numerical models qualitatively captures some of the key flow features, such as the pulse, with the two-layer version significantly more accurate. Although the work exposes the limitations of depth averaged numerical models, it also demonstrates promise in constraining the role of intra-flow surges in debris flow transition.

Fluid Dynamics 2015 Cohort

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What determined the motion of Typhoon Hagupit (2014)?

Tropical cyclones (TCs) are amongst the most destructive and dangerous weather systems in the world. Storms that make landfall can be both lethal and expensive. High risk areas, such as the Philippines, rely on accurate forecasts of the track and intensity of TCs. Whilst track predictions have improved over the last few decades, there are still cases where the numerical weather prediction models are unable to accurately predict the motion of the storm. One such storm to make landfall over the Philippines is Typhoon Hagupit (2014). Hagupit killed 18 people and caused £71 million of damage. Ensemble forecasts showed large uncertainty in the track of the storm, meaning the location of where the storm would make landfall was still unknown days in advance, making it difficult to take the necessary precautions. Using the Met Office's Unified Model, both global forecasts and 4-km local forecasts are analysed to investigate what determined the track of Hagupit and what could cause the uncertainty within the ensemble forecasts. Results from the global model show that the storm enters an area between two high pressure systems to the east and west at the time when the different tracks begin to diverge, i.e. the storm was positioned at the saddle point in the environmental flow. Accurately predicting the storm's interactions with its environment, such as upper and mid-level troughs, is likely to be of importance. These interactions, as well as the three-dimensional structure of the storm and its environment are investigated using both the global and convection-permitting model.

Fluid Dynamics 2015 Cohort

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Aerodynamic action on inclined stay cables in cable-stayed bridges

Fluid flow past cylindrical structures arises frequently in various engineering and environmental applications. A few notable examples are: aircraft landing gear, oil risers, and cable-stayed bridges. This study investigates the relationship between upstream fluid flow, wake dynamics, and flow-induced vibration (FIV). The majority of previous studies have focused on primary shedding structures and forces on the vertical rigid cylinder. This investigation elucidates previously overlooked observations, especially in the inclined configuration, where there exists contradictory evidence in the literature. Inflow conditions, inclination angle, and the effect on the wake dynamics are examined. Findings are related to the cable-stayed bridge, a favoured design, but susceptible to stay cable oscillation due to their 3-dimensional arrangement to the flow. Limitations of FIV models used in the engineering industry will be highlighted. Large eddy simulation of flow past an inclined cylinder has been carried out in OpenFOAM. The relationship between inclination and upstream turbulence is explored by considering the spanwise correlation of flow structures. Small-scale water flume experiments with particle image velocimetry will be undertaken, providing validation with numerical results. The aforementioned work aims to contribute towards greater understanding of inclined cylinder FIV, guiding better engineering design, and therefore reducing the probability of failures.

Fluid Dynamics 2015 Cohort

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Shark biomimetics: Drag reduction beyond parallel riblets

The hydrodynamics of shark skin has been the focus of much debate over the last few decades due to the small tooth-like structures found on their skin. While the shape of these dermal denticles ("skin-teeth") varies significantly between different species, most work has focussed on the riblet features which are often present on the denticle crown. While there is much agreement over the impact of riblets on a flow, literature concerning real shark scales is much more controversial. Some authors determine a drag increase of up to 50% while others report a drag decrease of up to 35%. There are several reasons that contribute to these discrepancies, such as replication methods, type of shark scales, and experimental technique. This project aims to investigate what effects the denticle geometry has on the flow, achieved using Large Eddy Simulation (LES) and Reynolds Averaged Navier-Stokes (RANS), validated against 3D Laser Doppler Anemometry (LDA) experiments. If the hydrodynamic impact of scale geometry can be properly understood, then this could lead to the design of similar biomimetic-inspired structures and applied to engineered surfaces.

Fluid Dynamics 2015 Cohort

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Identifying Optimal Eel Tile installation using Computational Fluid Dynamics

Eel tiles are increasingly used as a method to facilitate the passage of eel and elver over instream structures in response to the Eels Regulations 2009. However the hydraulic performance of the tiles and consequently the implications for passability of the eel tiles still remains uncertain. A series of computational fluid dynamics (CFD) models are developed to simulate the flow field over a model eel pass (eel tile). The models are based on the fully 3D Reynolds-averaged Navier-Stokes equations and use the volume of fluid (VOF) method to determine free surface location. The flow field is resolved for a range of eel pass inclinations and discharges, and compared to literature on the prolonged and burst swimming capability of European eels. Results indicate that CFD modelling is a useful tool in eel tile and fish pass design. Simulation results are used to develop a 2D parameter space such that practitioners can readily identify suitable eel tile inclinations and approach depths for eels and elvers of different body length.

Fluid Dynamics 2015 Cohort

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Modelling Infectious Aerosols

Airborne infection is of particular concern for people with Cystic Fibrosis (CF). There are several pathogens that concern those with CF, this project focusses on two: P. aeruginosa and M. abscessus. Bio-aerosols, such as the droplets people expel via coughing and sneezing, have long been understood as an important mode of transmission of infectious diseases. There is a lack of knowledge on the factors that affect aerosolisation. Microorganisms and drug treatments can influence the surface tension and rheology of the liquid that they are suspended in. This may affect the potential for the microorganism to be released in the aerosol as well as the size of the aerosol formed. An enhanced understanding of the evaporation and movement of pathogen-laden aerosolised droplets is essential to exploring the fundamental mechanisms that govern this transmission process. A 2D and 3D CFD model using FLUENT has been used to optimise the geometry of a previously used experimental rig. Bio-aerosol decay of previous work has been studied and will be compared to the CFD model. The optimised rig geometry will be used in future experiments that will analyse how pathogens affect evaporation and aerosolisation. This will be further analysed using an evaporating droplet model in MATLAB.

Fluid Dynamics 2015 Cohort

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Turbulence in Gravity Currents

Gravity currents are commonly found in both nature and industry, and as such there is significant interest in understanding their behaviour. There has, therefore, been extensive experimental and numerical work regarding such flows. Despite this, many aspects of their mechanics remain poorly understood. This work aims to improve understanding of the turbulence structure in gravity currents, particularly the formation of coherent turbulent structures within the current body and their effect on flow dynamics.

Particle image velocimetry is employed to measure the two-dimensional velocity field on a central plane in solute-driven constant-flux gravity currents. This is compared to a central plane in three-dimensional DNS simulations conducted for a similar flows using the spectral element solver NEK5000. These simulations, as well as previous numerical work, indicate that the turbulence structure in gravity currents is highly three-dimensional. To date, no fully three-dimensional experimental measurements have been made.

Moving forward, tomographic particle image velocimetry will be used to provide the first three-dimensional measurements of gravity currents. Flows with Reynolds numbers between 1000 and 5000 will be measured experimentally. After validation against the experimental data, simulations will be used to investigate how turbulence scales with Reynolds number, providing a valuable link between experimental and real-world flows.

Fluid Dynamics 2015 Cohort

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Modelling filaments produced by magnetically confined plasmas

Cross-field particle transport in magnetic confinement devices is dominated by intermittent ejection of coherent filamentary structures from the centre of confined plasma. These filaments are considerably denser and hotter than the surrounding background plasma. They move under the action of an effective gravity force that arises due to curvature and magnetic field gradients, transporting plasma across a region of open magnetic field lines known as the scrape-off layer and ultimately impacting on the surrounding material boundaries.

This is an issue for fusion reactors, since large fluxes of plasma impinging on material walls can cause significant erosion of the surface and component damage, and thus possibly limit the lifetime of the device. Surface particles can also become liberated from the material and enter the core of the plasma as impurities, degrading the performance of the reactor.

The goal of this research is to uncover the fundamental mechanism for generation of plasma filaments. The initial research consist of a theoretical investigation of an idealised fluid problem. We consider 2d electrostatic drift-fluid model of isothermal plasma with singly charged ions. The geometry is simplified to a local slab geometry with effects of magnetic curvature and gradient included through additional terms in the evolution equations, which consist of equations for plasma density and vorticity. These equations can be recast to resemble equations governing 2d Rayleigh-Bénard convection with additional terms. Through a linear stability analysis, we investigate the effects of these extra terms and also provide an interpretation in terms of the convection problem.

Fluid Dynamics 2016 Cohort

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Gravitational Collapse of Colloidal Systems

Small scale fluid dynamics is fundamental to the theory of colloids. Colloidal suspensions are mixtures containing very fine insoluble particles which are dispersed throughout a continuous phase. They can be found in many applications, such as consumers products, medicines and industrial waste. In consumer products, a crucial requirement is that the suspended colloids must not settle noticeably during the product's shelf-life for it to remain effective and convey quality to consumers. This combined experimental and modelling study has investigated the phase separation behaviour of colloidal suspensions. An existing settling model has been further developed to take into account additional effects, including rheological and chemical influences, within the framework of a convection-diffusion equation. It takes into account the influence of the ionic double layer which forms on the colloidal particles when dispersed in water. The settling model has been implemented numerically in MATLAB, using a finite difference solver with an adaptive spatial mesh and time-stepping scheme for improved efficiency. Further, models for the aggregation of the colloidal particles, which may occur depending upon various chemical parameters, have been investigated. The settling model compares favourably with highly controlled experiments for different dispersed phase volume fractions and electrolyte concentrations. Indeed, the settling behaviour of silica-water suspensions has been examined by tracking the evolution of the interface which develops between the suspension and supernatant (colloid-free fluid) above. These experiments have been conducted at both Earth and enhanced gravity, the latter using an innovative method for converting the results to Earth gravity conditions.

Fluid Dynamics 2016 Cohort

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Bubbly Flow in Steel Ladle Furnace

A study on the effect of bubble size and gas flow rate, on a ladle furnace during secondary refining of the steel making process, was carried out. Secondary refining in the ladle furnace plays an important role in the quality of steel. The refining process is used to increase homogenisation of alloy composition and temperature, whilst causing inclusions to be taken out of the melt by a slag layer. By studying the flow behaviour occurring in the ladle, we can better understand the phenomena that take place and optimise process parameters to produce higher quality steel. In this study, using a scaled water model of a ladle furnace, we measure and analyse the flow field produced by different bubble size distributions, via porous plugs, at different flow rates. A bottom-stirred ladle with centred and off-centred air plugs has been modelled. A PIV laser system has been used to measure and analyse the flow field inside the model. A Eulerian-Lagrangian multiphase computational fluid dynamics (CFD) model was created using ANSYS Fluent, and macro-scale mathematical modelling done for both the plume and bulk flow. The flow patterns and statistics of the flow were compared between the experimental results, CFD model and analytical model for validation of the modelling work.

Fluid Dynamics 2016 Cohort

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'Wetropolis' Flood demonstrator for Nature-Based Solutions

Extreme weather events are rare and due to a lack of data it is difficult to predict record-breaking floods such as the Boxing day floods of 2015. Flooding was the result of varying rainfall across numerous days. By increasing storage space and slowing the flow, we can mitigate the downstream flood risk.

The aim of this work is to develop the prototype of an interactive physical model combining the influence of Nature-Based Solution (more narrowly called Natural Flood Management) measures (e.g. floodplain roughness, soil structure) and hard engineering (by using real-time control for reservoir storage in naturally suitable flood plain areas) on downstream flood risk.

Initially, one-dimensional mathematical models of the different components in the physical model were developed; a groundwater level model for the moor and a scalar kinematic equation for the river.

These models have been implemented numerically using the finite element and finite volume methods, and have been successfully validated against Wetropolis. The numerical models now act as a tool for parametric studies to investigate the effect of nature-based solutions by using different channel roughnesses modelled by the Manning friction coefficient, thus aiming to reduce downstream flood risk. Furthermore, we refine this simple model to not only consider a uniform river channel but to include the different cross sectional areas seen at different sections along the river. Alongside this, a two-dimensional model has been implemented using a volume of fluid model to test its suitability, with promising results.

Fluid Dynamics 2016 Cohort

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Downdraughts in convective storms

During a thunderstorm, rain falls and cools the surrounding air causing it to drop towards the ground and form a downdraught. A downdraught occurs on a scale of about one kilometre, the code used by the Met Office to predict the weather works at scales much larger than this, and is hence unable to directly resolve the flow. To combat this, a downdraught is parametrised so that the effects are felt on the large-scale, but the flow is not resolved explicitly. A mathematical model of a downdraught must therefore be used to approximate the effect on large-scale weather systems. In this project we attempt to improve our understanding of a downdraught so that these effects can be better predicted. Three different aspects of the downdraught are studied: the effect of the raindrops on the descending air; an attempt is made to resolve the flow of air near the ground; and an intermediate regime between a thermal and a plume model, two limiting cases that have been widely studied, is considered. Laboratory experiments are used to visualise and quantify a downdraught, as well as validate theoretical models and numerical simulations. This research should give greater insight into the dynamics of a downdraught, the effect of a downdraught on the surrounding atmosphere, and the creation of new thunderstorms.

Integrated Tribology 2015 Cohort

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Poroelastic lubricity of micro-porous polydimethylsiloxane (PDMS)

With an ever increasing need to reduce the friction and wear of machines, work has turned towards bio-inspiration in order to improve tribological systems. Natural synovial joints display particularly favourable tribological characteristics; extremely low friction and wear. It is postulated poroelasticity is one of the mechanisms responsible for these properties.[1]

Microporous PDMS was prepared using a templating technique with heat sintered poly(methyl methacrylate) (PMMA) beads. Compression tests were carried out using a Mecmesin compressor with a load cell of 10 N. Tribological tests were completed under a range of conditions using both a bespoke tribometer and an Anton Paar NTR3 nano-tribometer with either water or glycerol as the lubricant.

Although the porous samples did not exhibit significant poroelastic behaviour with aqueous lubrication, using glycerol as a lubricant did result in the porous samples demonstrating poroelastic properties, halving the frictional coefficient as compared with water, and under some sliding conditions reducing the frictional coefficient to as low as 0.15.

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Integrated Tribology 2015 Cohort

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Bio-Inspired for Functional Aqueous Lubrication

Polymer brushes have been studied through experimental and theoretical means over the past three decades because of the huge potential and possibilities to greatly improve surface properties [1]. Replication takes place by grafting polymers to substrates where one end is tethered to a surface while the other end is free to extend from the surface, constrained only by its elasticity [2]. Charged and zwitterionic polymer [2-Methacryloyloxethyl Phosphorylcholine Polymer (MPC)] brushes surfaces can effectively achieve hydrated lubrication. The hydration layer can strongly hold and have the ability to support large pressures without squeezing out, but can also relax very quickly providing fluid response to shear. Such surfaces have been shown to be highly hydrophilic and as a result low friction coefficients (<0.001) have been achieved using nano-tribological methods [3]. The aim of this project is to investigate the feasibility of polymer brush technologies as a method of functionalizing a surface for use in water lubricated environments. This will be achieved through a systematic study in which the surfaces, polymer brush chemistry and tribological environment are varied. Whereby the focus will lie upon the effect of corrosion on zwitterionic polymer brushes under hydrated lubricated environments. Methods of optimizing and managing friction and wear response through functional grading and encapsulation within the films will be investigated. Surface characterisation will be conducted through AFM, ellipsometry and contact angle measurement as well as friction testing.

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Integrated Tribology 2015 Cohort

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Ionic liquids as lubricants additives for improved friction and anti-wear performance

Mechanical, primarily frictional, losses in automotive engines ranging from those in passenger cars to commercial vehicles account for approximately 15% of the energy loss. With tribological improvements capable of providing an 18% reduction in frictional losses in passenger vehicles, the need to design efficient engines and effective lubricants is clear. Lubricant and engine manufacturers are also called to consider environmental legislation which aims to reduce the levels of sulphated ash, phosphorous and sulphur (SAPS) emissions. Current trends in lubrication and engine manufacture are therefore focused on improving fuel economy, engine efficiency in addition to lubricant formulation to reduce these losses. At present, zinc dialkyl dithiophosphate (ZDDP) as one of the most commonly used anti-wear additives and a source of phosphorous and sulphur emission, ionic liquids have emerged as promising alternative. Ionic liquids have many promising properties which include high thermal stability, compatibility with different surfaces, low volatility etc. Since 2001, ionic liquids have shown positive results in reducing friction and wear as both neat lubricant and additives. However, there are several limiting factors that hinder the wider application of ionic liquids in engine oils. These include their immiscibility in non-polar base oils as well as their high cost. By using ionic liquids as additives, this can drive down the cost compared to using neat ionic liquids. More importantly, encapsulation of ionic liquids can improve the miscibility of ionic liquids in base oils and allow for their use as engine oil additives to improve friction and wear. My research therefore involves the microencapsulation of ionic liquids for use as engine oil additives to improve the anti-wear and friction properties of the oil.

Integrated Tribology 2015 Cohort

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An Investigation of the Soot- Induced Wear Mechanisms in Diesel Engines

The use of exhaust gas recirculation in diesel engines leads to the formation of soot as a result of poor combustion. Soot contamination in engine oil is known to induce high wear in engine components with the potential to cause engine failure however the wear mechanism is not fully understood. Salehi et al. found that adding carbon black to fully formulated oil produced much higher wear than when added to base oil. In this study, the tribological effect of dispersant and anti-wear agent was investigated in the presence of carbon black for boundary lubricated conditions. Findings show that when both dispersant and anti-wear additive are present, the wear is comparable to the wear seen in fully formulated oils. It was suggested that the corrosive- abrasive wear mechanism was responsible for increased wear however further investigation is required to confirm this theory.

Integrated Tribology 2015 Cohort

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High-Performance Polymer Composites for Extreme Conditions

The use of polymers is increasing throughout many different industries as their low weight and chemical resistance provide many advantages over metals. However polymers are limited by the temperature and load that they can withstand. By adding a reinforcement to a polymer, such as fibres or nanoparticles, the properties can be improved and the resulting composite material can be used over a much wider range of conditions. Extreme conditions are encountered in particular by aerospace components. The most commonly used polymer in aerospace is polyetheretherketone (PEEK), however interest is growing in other high-performance polymers such as polyphenylene sulphide (PPS). As a preliminary study, the tribological behaviour of both pure PEEK and carbon fibre-reinforced PEEK (PEEK-CF) was investigated. These experiments formed the groundwork and established a suitable methodology for a larger investigation involving other high-performance composites.

Tribological tests were carried out in dry sliding on a pin-on-reciprocating-plate rig. A spherical pin of aerospace grade steel (AISI 440) was used against a polymer plate, manufactured from either pure PEEK or PEEK with 30% carbon fibre content.

The sliding speed and test time were kept constant, while the load was varied. The coefficient of friction could be calculated for the duration of the test. Analysis of the wear scar was carried out using microscopy, and the effect of the carbon fibres could be evaluated with regards to the mechanisms at work in the contact. Future tests will be carried out at low temperatures to simulate some of the extreme conditions encountered in service.

Integrated Tribology 2015 Cohort

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Nano-mechanical characterisation of DLC coatings for tribological performance

DLC coatings are becoming increasingly popular in the automotive industry due to their high hardness, resistance to wear and low friction coefficient (Johnston and Hainsworth, 2005). They can suffer from poor adhesion at high loads and impact stresses (Horiuchi et al., 2009). Well characterised coatings will enable the relationship between mechanical properties and impact behaviour to be studied. PVD coatings will be deposited on tool steel and stainless steel, adhesion will be varied with Cr and Ti interlayers and varying substrate roughness. Characterisation will take place with nanoindentation, nano-impact, microindentation, AFM, Raman spectroscopy, SEM, SIO modelling and x-FIB of nano-impact craters.

Nanoscratch measurements will assess coating adhesion. Determination of ploughing contribution to friction measurement will be assessed as will the influence of surface roughness and indenter properties.

Tribocorrosion measurements of DLC will be taken and wet and dry scratch tests will be performed to investigate the influence of moisture on DLC coating performance.

Fretting tests will be performed to determine the influence of mechanical properties on friction and wear behaviour. Impact testing will be used to compare with the fretting results. Raman spectroscopy will be used for monitoring tribo-film formation.

Performance of an older model Nano-POD tribometer will be critically analysed and compared with nano-fretting results to determine its potential and compare reciprocating and unidirectional sliding. SEM and Raman spectroscopy will monitor the formation of tribo-films.

Macroscale tribometer tests will be performed to observe the difference in results and attempt to narrow the gap between the nanoscale and macroscale in tribology.

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Integrated Tribology 2015 Cohort

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Implementation of MCA in the framework of LIGGGHTS: Towards predictive modeling of dry friction and wear

The Movable Cellular Automata (MCA) method was first introduced by Psakhie, Horie et al in 1995 as a hybrid particle-based method based on the classical cellular automata (CA), discrete element (DEM) and molecular dynamics (MD) methods; combining their advantages. It allows the modelling of complex materials behaviour and processes, such as crack generation and growth, mass mixing, phase transformation, etc. Many developments have been made and MCA is now presented as a discrete approach to model the behaviour of materials on different scales and is used as multi-scale modeling approach. This paper focuses on the implementation of the MCA method within the framework of the opensource code LIGGGHTS; which stands for LAMMPS Improved for General Granular and Granular Heat Transfer Simulations. LIGGGHTS is based on DEM to simulate granular materials, MCA is implemented to simulate complex solid behaviour, most importantly plastic deformation. The main difference between MCA and DEM is that the interaction between the particles is based on manybody forces of inter-automata interactions; similar to the embedded atom method used in MD; because pair-wise interactions between elements are insufficient to simulate irreversible strain accumulation (plasticity) in ductile consolidated materials. LIGGGHTS was chosen as a framework due to its massive parallel computing capabilities, giving MCA the capability of simulating more complex systems on higher scale levels. The testing and verification of the code includes 1- showing the macroscopic isotropic mechanical response for the simulated material by simulating loading and unloading of uni-axial compression, tension and shear loading of 3D material samples, 2- nano-indentation and scratching models similar to the ones simulated in [4]. Nano-indentation simulations will show the capability of modeling plastic deformation in contact interaction, and scratching simulations will show the capability of modeling fracture. The results show good correlation with analytical solutions. The code could potentially be used in many different applications on different scales; such as the modeling of wear.

Integrated Tribology 2015 Cohort

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Fatty amine/ZDDP interactions for improved tribological performance.

Reduction in fuel consumption and tighter environmental restrictions on the combustion emission products are among the key challenges of automotive industry. One way to address these challenges is by developing more efficient and environmental friendly lubricant additives. Organic friction modifiers (OFMs) are long chain compounds with polar end groups, including amine, amide, carboxylic acid, ester, alcohol, borate and phosphate are few of them. Zinc dialkyldithiophosphate (ZDDP) is an effective anti-wear additive used in the formulation of the lubricant but at the same time it also increases the boundary friction coefficient, which affects the fuel consumption of the automotive engine. ZDDP is the main source of phosphorus in the lubricant which suppresses the catalytic activity of catalyst components and reducing their efficiency to convert CO to CO2.

The current study will reveal the friction and wear performance of fatty amine (FA) along with reduced concentration of ZDDP by using unidirectional pin on disk arrangement and furthermore analyze the growth kinetics, physical and tribological properties, chemical composition and thickness of the tribofilm generated.

Integrated Tribology 2015 Cohort

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Tribological Performance of Through-Hardened and Case-Hardened (Nitrided) Steel Systems in the Boundary Lubrication Regime

Often, engineering systems with interfaces that operate in the boundary lubrication regime are susceptible to increased friction and wear. This reduces the working efficiency of the systems, sometimes resulting in complete failure of the system. To improve the tribological performance at the interfaces, the intrinsic and/or surface properties of these components can be modified via various thermochemical treatments. Nitriding is a popular surface modification technique, well-known for its ability to create a hard nitrogen-rich surface layer that can offer a reduction in friction and wear at the interface, as well as enhancing corrosion resistance. This treatment has been applied to gear and hydraulic components, to name a few. Lubricant-additives also play a crucial role in improving their tribological behaviour. The current study investigates the influence of different additives on the tribological performance of through-hardened and nitrided EN31 steel. Interesting synergies were observed with the nitrided systems in the presence of the different oil formulations, and although generally the hardened EN31 was more wear-resistant than the nitrided steel, friction performance of the nitrided steel systems was strongly influenced by the oil additives. EDX analysis within worn regions indicate formation of a tribofilm. The poster discusses the formation of these tribofilms on nitride surfaces and their effect on tribological performance.

Integrated Tribology 2016 Cohort

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Tribology of Fuel Contaminated Engine Oils

Investigations were undertaken to evaluate gasoline contamination in oil at elevated temperatures and to attempt to develop a top up method for the maintenance of constant gasoline contamination in oil during tribological testing. Samples were prepared with 2-12% gasoline contamination and heated to 25-120°C (typical internal combustion engine temperatures) for a period of 2 hours. Half of the samples were heated in open air to allow evaporative losses to take place whilst the other half were heated while fitted with a reflux condenser to prevent evaporation.

The samples were then analysed by GC-FID, FTIR and viscometry. FTIR displayed that no new functional groups were being formed at the temperatures and therefore it is unlikely that gasoline triggered the ageing of the motor oil. GC-FID results found that total gasoline contamination decreased as temperature was increased, with lighter compounds (9 carbons and below) being evaporated at a higher rate. This means heavier carbons from gasoline may accumulate within motor oil over time. Viscometry showed that gasoline contamination significantly decreases the viscosity of oil, and although evaporative loss of gasoline with temperature did increase viscosity this effect was relatively small. This suggests that heavier gasoline compounds may have a lasting effect to decrease the viscosity of oil.

Integrated Tribology 2016 Cohort

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Binding and tribological properties of layered mucin and lactoferrin for drug delivery applications

The oral cavity presents many challenges when investigating possible drug delivery routes. In particular creating a multi-layered oral mucosal layer can be an effective technique to simulate oral mucosal layers and study in vitro oral drug delivery. This study aims to investigate the creation of such multi-layered scaffolds using the binding of anionic mucin to cationic lactoferrin. Mucins are highly glycosated proteins that play a pivotal role in creating gel-like secretions to act as lubricants in addition to creating a smooth surface to minimize shear stress. Lactoferrin, also present in saliva, is a glycoprotein with anti-microbial properties with unique isoelectric point at pH 8.5. In this study, multi-layer films consisting of porcine gastric mucin and lactoferrin were prepared on gold substrates using layer-by-layer assembly. Six protein bilayers were deposited on a Quartz Crystal Microbalance to observe the electrostatic binding behaviour. The lubricating ability of the protein multi-layers was measured using a Micro Tribometer with a gold sphere exerting 0.2N load, sliding uni-directionally along a gold plate. Atomic force microscopy was used to observe the topography and ellipsometry was used to measure the final film thickness. This preliminary study offers a fundamental understanding of multi-layered protein scaffold which has potential for the development of more advanced oral drug delivery systems.

Integrated Tribology 2016 Cohort

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Comparing Ultrasonic Viscosity Measurement Techniques and Their Ability to Measure Degraded Oils

As oil undergoes extreme conditions for long time periods it will inevitably degrade, therefore increasing the viscosity. If the oil viscosity could be measured continuously then a warning system could be put in place to alert the operator whenever the oil needs changing, thus optimising the oil change interval. In previous research two different ultrasonic methods have been used to measure fluid viscosity: the pulse-echo method and the continuous wave method. Both methods calculate viscosity from the amount of energy reflected at the solid liquid interface; a more viscous fluid will reflect less energy as more energy has been transmitted into the fluid. This project investigated these techniques' ability to accurately measure the viscosity of degraded engine oils, and compared the measurements with those of a work bench rotational viscometer. The ultrasonic techniques produced lower viscosity measurements than results obtained from the rotational viscometer in all but one case, in which the viscosity measurement produced by the continuous wave method was slightly larger than the rotational viscometer's measurement. A possible hypothesis is that these results are due to the transmitted shear wave entraining and measuring only the smaller molecular weight substance, thus giving an artificially low viscosity. In addition, the continuous wave method's viscosity reading was consistently higher than the pulse echo method's reading; this could be due continuous wave method transmitting more energy into the system, therefore entraining more of the heavy molecular weight substance and giving a more realistic viscosity measurement.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Developing Graphene oxide biomaterials for Neural tissue engineering

Graphene oxide (GO) is a two dimensional nanomaterial with promise as a biomaterial. Though biologically inert, GO is physically strong and flexible at macroscale, comprising a single atom thick planar lattice of carbon featuring oxygen containing functional groups available for chemical modification such as reduction to restore electrical conductivity, or covalent modification to permit polymerisation to hydrogel matrices. GO has generated substantial international interest in tissue engineering as a scaffold substrate.

The properties of graphene materials align with the culture requirements of neural cells, including conductivity, microporous topographical structures such as tube and filament structures for attachment, and an affinity for peptides through electrostatic binding interactions and disulphide bridges when properly modified. Additionally, previous studies suggest graphene based culture environments may inherently drive differentiation of neural progenitor cells to neuron and oligodendrocyte lineages.

This work has begun to develop Graphene Oxide as a platform for chemical modification and subsequent integration to polymeric hydrogels as a scaffold for culture of heterogeneous 3D neural tissue from neural progenitor cells. Currently work has focused on biocompatibility and cell growth characteristics in two dimensions on as-supplied and thiol modified graphene oxide films using SH-SY5Y cell lines.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Rapid label free separation of stromal cell cultures for musculoskeletal disease

Introduction: Musculoskeletal diseases represent the second greatest cause of disability worldwide. Current strategies include the use of stem cells to coat engineered scaffolds in order to repair the damaged tissues. For this, the patients' autologous cells are harvested and amplified in the laboratory. This process requires time and cell manipulation which can have an impact on the patients' safety and on the final cost of the therapy. In order to make this approach easier and more cost-effective, there is a need for a device.

Methods: By using remote dielectrophoresis, where an electric field is coupled into a microfluidic channel using surface acoustic waves, cells can be separated with minimal manipulation. The device will be first optimised with the use microfluidics modelling and tested with a complex mixture of cells. After separation, the cells will be tested by seeding them on scaffolds and staining for osteogenic potential markers. After in vitro validations, cell seeded scaffolds will be implanted into athymic rats with calvarial defects. The performance of the cell separation will be compared to that obtained with magnetic activated cell sorting.

Results: Proof of concept of this technology has been already done on yeast cells and dental pulp cells. Experiments on latex beads showed critical parameters of the channel needed to optimise particle alignment.

Conclusion: This research aims to scale up this technology to provide a safe and label free separation of stem cells in a real intra-operative time while maintaining their osteogenic potential.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Molecular Imaging of Abdominal Aortic Aneurysms

Abdominal aortic aneurysms (AAAs) are localised dilatations of the abdominal aorta that progress over time and eventually rupture. Current diagnosis and monitoring approaches are limited to visualising anatomical changes in the vasculature once the disease progresses to more severe stages, at which point surgical intervention poses a greater risk. In vivo molecular imaging is a promising approach in AAA, with its ability to combine functional and anatomical information. The aim of this project is to use molecular imaging modalities to study molecular mechanisms underlying AAA in murine models; in particular, bioluminescence imaging and hybrid positron emission tomography–computed tomography (PET-CT) will be used to characterise and quantify pathological cell proliferation and vascular remodelling. Dynamic PET-CT imaging will be performed with the radioactive tracer 18F-fluorothymidine (18F-FLT), the use of which will be demonstrated for the first time in AAA models. 18F-FLT activity correlates with cell proliferation, as its expression is reflective of the synthesis phase of cell division, and has been used extensively in tumour imaging. Herein, 18F-FLT PET-CT may facilitate a more in-depth picture of underlying biological mechanisms by using tracer kinetic modelling to fit time–activity curves of specific regions of interest. Parametric or quantitative images can then be constructed and assessed to describe the pharmacodynamics and biodistribution of the tracer molecule. In this way, implementing multimodal molecular imaging technologies can enable quantitative evaluations of pathological vascular remodelling and cellular proliferation in AAA disease.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Aligned nonwoven fibre guides and tunable hydrogel combine to form a versatile fibre-reinforced scaffold for tissue engineering applications

Spinal cord injury (SCI) affects 40,000 people in the UK at present, with 1000 new injuries annually. The sudden and severe impact results in immediate physical impairment and prolonged emotional distress. High costs are inevitable due to poor regenerative capacity of the tissue, leaving the patient with a poor quality of life for years. Previous attempts to promote regeneration have largely focused on the neuronal component with less importance placed on the supporting environment. Combining materials to promote both may have a positive impact on regeneration.

Aim: Manufacture of a fibre-reinforced hydrogel capable of promoting regeneration of parenchyma and supporting cells simultaneously.

Methods: Electrospinning of aligned fibre scaffold using FDA approved polycaprolactone; tuneable hydrogel production using collagen; effective and reproducible combination of the two materials; evaluation of neuronal guidance and extracellular matrix growth; optimisation of mechanical properties and degradation profile.

Results: Individual components have been produced and characterised alongside partial characterisation of the combined system.

Conclusion: Going forward, biological evaluation of the combined scaffold will accompany optimisation of individual components for appropriate growth and degradation.

Impact: A device evaluated mechanically at the macroscale for handling consideration and the microscale for multi-cellular consideration may promote regeneration better than previous attempts. A device of this nature may have other applications, including peripheral nerve injury, non-union fracture and in vitro modelling.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Development of an in vitro model of traumatic spinal cord injury using the BOSE Electroforce BioDynamic 5110 to investigate different injury mechanisms

Traumatic spinal cord injury (SCI) creates immediate and long-term physical and emotional pain for 1,000 patients every year, in the UK. The intrinsically poor regenerative capacity and inhibitory microenvironment of the lesion post-injury has resulted in slow progress in the development of effective treatments, in humans.

The aim of this project is to develop and implement more clinically relevant injury scenarios, such as high energy, high velocity burst fractures, using neural cell-seeded collagen hydrogels as a physiologically relevant in vitro model of the spinal cord. The relationship between mechanical input and its effects on neural cellular responses, such as viability and astrocyte reactivity, will be investigated.

This project utilises the materials testing machine, BOSE Electroforce BioDynamic 5110 (TA Instruments), which is capable of testing samples within a biodynamic tissue culture chamber. Preliminary tests show the BOSE is capable of simulating contusion type injuries on relatively soft collagen hydrogels, in a reproducible and highly controlled manner. Current optimisation work involves determining the optimal hydrogel height and seeding density for C6 and PC12 cell lines for reproducible injury simulation, and downstream analyses and imaging.

Advancements to scientific knowledge will be achieved through increasing the biological complexity of the model, by incorporating not just glial but neuronal cells as well. In order to establish a more in depth understanding of the potential differential cellular responses to different mechanisms of spinal cord injury, burst fracture/contusion, distraction, and dislocation mechanics will be developed, and compared, using the BOSE.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Rapid Label-free Separation of Specific Stem Cell Populations

Introduction: Autologous stem cell therapies have a huge potential to address clinical challenges in oncology, Parkinson's disease, spinal cord injuries, bone, muscle or cartilage defects and diabetes. Using autologous stem cells is advantageous due to their immunological safety but a major limitation is the isolation of the rare stem cell population in adult tissues. The ability to separate and concentrate cell subpopulations intraoperatively and without labelling would provide a step change in the delivery of cell-based therapies.

Methods: This project will use remote dielectophoresis to separate cells based on their dielectric properties combined with protein-binding proteins (Affimers) to capture stem cells via surface marker recognition. The combination of these two novel technologies will provide high throughput and high specificity with minimal manipulation. There is evidence to suggest the surface marker CD271 isolates a population of cells with therapeutic potential however it is necessary to eliminate hematopoietic CD45(+) cells to achieve high purity. This strategy will be used for specific stem cell separation in this device – positive selection via CD271 and negative selection via CD45.

Results: Phage display screening of the existing Affimer library has identified 3 unique binders for CD271 and 2 unique binders for CD45. Characterisation of these binders is ongoing to select the most suitable for this application. Binders must be highly specific but relatively weak to allow release of cells after capture.

Conclusion: This research will deliver a novel device capable of isolating a minimally manipulated, enriched population of specific stem cells for regenerative therapies.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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The Effects of Experimental Conditions on the Structural and Material Properties of Porcine Patellar Tendon

Several studies have performed mechanical characterisation of tendinous/ligamentous tissues under varying experimental conditions. The effect of freeze-thaw and strain rate is understood however the effect of tissue hydration is disputed and freezing pre-dissection vs post-dissection is not widely reported. The aim of the study was to validate experimental testing conditions of future human ligaments. Twenty-four porcine patellar tendon bone-ligament-bone specimens were dissected, placed into small independent groups (n=3) and tested using an Instron E10000 under a range of experimental conditions including differing number of freeze-thaw cycles, strain rates, hydration levels and specimen storage conditions identifying the effects on the structural and material properties. Freezing pre-/post-dissection had no significant effects on the structural and material properties. Both higher strain rates (100%.s⁻¹) and submerged in, rather than sprayed with, phosphate-buffered saline, resulted in the transition point between the toe and linear region to be extended and elevated for both structural and material results. The toe-region elastic modulus was on average 31% larger for specimens submerged in rather than sprayed with phosphate-buffered saline. Mid-substance failure occurred for 51.8% of specimens, where typically some weak fibrous attachment remained after failure, and an avulsion of the patellar enthesis occurred for the remaining 48.2%. Strain rate effects are an important observation for future human ligament testing of sprain scenarios. Although slightly limited by the intrinsic variability of soft tissues the results suggest that neither tissue hydration nor freezing pre-/post-dissection have a significant effect on structural and material properties of ligamentous tissue.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Development of a Gelatin-Norbornene Hydrogel System with Tuneable Mechanical Characteristics

The use of specialised 3D scaffolds for cell culture has become accepted as the most physiologically relevant way to culture cells in both model systems and tissue engineering applications. Hydrogels are one such class of material that allows culture of cells in 3D, and have been favoured by researchers due to their suitability for facile transport of nutrients and waste, and similarity to native extra-cellular matrix.

As interest in hydrogels has grown, it has been shown that naturally derived hydrogels offer desirable levels of bioactivity and biocompatibility, but generally lack the structural control afforded by synthetically made hydrogels. Conversely, though synthetic hydrogels offer good structural control, they lack the amino-acid sequences of synthetic hydrogels, resulting in poor cellular response to the scaffolds.

Gelatin is a natural polymer that can be functionalised through chemical grafting of different side-chains to achieve a natural/ synthetic hybrid hydrogel which combines bioactivity with structural control. Here, testing is described of a gelatin based, norbornene functionalised hydrogel, crosslinked with a range of chemicals at different concentrations. The result was a highly tuneable system with a wide range of mechanical properties, likely making it suitable for use across a range of different tissue engineering applications.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Tissue Repair Capacity of an Antimicrobial Releasing Scaffold

The design of advanced biomaterials is a promising strategy to aid the regeneration of soft tissue which can be lost during surgery or disease. Bacterial infection is a common surgery-associated complication which could prevent successful tissue integration. Misuse of antibiotics has led to the concerning spread of antimicrobial resistance (AMR) so alternative antibiotic-free strategies are being explored. PhotoTherix^{TM} is a bioresorbable electrospun scaffold equipped with photodynamic therapy (PDT) technology aimed for use in maxillofacial applications. Typically, a photosensitiser (PS) is loaded in its inert form and then activated on-demand through a light source to enable its antibacterial function. To enable translation to clinical use, this study aims to investigate how both the regenerative and antimicrobial capacity can be controlled via variation of chemical and physical parameters of the scaffold architecture. Scaffolds based on FDA-approved biodegradable polyesters (poly(ε-caprolactone) (PCL) and poly(lactic-co-glycolic acid) (PLGA)) have been produced via electrospinning with various parameters being considered to establish structure-function relationships. The incorporation and controlled release of PS dyes (methylene blue and erythrosine) from the material will be studied with regards to scaffold bactericidal effectiveness against bacteria (*Lactobacillus Casei*). Evaluation of the viability of cells (human oral mucosal keratinocyte and fibroblast cells) populating the scaffold will then be performed to determine tissue cell-scaffold relationships. The selectivity achievable between the bacteria and human cells from *in vitro* models will be established. The resulting prototype would improve patient outcomes, reduce the health economic burden and control the spread of AMR.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Biochemical heterogeneity of perineuronal nets

Perineuronal nets are a molecular assembly of extracellular matrix molecules tethered to the surface of a defined population of neurons that regulate plasticity in the central nervous system (CNS). This project aims to understand how the formation of perineuronal nets could change the microenvironment and local mechanics of the neuronal surface, therefore affecting neuronal behaviour.

Perineuronal nets have been implicated in a variety of neurological disorders such as epilepsy, schizophrenia and dementia. They have also been implicated in memory formation and fear conditioning. So far the mechanisms by which perineuronal nets exert their function has been harder to identify, with a variety of hypotheses being put forward.

To help elucidate possible mechanisms of action it is important to identify the components that are responsible for forming perineuronal nets. A variety of molecules have so far been implicated, however no study has looked systematically at where these components are located in different parts of CNS. Interestingly, in different parts of the CNS perineuronal nets appear morphologically distinct. This study aimed to understand if the morphological differences are related to changes in the molecular composition of perineuronal nets.

Understanding the molecular composition of these cell surface structures will be the first part of a wider piece of work that will look to understand if changes to the molecular composition affects their biophysical properties, which in turn may affect neuronal behaviour.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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Developing Experimental Models of Non-Traumatic Spinal Cord Injury and Surgical Interventions

Introduction: Non-traumatic spinal cord injuries are caused by degenerative spine disease or cancers which slowly compress the spinal cord. Up to 33000 people in the UK are affected, with symptoms including gait instability, lack of co-ordination and sensory deficits. Non-traumatic injuries themselves, and the disease process are poorly defined in the literature. Surgery to decompress and stabilise the spinal cord is undertaken based on surgeon preference. Again, both decompression and instability are poorly defined, with unclear risks and benefits to patients.

Aim: The aim of this research is to evaluate responses to mechanical insults of the type observed in non-traumatic spinal cord injury, and subsequent surgical interventions.

Methods: In-vitro, controlled displacement will be applied to a 3D collagen hydrogel model of the spinal cord. Changes in cellular phenotype, viability and spatial distribution will be evaluated. In-vivo, a volume-swelling material will be implanted inside the spinal canal. Over time, this will expand and impinge the spinal cord to clinically-relevant levels. Further, a bespoke stabilisation device will be designed based on anatomical dimensions from CT scans. Outcomes will be compared in control, injured, decompressed and stabilised groups.

Results: The in-vitro system has been characterised and assays optimised using cell lines as a surrogate for primary cells. In-vivo, rodent anatomy has been evaluated using FIJI software.

Conclusion and Impact: Progress is being made towards an experimental model of non-traumatic spinal cord injury. Overall, understanding injury pathology and the effects of surgical interventions will help guide clinical practice, improving outcomes for patients.

Tissue Engineering & Regenerative Medicine 2015 Cohort

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The development of a patient specific foot scaling method for dynamic musculoskeletal analysis

Introduction: The promise to deliver personalised methods to solve complex biomechanical problems is a large field of research where multibody dynamics is one approach that offers advantages such as dynamic measurements of kinematics and kinetics in the musculoskeletal system which can be directly applied to the foot. Inverse dynamics can be applied to the biomechanical models to compute the distribution of muscle forces, but requires inputs through segmentations from medical images as a starting point.

Methods: Rigid body segments are exported locally from the AnyBodyModelling system. In parallel the source MRI images are segmented using Imorphics in-house software. These source and target files are then imported into MeshLab software where an anatomical landmark based registration process is used to create correspondence and finally, the stl files and points from the landmark based registration are run through an STL transformation using an affine radial basis extra/intrapolation as a pre transformation. To verify the inter/extrapolation method the RMS error between meshes is computed by calculating on the Hausdorff distance between source and morphed meshes.

Results: Based on 26 landmark points the Hausdorff distance calculation between source and morphed meshes was Min: 0.0000 Max: 1.25mm Mean: 0.785mm RMS: 1.5mm. The results indicate a small measure of error between the target and morphed meshes.

Discussion: The results verify the scaling method and acts as a milestone in the progression towards generating a full patient specific multibody dynamics model that could be capable of measuring the kinematics and kinetics of the foot.

Tissue Engineering & Regenerative Medicine 2016 Cohort

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Engineering biological bridges to reconnect a severed spinal cord

Spinal cord injuries can have devastating, permanent impacts, including pain, numbness, incontinence and paralysis. Currently, functional recovery is highly unlikely after severe injury, with no successful treatments available. Using biomaterials to bridge severed spinal cords is an attractive method to promote axonal regeneration. However, functional recovery is a complex problem: chronic injuries form glial scar tissue, and the surrounding environment is unstable and inhospitable to regenerating nerves. Therefore, as well as encouraging axons to grow into grafts, another challenge is to encourage them to grow out of the grafts into the surrounding environment in order to reconnect the distal cord. Decellularised peripheral nerve grafts (DPNG) have been developed, which have advantages over previous biomaterial bridges, including the presence of pro-growth factors and absence of immunogenicity. This project will investigate the use of DPNG to bridge complete spinal cord transections. The initial aims will be to produce DPNG bridges suitable for transplantation, and to determine optimal conditions for axonal growth through DPNG bridges, using an in vitro model of dorsal root ganglion neuron culture. This will be followed by the optimisation of an in vivo model of rodent spinal cord transection and implantation of DPNG bridges into the chronic injury. This will include chemical manipulation of local inhibitory factors, vertebral fixation to stabilise the injury site, and rehabilitation using electrical stimulation and locomotor training. Ultimately, physiological, morphological and behavioural measurements will be used to evaluate the in vivo ability of DPNG bridges to induce functional reconnection of the severed spinal cord.

Tissue Engineering & Regenerative Medicine 2016 Cohort

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Developing, refining, and validating patient specific tuneable activity monitor algorithms which are integrated into the healthcare record

An essential factor for humans to be healthy is their physical activity. It is a fact that both mortality and morbidity are associated with inactivity. Different types of diseases, such as cancer, musculoskeletal, cardiovascular are responsible for the patients' reduced physical activity. Therefore, one of the main goals of clinicians is to restore both the activity and function of patients. Activity monitoring is a tool that clinicians should consider along with clinical assessment and their experience when take decisions about the treatments given to their patients with long term conditions. Additionally, they are useful for patients to track their activity. However, the current monitors used in the clinical populations are not suitable for patients with abnormal gait and thus the data recorded is not accurate and it cannot be used effectively. The reason for that is because patients walk slower or by using crutches for support and hence the acceleration signals produced through the activities are much lower than the ones specified in the healthy range and they cannot be detected easily. Therefore, there is a clinical need to develop algorithms that can be used for specific patient types with atypical gait. With the use of these algorithms, more robust and accurate activity measurements will be produced, and consequently clinicians would be able to take better decisions about the medication of the patients. Equally important, it is the development of an electronic platform that will integrate activity information and PROM data with EPRs for the detection of any sudden deterioration and the monitoring of long-term improvements in activity by clinicians.

Tissue Engineering & Regenerative Medicine 2016 Cohort

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The evaluation of biomechanical and wear performance of total ankle replacement

Total ankle replacement (TAR) is a substitute for ankle arthrodesis, replacing the degenerated joint with a mechanical motion conserving alternative. TAR has not been subject to the same pre-clinical testing and validation requirements as hip and knee replacements, as it has only recently been given an equivalent medical device classification. Limited experimental and computational methods for assessing the performance of TAR have been developed, but presently use standard test conditions. Therefore, the purpose of the study is to develop more clinically-relevant models for the evaluation of biomechanical and wear performance of TAR. Biomechanical gait analysis of the ankle from TAR patients and normal patients will be used to identify key parameters for application in experimental simulation. Collaboration, through the industrial partner, with clinicians, will be used to investigate the envelope for implant positioning clinically. Short-duration experimental biomechanical simulations will be used to examine the effect of alignment and inputs derived from study on the contact mechanics of the TAR. These studies will be used as a screening method to determine the optimal test conditions for longer-term wear studies. A number of clinically relevant kinematic and kinetic conditions will also be used to create ‘normal’ and ‘adverse’ situations to assess the wear performance of TAR. This study will be the first to develop clinically relevant experimental simulation for the evaluation of TAR. The development of such methods will be crucial in the ongoing improvement of TARs, and in enhancing clinical functionality, through understanding the envelope of TAR performance.

Tissue Engineering & Regenerative Medicine 2016 Cohort

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The effect of mechanical forces on tissue regenerative properties of mesenchymal stem cells in the ankle joint

Ankle arthritis affects 1.7 million adults in the UK, most of which onsets post-traumatic injury. This means patients are younger, of mean age 51.5 years. Treatment by ankle fusion or total ankle replacement is only employed in 10% of cases. Replacement has a failure rate of 15% within 10 years, which is superseded by ankle fusion, potentially leading to progressive osteoarthritis throughout the foot due to alteration of the biomechanics. Studies of hip osteoarthritis have found evidence of initiation of repair, with hyperplasia of subchondral bone multipotential stromal cells (MSCs) below cartilage defects. However, these show reduced osteochondral differential potential. This suggests modulation of biomechanical forces on bone-resident MSCs may potentially induce spontaneous regeneration.

This project will evaluate if medical imaging can identify more and less damaged areas of osteoarthritic ankle joints, using cadaveric ankle tissues for mechanical characterisation and medical imaging. The correlation of mechanical properties of the tibia and talus with medical imaging will be examined. Histological characterisation of bone and cartilage from total ankle replacement and fusion samples will be performed, with immunohistochemistry of MSCs and osteoclasts in bone specimens to identify topography in relation to tissue damage. New experimental methods for testing ankle bone biomechanics will be developed, and novel CT imaging of cadaveric specimens and correlation with measured properties will be applied to patient-specific computational modelling to aid pre-surgery design and predict mechanical properties based on medical imaging. This research will contribute to the development of a novel therapy for ankle osteoarthritis by endogenous regeneration.

Tissue Engineering & Regenerative Medicine 2016 Cohort

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Mesh morphing strategies for image-based in-silico musculoskeletal biomechanics

The aim of this PhD project is to develop mesh morphing strategies which will encourage the generation of reproducible and high-quality in-silico models and meshes to an automated standard. This research attempts to minimise the influence of human-error on the quality of the final mesh and models, which can be highly subjective. Musculoskeletal-based surgical intervention and the development of new therapies are expected to increase in the ageing population over the next couple of decades. Hexahedral meshes provide biomedical engineers greater predictive capabilities for musculoskeletal-based simulations [1]. This project seeks to achieve three objectives:

1. Development of tools to automate the registration, segmentation and hexahedral meshing of anatomical sites of interest

2. Development of mesh morphing tools with respect to the built meshes

3. Validation of the developed tools and demonstration of the superiority of hexahedral meshes through the assessment and comparison of contact mechanics with respect to tetrahedral meshes

The current state-of-the-art in image segmentation algorithms will be reviewed and implemented to determine their suitability. Successful automation will involve specific programming and/or implementation of learning models for each load-bearing joint. These regions have been identified due to their clinical significance and importance with respect to degenerative diseases and debilitating conditions [2]. Subtle interventions precisely coordinated with individual-specificity could lead to drastic improvements to a patient's overall quality of life. If successful, this research will lead to improvements with respect to: the development of future therapies; treatment optimisation; providing frontiers for physical intervention and easing the development of clinical-grade patient-specific FE models.

References:

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Characterising the properties of bone in the arthritic ankle – could we use a more conservative intervention?

1.7 million adults in the UK suffer from arthritis of the foot and ankle, with a growing number of younger patients being treated for post-traumatic osteoarthritis. Around 10% of cases are treated through surgical intervention, such as total ankle replacement or fusion, but are not without their failings. Current treatments significantly disrupt the joint, even with efforts to minimise the damage to the local area. Hence researchers are looking for alternative treatment that is effective, long-lasting and conserves tissue.

The viability of new interventions is dependent upon determining the relationship between the tissue degeneration and the mechanical forces experienced within the joint. A portion of the tibia-talus joint can be harvested during an ankle replacement or ankle fusion surgery. This provides a source of tissue from which to study the tissue quality and the effect of mechanical forces on tissue degeneration. Using a combination of tissue imaging techniques and biomechanical testing of the joint, one can determine whether the arthritic ankle bone is of sufficient quality to support a more conservative, tissue-preserving intervention. The development of novel CT imaging techniques and experimental methods to characterise the ankle bone will aid in the development of future patient-specific computational modelling using finite-element methods.

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Development of Methodology for Wear Particle Isolation and Assessment of the Biocompatibility of Poly-Ether-Ether-Ketone (PEEK) and Carbon Fibre Reinforced-PEEK

Concerns regarding the incidence of osteolysis and subsequent failure of implants containing ultra-high molecular weight polyethylene (UHMWPE)[1], have prompted research into alternative bearing materials. Components made from poly-ether-ether-ketone (PEEK) and carbon-fibre-reinforced-PEEK (CFR-PEEK) have shown reduced wear in hip and knee implants compared with conventional polyethylene[2-4]. As such, interest has grown in the use of PEEK in a metal-free knee replacement, where the femoral component is manufactured from PEEK Optima®, articulated against a UHMWPE tibial component. In these systems, the wear of UHMWPE tibial components of total knee replacements (TKRs) was shown to be similar when articulated against PEEK Optima® and cobalt chromium alloy[5]. Currently, little is known about the size, morphology and biological responses to wear particles produced in PEEK and CFR-PEEK articulations, and there is no methodology that allows differentiation of PEEK from UHMWPE wear debris. This project will therefore look to develop particle isolation methodology to allow isolation of PEEK, UHMWPE and cement debris from simulations of PEEK on UHMWPE TKR components; and from these isolates, the particle size distributions will be determined. Additionally, questions about the mechanical performance of PEEK in its application in an all-polymer TKR, as well as potential issues with fixation of the device will be addressed; as will the characterisation of inflammatory responses to PEEK particles, in terms of cytotoxicity and inflammatory cytokine release. We will also be determining the suitability of additive manufacturing for the production of components for TKR applications in terms of wear characteristics and particle release.

[1] Ingham & Fisher Biomaterials 2005; [2] Wang et al Tribology International 1998; [3] Scholes & Unsworth Proc IMechE Part H 2008; [4] Grupp et al Acta Biomateriala 2010; [5] Cowie et al. Trans 2nd International PEEK meeting 2015.

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Vascular Biomechanics in Non-traumatic Spinal Cord Injury

In Europe, there are approximately 330,000 people who suffer from spinal cord injury (SCI): a growing area of concern within this field is non-traumatic (NT) injury. NT-SCI thought to have twice the incidence rate of traumatic injuries, but is under-researched due to its secondary pathological nature. NT-SCI involves a continual impaction on the cord, via tumour or bone ingrowth, resulting in disruption of the surrounding spinal vasculature and neural function. Stenosis and re-modelling of the vasculature can lead to inefficient diffusion of vital nutrients and therefore inefficiency of the cord itself – which manifests as a spectrum of symptoms of varying severity. The changes in vessel flow, biomechanics and biology are key factors for understanding these phenomena. There is currently no anatomically correct model of the cord vasculature in NT-SCI, which impedes understanding of the injury pathology and therapeutic development.

As a means of creating a model of NT-SCI, a computational simulation will be developed alongside in vitro and in vivo models. Histology of an impacted rat spine will be used to develop the initial model before simulation with applied fluid dynamics. In vitro and in vivo models will be used to validate the computed model, as well as investigate various other research questions.

The key research question asks what changes in the vasculature lead to vessel stenosis and the resultant effect on cord function. Tissue tolerances and plasticity post-injury will be investigated, alongside further questions such as the effect of injury method and treatment efficiencies.

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