NPCEC 2013

1st Northern Postgraduate Chemical Engineering Conference

8th & 9th August 2013

Conference Booklet

Dear Delegate,

I would like to welcome to you to Newcastle University for the 1st Northern Postgraduate Chemical Engineering Conference 2013 (NPCEC 2013).

This novel event organised by students and for students will allow early stage researchers to present their work, both orally and via poster sessions, to peers in an encouraging and supportive environment, while still providing them the experience of presenting to the greater research community in a professional setting. This conference will bring together scientists, engineers, industrial professionals and students to discuss current challenges and establish new partnerships.

Further to presentations given by postgraduate students, I am delighted to welcome four world-leading scientists who have kindly agreed to give up their time to discuss and hopefully inspire us about the fantastic research they conduct.

I hope this new event will become an annual conference taking place in various chemical engineering institutions each time. Perhaps some of you over the next two days will be inspired to organise the conference in years to come. Please come and talk with us if you are interested to learn more.

I would like to thank all of our academic, industrial and societal sponsorship and advertisement, without which this event could not have been possible. I would also like to express my gratitude to all members of the NPCEC 2013 Conference Committee who have worked very hard to make this event a success.

Finally, I would like to thank you for attending this conference and I hope you will enjoy what promises to be a great occasion.

Glenn Adam Hurst

Chairman

1st Northern Postgraduate Chemical Engineering Conference

Day One: Thursday 8th August

08:30 - 09:10	**Registration & Opening Address**
	Session Chair : Samet Sahin
09:10 - 09:40	**Keynote Presentation** *The Application of Ceramic Membranes in Chemical Processes* Prof. Ian Metcalfe Newcastle University
09:40 - 10:10	
10:10 - 10:30	*Air Separation by Porous Organic Cage Molecules* Jayne Armstrong Newcastle University
10:30 - 11:20	**Morning Coffee Break & Poster Session** **[kindly sponsored by the RSC Newcastle upon Tyne and North East branch]**
11:20 - 11:40	*Gas Separation and Purification on Porous Framework Materials* Nwali C. Joseph Newcastle University
11:40 - 12:00	*Elimination of Volatile Organic Compounds by Catalytic Oxidation at Low Temperature* Emmanuel Iro Teesside University
12:00 - 12:20	*Influencing the Filtration Flow Rate by Coating the Particulate Substance* Abdul Shakoor Loughborough University
12:20 - 12:40	*Diffusion Controlled Structure Selection for Energy Efficient Operation* Funmilayo Osuolale Newcastle University
12:40 - 13:00	*Computational Fluid Dynamics for Microreactors Used in Catalytic Oxidation of Propane* Sunday Odiba Teesside University
13:00 - 13:40	**Lunch**

	Session Chair: Richard Law
13:40 - 14:40	**Keynote Presentation** *Networking Complex Chemical Systems* Prof. Leroy Cronin Glasgow University
14:40 - 15:00	*Advanced Configurable Reactors in Complex Chemical Systems* Andreu Ruiz del la Oliva Glasgow University
15:00 - 15:20	*An Overview of Marine Coating Embrittlement in Water Ballast Tanks* Emmanuel Oriafo Northumbria University
15:20 - 15:50	**Afternoon Coffee Break & Poster Session** **[kindly sponsored by the RSC Newcastle upon Tyne and North East branch]**
15:50 - 16:10	*Safe Solar Hot Water Systems* Felicity Tipping Newcastle University
16:10 - 16:30	*Hydrogen Production During the Pyrolysis-Gasification of Refuse Derived Fuel by Nickel Based Catalysts* Paula H. Blanco University of Leeds
16:30 - 16:40	**Day 1 Summary**
18:00 - 22:00	**Social Programme**

Day Two: Friday 9th August

08:45 - 09:00	**Registration & Opening Address**
	Session Chair: Selgin Al
09:00 - 10:00	**Keynote Presentation** *Recent Developments in Process Integration Design Techniques* Prof. Robin Smith University of Manchester
10:00 - 10:20	*Intensified Synthesis of Fine Chemicals via Heterogeneous Catalysis* Valentine C. Eze. Newcastle University
10:20 - 10:40	*Algal FAME Production with a Novel Surfactant Based Catalyst in a Reactive Extraction* Kamoru A. Salam Newcastle University
10:40 - 11:10	**Morning Coffee Break & Poster Session** **[kindly sponsored by the RSC Newcastle upon Tyne and North East branch]**
11:10 - 11:20	*Catalytic Hydrothermal Processing of Different Vegetable Oils Using HZSM5* Thomas Robin University of Leeds
11:20 - 11:40	*Process Intensification: Nanoparticle Production in Spinning Disc Reactor* Somaieh Mohammadi Newcastle University
11:40 - 12:00	*On the Investigation of Nucleation Mechanism in an Oscillatory Baffled Crystallizer* Craig J. Callahan Heriot-Watt University
12:00 - 12:20	*Reversed Crystal Growth of ZnO Microdisks* Katherine Self University of St. Andrews
12:20 - 12:40	*Preparation of Biodegradable Polymer Nanoparticles for Pharmaceutical Applications in Co-Flow Microfluidic Devices* Rahimah Othman Loughborough University
12:40 - 13:00	*Development of Non-Esterified Fatty Acid Electrochemical Biosensor* Anisah T. Hussain Newcastle University
13:00 - 13:40	**Lunch**

	Session Chair: Glenn Adam Hurst
13:40 - 14:40	**Keynote Presentation** *Principles of Adhesion* Prof. Mike Adams University of Birmingham
14:40 - 15:00	*Improving Yield and OEE Filling Unit Operation within the Manufacturing Process for Multi Dose Powder Inhalers* Christopher Davis Newcastle University
15:00 - 15:20	*An Investigation on Cake Permeability Measurement and Prediction* Faiz M. Mahdi Loughborough University
15:20 - 15:50	**Afternoon Coffee Break & Poster Session**
	[kindly sponsored by the RSC Newcastle upon Tyne and North East branch]
15:50 - 16:10	*Hydrogen Energy-Development of Non-Noble Catalysts For Hydrogen and Oxygen Evolution in Alkaline Polymer Electrolyte Membrane Electrolysis* Luke Watkins Newcastle University
16:10 - 16:40	**Day 2 Summary/Prize Presentations**

List of Posters (8th & 9th August)

Dynamic Process Monitoring Using Partial Least Squares and Extension Botinah Alaf Newcastle University
Harnessing Stranded and Flared Associated Natural Gas: The Role of Heat Transfer in Combined Micro-Channel reactors / Heat Exchangers A O Odunsi Herriot Watt University
Hierarchical Growth of ZnO Crystals Hydrothermally from Zinc Acetate Faith Bamibduro University of Leeds
Modelling of Waste Recovery via Pyrolysis Haoyu Li Herriot Watt University
Organic Matter Transformation in Sewer Processes Afifah Abd Rahim University of Sheffield
Investigations into Parameters Affecting Purity in Oscillatory Baffled Crystalliser and Stirred Tank Crystalliser H.R. McLachlan Herriot Watt University
Development of Algal Biodiesel via Synthetic Biology Danying Wu University of Sheffield
Iron for Nitrobenzene Reduction Goh Sher Leen University of Strathclyde
Production of Microparticles for Drug Delivery in Flow Focussing Microfluidic Devices Ekanem Ekanem Loughborough University
Novel amine functionalised silica based adsorbent for CO_2 *capture* Esegboria Obhielo University of Strathclyde
Characterisation of High Shear Rotor Stator Devices Prisola Isaac University of Liverpool
Feasibility of the Microwave Regeneration of adsorbents for CO_2 *capture* Javier Cardona University of Strathclyde
Nucleation of Crystals under Controlled Flow Conditions Carol Forsyth University of Strathclyde
Physicochemical Characterisation Of A Solid Torrefied Biomass Raimie Hebriyah Haji Ibrahim University of Leeds
Bio-inspired Silica Nanoparticles Optimisation for Delivery Applications and Understanding Biological Safety Scott Davidson University of Strathclyde

Characterisation of Spatially Resolved Spectroscopic Measurements for Use in Monitoring Pharmaceutical Fermentation Sarra Tiernan University of Strathclyde
Software Framework For A Holistic Approach To The Analysis And Reduction Of Environmental Burden In Food Production Christopher J Fishlock Newcastle University
Complex Flow of Concentrated Suspensions Claire Forsyth University of Strathclyde
Efficiency of Steam Generation and Waste Utilisation in a Spirits Plant Eric Siqueiros Newcastle University
Development of a Potential Immunocontraceptive Nanomaterial using Molecular Dynamics Simulations David Connell University of Strathclyde
Optimising Conical Inline Filter Design by Manufacturing using Additive Technology Bhavani Vijayakumar Lancaster University
A Novel Procedure in Ambient Pressure Dried Silica Aerogels Xiao Han Newcastle University
CFD Investigation on different Unit Cell Model of Porous Media Faiz M. Mahdi Loughborough University
A Generic Selection Criterion for Three Phase Separations MaryJane A Obah Teesside University
Comparison of Nano-Inorganic Catalyst for Reversible Hydration of Carbon Dioxide Shun Toei Newcastle University
Continuous Screening of an Imine Synthesis Reaction using Mesoscale Oscillatory Baffled Reactor Fatimah Rubaizah Newcastle University
Pyrolytic characterization and Kinetics of microalgae (Chlorella vulgaris and Nannochloropsis ocutala) using thermo gravimetric analyser Auwal Aliyu Newcastle University

Conference Committee

Name	Role
Glenn A. Hurst	Conference Chairman
Richard Law	Conference Vice-Chairman
Selgin Al	Committee Member
Gaurav A. Bhaduri	Committee Member
Simon Coleman	Committee Member
Samet Sahin	Committee Member

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Keynote Presentations

Mike Adams

Professor of Product Engineering and Manufacturing

School of Chemical Engineering

University of Birmingham

Birmingham, UK

Ian S. Metcalfe

Professor of Chemical Engineering

School of Chemical Engineering and Advanced Materials

Newcastle University

Newcastle upon tyne, UK

Lee Cronin

Professor-Gardiner Chair of Chemistry

School of Chemistry

University of Glasgow

Glasgow, UK

Robin Smith

Professor

School of Chemical Engineering and Analytical Science

Manchester University

Manchester, UK

The application of ceramic membranes in chemical processes

Ian S Metcalfe

School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle upon Tyne NE1 7RU

Membranes and membrane reactors are of great interest in the chemical industries because they offer the possibility of improved yields and more compact plant. Clearly the availability of membrane systems having suitable performance at an acceptable cost is an important consideration. Organic membranes can be difficult to use at high temperatures, while porous inorganic membranes tend to have problems associated with selectivity. In this talk we will focus on the use of inorganic, dense, ion-conducting membranes. Such membranes can be highly selective. We will explore their use in new membrane-based chemical process applications.

Mixed ionic and electronic (MIEC) conducting metal oxides can be employed as oxygen permeable membranes (in the case of coupled oxygen ion and electron transport) or hydrogen permeable membranes (in the case of coupled proton and electron transport). Dual ion conducting materials can be used to design membranes for e.g. water and carbon dioxide permeation. This presentation will describe transport mechanisms within these solids and show how these lead to permeation models.

The talk will also focus on the application of such membranes in chemical processes. For example, under an oxygen chemical potential difference an oxygen permeable ceramic membrane can supply pure oxygen to a hydrocarbon for e.g. partial oxidation. This permits the use of air as the oxidant and can lead to more intensified, efficient hydrocarbon processing. Other novel processes involving hydrogen production, internal reforming within a solid oxide fuel cell and carbon dioxide capture will also be demonstrated and discussed.

Parallels will also be drawn with chemical looping processes in which an oxygen carrier undergoes periodic redox reactions leading to reaction and separation. We will show that any chemical looping process has a membrane analogue and vice versa.

Networking Complex Chemical Systems

Lee Cronin,
WestCHEM, School of Chemistry, University of Glasgow, Glasgow G12 8QQ.

Traditionally much of chemical synthesis, molecular discovery and transformations have been done in one pot reaction systems whereby reagents are added and the reaction conditions are controlled in terms of temperature, solvent, atmosphere and pressure. Although this general approach has been incredibly successful, the manipulation of complex reaction networks and the development of systems showing emergent properties require a fundamentally new approach.

In this lecture I will outline our recent efforts, investigating the self-assembly and self-organization of inorganic molecules and the engineering of complex systems and reaction networks that lead to the emergence of system-level behaviours. To do this we have developed new reaction techniques to control the assembly of nanoscale molecular metal oxide clusters, some of the largest non-biological molecules known, as well as new physical techniques e.g. the development of new cryospray and variable temperature mass spectrometry (for the elucidation of reaction mechanism and the observation of highly reactive intermediates). Ultimately our aim is to develop new approaches to molecular discovery and the assembly of complex chemical systems, as well as the development of new reaction formats for complex chemistry e.g. flow systems and 3D-printing (see publications below)[1-5].

Figure Images depicting our different approaches to new reactor formats: Networks, flow array and 3D printing.

1. H. N. Miras, G. J. T. Cooper, D.-L. Long, H. Bögge, A. Müller, C. Streb and L. Cronin, ‘Unveiling the Transient Template in the Self Assembly of a Molecular Oxide Nano-Wheel’, *Science*, **2010**, *327*, 72-74. DOI: 10.1126/science.1181735.

2. C. J. Richmond, H. N. Miras, A. R. de la Oliva, H. Zang, V. Sans, L. Paramonov, C. Makatsoris, R. Inglis, E. K. Brechin, D-L. Long, L. Cronin, ‘A flow-system array for the discovery and scale up of inorganic clusters’ *Nature Chem*., **2012**, 4, 1037-1043. DOI:10.1038/nchem.1489

3. M. D. Symes, P. J. Kitson, J. Yan, C. J. Richmond, G. J. T. Cooper, R. W. Bowman, T. Vilbrandt, L. Cronin, 'Integrated 3Dprinted reactionware for chemical synthesis and analysis', *Nature Chem.,* **2012,** *4,* 349-354.DOI :10.1038/nchem.1313

4. A. R. de la Oliva, V. Sans, H. N. Miras, J. Yan, H. Zang, C. J. Richmond, D.-L. Long, L. Cronin, 'Assembly of a Gigantic Polyoxometalate Cluster {W200Co8O660} in a Networked Reactor System', *Angewandte Chemie International Edition*, **2012,** *51*, 12759-12762

5. P. Kitson, M. Rosnes, V. Sans, V. Dragone, L. Cronin, 'Configurable 3D-Printed millifluidic and microfluidic 'lab on achip' reactionware devices', *Lab on a chip,* **2012,** *12,* 3267-71.

Recent Developments in Process Integration Design Techniques

Robin Smith

Centre for Process Integration, University of Manchester, Manchester M13 9PL.

Process integration focuses on the design, optimization, operational optimization and control of chemical and biochemical processes. This relates to processes in the petroleum, petrochemical, chemical, pharmaceutical and food processing industries. The emphasis is on a holistic approach to the process, rather than concentrating on individual operations, or the phenomena occurring in individual operations. The research in process integration started in the late 1970s and early 1980s with an emphasis on energy efficiency. The early focus was on systematic methods for the design of heat exchanger networks. Later, the ideas and techniques developed to solve the heat exchanger network problem provided the basis for the extension of the methodology into new areas. Although research in process integration now covers a much wider area than energy efficiency, the greatest emphasis is still placed on process design, retrofit and operational optimisation for energy reduction.

The earliest tools to become established in process integration were basic thermodynamic tools. Perhaps the most important concept underlying these early tools was the idea of setting energy targets before design. However, there is a general lack of understanding of the limitations of such targets and just how achievable they are in practice.

Since the early development of thermodynamic approaches to process integration, there has been huge progress in the development of approaches based on optimisation. The basis of many of these approaches is to set up a superstructure for the process design or retrofit that includes all the features that are candidates for the final solution. This is then subjected to optimisation that removes redundant (non-optimal) parts of the design and adjusts the continuous parameters to their optimum settings. Whilst it is very tempting to think of this as being the ultimate solution to the problem, the size and difficulty of the optimisation required remains an obstacle.

Most of the process integration activity carried out industrially relates to the retrofit of existing processes for reduced energy demand or the retrofit of energy systems for increased process throughput. Whilst the methods for the design of new energy systems have become relatively sophisticated, methods for the retrofit of energy systems are still far less well developed.

The importance of exploiting degrees of freedom within the process for improving energy performance has been a feature of process integration from the earliest days. Combining process changes with changes to the heat recovery system, leads to far better results compared with changes to the heat recovery system alone. If process models and heat recovery models can be combined effectively, then there are not just opportunities for design and retrofit, but also operational optimisation.

The drive towards sustainability in manufacturing requires the application of process integration techniques across all material and energy flows for the goal of resource conservation. Although the history of process integration is relatively short, it has by now seen many successful industrial applications towards that goal.

Principles of Adhesion

Mike Adams

School of Chemical Engineering, University of Birmingham, Birmingham B15 2TT.

The fouling of processing equipment arises from a number of mechanisms such as particle impact and the shear of a paste. Its extent and the difficulty of removal depend on the adhesion between the fouling deposit and the equipment walls. Adhesion is governed by molecular, microstructural, topographical and mechanical length scales. The interactions at the deposit-wall interface may be modelled by discrete particle schemes for agglomerates and granular solids unless the primary particle size is less than that of the asperities when a continuum description is required. In either case, the stored elastic strain is the critical factor in attenuating adhesion.

The autoadhesion of elastic and elastoviscoplastic particles will be considered together with the role of liquids in terms of their influence on wetting, tack and the capillary forces. The description of continuum scale modelling will be based on the application of engineering plasticity and fracture mechanics approaches. Examples will include impact, scraping and shear.

Oral Presentations

Air Separation by Porous Organic Cage Molecules

J. Armstrong[a]*, J. Jones[b], T. Hassel[b], S. Chong[b], K. Jelfs[b], M. Thomas[a], A. Cooper[b]

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The separation of oxygen and nitrogen is achieved commercially using carbon molecular sieves and the pressure swing adsorption (PSA) technique. The development of new porous materials for the improvement of air separation processes has increased rapidly over the past decade, dominated mainly by metal organic frameworks, covalent organic frameworks, nanoporous polymers and, most recently, porous organic cage molecules.

Porous organic cage molecules contain C-C, C-H, N-H and C-N bonds and are assembled without the use of directional covalent bonding, which is found in metal organic frameworks. Cages are assembled instead through weaker intermolecular interactions allowing the potential for flexibility in the materials, through both reorientation and complete relocation of the discrete cage units within the crystal lattice (Cooper 2011).

The 1 nm diameter tetrahedral cage molecules formed by the condensation reaction of 1,3,5-triformylbenzene with 1,2-ethylenediamine can exist in a number of stable polymorphs, Cage 1α, Cage 1β and Cage 1γ (Jones et al 2010). Cage 1α has voids between the cages, which are connected by very narrow constrictions that allow the kinetic molecular sieving of oxygen, carbon dioxide and nitrogen, a property which is not present in the polymorph Cage 1β. It was found that oxygen adsorbs approximately ten times faster than nitrogen on Cage 1α, with selectivity and rate constants similar to those observed for carbon molecular sieves. This material was found to be extremely stable, and repeatable isotherms of carbon dioxide, oxygen and nitrogen adsorption were collected after over 30 cycles of adsorption, heating to 120°C and desorption, with isotherms collected over a pressure range of 0 - 1000 mbar.

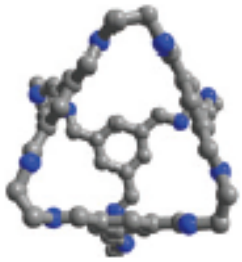

Figure 1. Cage 1α Porous Organic Cage Material

A. I. Cooper, (2011) Nanoporous *Organics Enter the Cage Age,* Angew. Chem. Int. Ed. 50, p996

J. T. A. Jones, D. Holden, T. Mitra, T. Hasell, D. J. Adams, K. E. Jelfs, A. Trewin, D. J. Willock, G. M. Day, J. Bacsa, A. Steiner, A. I. Cooper, (2010) *On-Off Porosity Switching in a Molecular Organic Solid*, Angew. Chem. Int. Ed. 50, p 749

Gas Separation and Purification on Porous Framework Materials

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Gas separation and purification is an important component of chemical, petrochemical and related industries; often has high energy demands. Many porous materials have been applied, including zeolites and activated carbons (Li et al, 2009). Porous framework materials, a relatively new class of porous materials, are extremely desirable as a replacement of traditional adsorbents (Yaghi et al, 2003, Rowsell and Yaghi, 2004, C. Janiak and Vieth, 2010). To assess the suitability of the materials, it is necessary to determine the adsorption capacity and kinetics of the porous framework materials (Li et al, 2009; Li et al, 1999). In the present study a new class of porous material, CuL2Py MOFs (Figure 1), metal organic framework is investigated due to the dynamic structural flexibility and high micropore volume possessed by the material. The adsorption capacity and kinetics are determined through the study of the isotherms obtained using an Intelligent Gravimetric Analyser. The material is characterised fully from carbon dioxide adsorption at 273 K, 195 K and nitrogen adsorption at 77 K. Results showed that CuL2Py MOFs (Figure 1) is a highly micro-porous material with high adsorption capacity and good kinetics, which are desirable properties for efficient gas separation.

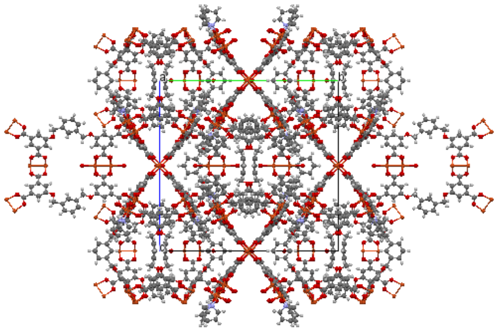

Figure 1: CuL2Py MOF

Keywords: Gas Separation, Porous Framework Materials, MOFs, CuL2Py.

J.R. Li, Ryan J. Kuppler and Hong-Cai Zhou, (2009) *Selective gas adsorption and separation in metal-organic frameworks.*, Chem. Soc. Rev., 38, pp. 1477 – 1504.

O.M. Yaghi, M. O'Keeffe, N.W. Ockwig, H.K. Chae, M. Eddaoudi, J. Kim, (2003). Nature, 423, 705-714.

J.L.C. Rowsell, O.M. Yaghi. (2004), *Metal–organic frameworks: a new class of porous materials*. Micropor. Mesopor. Mater., 73, pp. 3-14.

H. Li, M. Eddaoudi, M. O'Keeffe, O.M. Yaghi, (1999), *Nature,* 402, 276–279.

C. Janiak, J.K. Vieth, (2010), *New J. Chem.* 34, 2366–2388.

Elimination of Volatile Organic Compounds by Catalytic Oxidation at Low Temperature

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Volatile organic compounds (VOCs) constitute most of the toxic air pollutants found indoors, prompting the need to develop a safer, cheaper, more robust indoor air purification technology that can destroy VOCs completely at low temperatures. Catalytic oxidation method which breaks down VOCs completely into environmentally healthier carbon dioxide and water holds the greatest potential due to its ability to operate with dilute effluent VOCs streams of less than 5000ppm. The problem with the current catalysts used for VOCs oxidation is that they are active at temperatures above 180˚C only, increasing the operational cost and in some cases unwanted intermediate products are produced with high temperatures. Our first step in the design of low temperature catalyst for VOCs oxidation is to develop a suitable catalytic support for the active phase, one that provides high surface area for active sites, with large pore diameter to allow passage of the large VOCs molecule through active sites, stable to moist environment and also cost effective. Using sol gel method, we have successfully synthesized SBA-15 mesoporous silica support with ordered structural arrangement as confirmed by Energy Dispersive and X-ray Diffraction characterization. Moreover, Scanning Electron Microscope imaging revealed fibre-like agglomeration, bended tube and spherical morphology. Nitrogen adsorption measurements will be done to calculate the BET surface area, pores size and volume. The support will then be loaded with the active phase. A mobile device will be designed and built to work with the new catalyst to eliminate VOCs indoors.

Influencing the filtration flow rate by coating the particulate substance

A. Shakoor*, F. Mahdi

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Conventional fillers, such as talc, have been used for many years as reinforcing fillers and nucleating agents in commodity polymers and have the potential to provide significant and cost-effective improvements in thermoplastic formulations. It was found that talc has increased the crystallinity and mechanical properties of the composites [Shakoor and Thomas 2013]. It has a plate-like structure and has a tendency to agglomerate and make clusters during separation applications. It has reported that cluster improves the flow rate but difficult to predict and control [Di Giovanni et al. 2012]. Stearic acid as a surfactant used in coating of mineral fillers like talc to disperse the particle effectively for better properties in the composites [Kim et al. 2006]. The effect of coating on the talc can be used to find the influence of the filtration flow rate of particulate substance. The aims of this work are to investigate the effect of stearic acid coating on the particle structure and the flow rate of the talc.

Methodology: Talc is coated with 1(%) stearic acid and is carried out in a bench top high shear mixer running at 16,000 (rpm) for about 5 minutes at a temperature of 80 ($_{o}$C). The filtration methodology is discussed [Mahdi and Holdich 2013].

The measured values for pure and coated talc show significant difference in the results as in Table 1. Fig.1 shows the FTIR spectra for pure and coated talc and significant peaks are observed mainly between frequencies at 3000 to 2750 cm$_{-1}$, thus shows that the coating has taken place. As a result, the filtration flow rate significantly improved by 80% due to particle clustering during the process, see Fig. 2. In conclusion, the increase in filtration flow rate can be attributed to changes in the particle surface charge.

Table 1 Particle characterization for pure and coated talc

	Nat. pH	**ζ (mV)**	**IEP**	**Density (g/cm3)**	**D50 (μm)**	**Mean D (4,3) (μm)**	**Span**
Pure	9.4	-16	*pH 2.0*	2.98	8.1	10.2	2.2
Coated	7.1	-7.8	*pH 10.3*	2.8	11.8	15.2	2.3

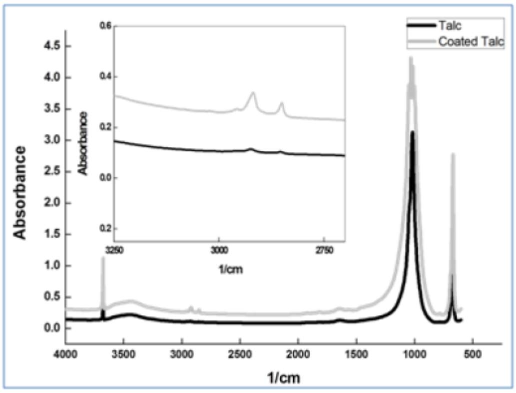

Fig.1: FTIR Spectra of pure and coated talc

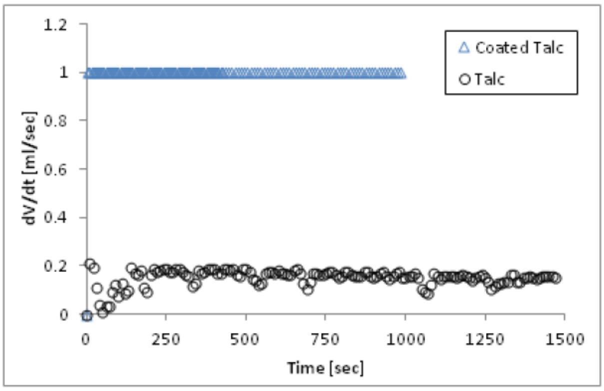

Fig.2: filtration flow rate of pure and coated talc

Di Giovanni B.A., Mahdi F.M., Starov V.M., Holdich R.G, 2012, Chem. Eng. Res. Des. **90**(A), pp.1168-1176
Kim H., Biswas J., Choe S., 2006, *Polymer*, **47**(11), pp. 3981-3992
Mahdi F.M., Holdich R.G., 2013, *Chem. Eng. Res. Des* [**In press**]
Shakoor A., Thomas N., 2013, *Polymer Eng. & Science*. [**In press]**

Distillation Control Structure Selection for Energy Efficient Operation

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* Corresponding author. Email f.n.osuolale@newcastle.ac.uk

Distillation is the major separation process in the chemical and petrochemical industries and is energy intensive. A little increase in the efficiency of a distillation column translates to a large amount of reduction in operation cost. For instance, distillation columns consume 2.87×10^{18} J a year which is equivalent to a continuous power consumption of 91GW or to a 54 million tonnes of crude oil (Soave and Feliu, 2002). In this work a method of improving the efficiency of distillation process operations through appropriate selection of control configuration is presented. Thermodynamic analysis is incorporated in the choice of control structure (Montelongo-Luna *et al.*, 2011).

Two binary distillation systems of methanol-water and benzene-toluene were considered. Steady state and dynamic simulation of the two binary systems were performed. Detailed thermodynamic analyses of the two distillation processes were considered and the results reveal a great deal of irreversibility within the systems. Relative gain array (RGA) and Relative exergy array (REA) were used to screen for energy efficient control configurations for the systems. Control structures were tested in dynamic simulation under disturbances and set point changes. The reboiler energy, exergy efficiency and exergy loss of each simulated system were calculated. Table 1 gives the results for the benzene-toluene system showing the DV configuration as the control structure of choice. The results reveal the screened energy efficient control configurations for each system consume the least reboiler energy, has the least exergy loss and the highest exergy efficiency. The method could be applicable in determining feasible and energy efficient operating conditions for a distillation process.

Table 1. Results for Benzene-Toluene system

Control configuration	**Exergy eff (%)**	**Exergy loss (kJ/hr)**	**Reboiler energy (kJ/hr)**	**RGA**	**REA**
LV					
Steady state	25.35	5.78×10^7	2.161×10^7	-0.4539	-0.3322
ΔReflux rate	23.32	6.46×10^7	1.22×10^8		
ΔReboil energy	29.41	4.7×10^7	1.18×10^8		
DV					
Steady state	25.35	5.78×10^7	2.161×10^7	0.9801	0.8499
ΔDistillate rate	32.80	3.76×10^7	7.856×10^7		
ΔReboil energy	38.33	3.90×10^7	7.17×10^7		
LB					
Steady state	25.35	5.78×10^7	2.161×10^7	-2.4542	1.0349
ΔReflux rate	29.49	4.38×10^7	1.17×10^8		
ΔBottoms rate	22.14	6.66×10^7	1.17×10^8		

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Computational Fluid Dynamics for Microreactors Used in Catalytic Oxidation of Propane

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Recent advances in microfabrication technology have been adapted in the field of chemical engineering to realise microreactor devices with higher efficiency than those in conventional systems mainly due to their large surface area to volume ratio which leads to higher heat and mass transfer properties. The optimal design for a specific application can be proposed based on simulation results obtained by using CFD package of COMSOL Multiphysics. This research deals with the design of suitable microreactors for the catalytic oxidation of volatile organic compound (VOCs), using propane as model molecule. First step was the selection of the most suitable microreactor geometry based on cold flow (without reaction) and the simulation results obtained using the above software. Second step consisted on the simulation of the operation of the selected microreactor for propane oxidation. As such four different geometries have been proposed and simulated in 2D to evaluate the fluid behaviour in the microchannels. So called A2 geometry gave the optimum flow distribution from laminar to transitional (the lowest relative standard deviation). Geometry A2 was modified in a 3D model to further investigate the catalytic oxidation of the model VOCs.

The catalytic microreactor was simulated for temperatures between 563 and 663 K and inlet flow velocities between 0.05 and 1 m/s. As expected, conversion increased with temperature for a fixed inlet flow velocity. Propane conversion increased as the inlet flow velocity decreased. For a fixed temperature, the propane conversion increased as the inlet flow velocity decreased. As the target conversion was set to 99.99%, a number of isothermal microreactors with A2 geometry were connected in series and the conversion profile in each of them was determined. Their number decreased as the temperature increased and the inlet flow velocities decreased (as such, the residence time within each reactor increased).

Advanced Configurable Reactors in Complex Chemical Systems

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The conventional polyoxometalate (POM) synthetic methods and fundamental self-assembly mechanisms are under intensive review because one-pot reactions mask a vast and complex range of intricate self-assembly processes (Gao et al, 2013). Therefore it is difficult to predict / control the assembly processes, and flow systems were employed in POM chemistry unravelling the mechanism of formation of giant polyoxomolybdates (Miras et al, 2010). Since this fundamental discovery, a new generation of PC-controlled configurable reactors has been designed for automating/accelerating the discovery of new complex inorganic architectures. The advantage of the automation of inorganic reactions is focused on rapid discovery of new nano-scale clusters / materials in a reproducible and fashion way. POMs are good chemical system candidates to study in automated reactor systems helping to investigate and discover new POM clusters accelerating reaction number, optimizing chemical compositions and improving reproducibility issues. Herein, we present two Advanced Configurable Reactors (ACRs) which enable to control chemical composition, order of addition and space networking in pre-designed reaction mixtures in basis on space and time dependency fashion. The Continuous Processing System (CPS) shows the potential of continuous flow-conducted systems to synthesize a wide range of nano-sized inorganic clusters in a highly controlled and reproducible fashion (Richmond et al, 2012). The Networked Reactor System (NRS) is employed to dynamically control in space and time the self-assembly of tungsten-based nano-scale clusters by interfering multiple "one-pot" reactors (de la Oliva et al, 2012). The NRS (Figure 1) allowed to automated synthesis of polyoxometalate clusters in very precise control of chemical composition of initial starting materials and pH overall the system, yielding a gigantic $[H_{16}Co_8W_{200}O_{660}(H_2O)_{40}]^{80-}$ anion cluster. The advantages of NRS in confining reaction conditions in different time scales may provide a completed new vision of performing chemical reactions as showing modularity and interference of inorganic transient building block.

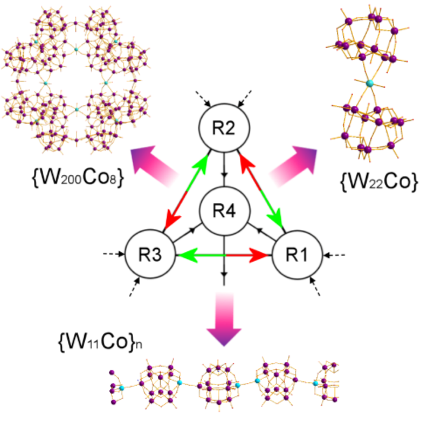

Figure 1. The NRS reactor design to synthesize polyoxometalate clusters.

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An Overview of Marine Coating Embrittlement in Water Ballast Tanks

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Coating degradation plays a significant role in structural failure with corrosion occurring once the steel substrate is exposed. The effective service life of ships is determined by the condition of the coating in water ballast tanks coatings (W.B.T.s) (*Vold, 1997*). Evidence obtained in the last two decades showed that the alarming loss of ships and lives at sea was attributed to severe corrosion of W.B.Ts (*George et al, 2005*).

Based on the available evidence, the International Maritime Organisation (I.M.O) developed the Performance Standard for Protective Coating (P.S.P.C.) which was adopted in July, 2008 (*George et al, 2005 and Thorsten, L. 2009)*. This requirement for type approval of WBT coatings addressed the majority of issues and has resulted in a significant reduction in accident occurrences.

The target performance lifetime of P.S.P.C. type approved W.B.Ts coatings is 15 years (*Thorsten, 2009*) with minimum maintenance. This service lifetime is an estimate based on the results of laboratory testing. In practice however, coating failure in the form of cracking, is found to occur around welds and joints as the coating ages and becomes embrittled. There is therefore renewed industrial research aimed at understanding this issue in order to eliminate cracking and achieve the intended coating lifespan of 15 years with minimum maintenance.

Coatings in a WBT may be applied as very thick films to poorly prepared steel substrates. Factors such as hygrothermal cycling resulting from cargo loading and unloading produces stresses in the paint film which can ultimately result in cracking. This paper will describe the in service challenges faced by these coatings as well as some of the issues affecting performance and embrittlement of WBT coatings.

Figure 1. Marine coating degradation showing cracks and rust in water ballast tanks

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Thorsten, L. (2009) Implementing The IMO PSPC for Ballast Water Tanks. JPCL February
Vold, H. (1997) Protective Coating for ballast Tanks. PCE, June.

Safe Solar Hot Water Systems

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This project was completed over ten weeks in the Summer of 2013 at the Estates Department following solar thermal installations for NHS South of Tyne and Wear. The organisation had installed a number of solar thermal hot water systems with the aim of reducing their carbon footprint and increasing the amount of energy consumed from renewable sources.

Following routine system testing elevated coli form and legionella counts were seen in hot water systems that had solar hot water devices installed. Accordingly all solar hot water systems were isolated and disconnected from the properties primary hot water systems with corresponding tanks drained. Since removing the solar thermal element from the hot water systems, the coli from counts have returned to safe levels.

Legionella bacteria are common and are found in natural water systems, however at low levels they represent little to no risk. Hot water systems are designed to minimise conditions that allow bacterial proliferation hence reduce the risk of disease. The project initially analyses and explains potential causes of increased coli form counts when using solar thermal systems to pre heat hot water. The aim of the project is to offer a solution to the problem and enable to the solar thermal hot water systems to be safely put back online, or give proof it this not possible while complying with the relevant legislation.

A cost benefit analysis was carried out for each potential solution ensuring that any gains were greater than the expense.

Hydrogen production during the pyrolysis-gasification of refuse derived fuel by using nickel based catalysts.

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Hydrogen has a potential for power generation as can be used as fuel in further power generation processes (Wu and Williams, 2008); however the current hydrogen production processes are not effective as they require high energy inputs and involve CO_2 generation. The thermal treatment of solid wastes has been regarded as an alternative waste treatment with energy recovery (Morris and Waldheim, 1998). For example refuse derived fuels (RDF) obtained from the main municipal solid waste stream (Dalai et al., 2009), have been used as raw material during combined thermal treatments such as pyrolysis and gasification, in order to obtain a high value gas rich in hydrogen. One of the major challenges during the application of the combined pyrolysis-gasification process is the tar formation. Tar is a condensable fraction composed mainly of aromatic compounds; due to its variable composition tar tends to condense at different gasification stages originating diverse operational problems; as a result the overall process yield is reduced (Li and Suzuki, 2009). Different methods have been tested to reduce tar formation; however the most common is the use of nickel based catalysts as its use promote tar cracking and increase the hydrogen content in the produced gas (Wu and Williams, 2010). A high catalytic performance is related to the catalysts properties such as surface area, porous properties, and pore size distribution; for this reason the catalysts characterisation is a relevant criterion while testing catalysts. In the present work a series of nickel based catalysts were prepared, characterised and tested for their activity in terms of hydrogen production and tar reduction during the pyrolysis gasification of RDF. The pyrolysis process was undertaken at 600 ºC whereas the second gasification stage was carried out at 800 ºC, the produced gases were passed through a cooling system and the non-condensed fraction was collected in a gas bag for further gas chromatography analysis. The results showed that using Ni/SiO_2 catalyst, the hydrogen content in the produced gas can be increased up to 55wt.%.

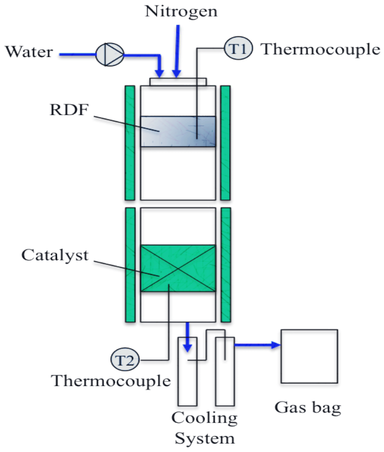

Figure 1. Two-stage pyrolysis-gasification reaction system

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Intensified Synthesis of Fine Chemicals via Heterogeneous Catalysis.

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Carboxylic acids esterification is an important reaction in the productions of fine and specialty chemicals used in fragrances, pharmaceuticals, and pesticides (Lilja et al, 2002). This reaction is commonly catalysed by homogenous acid catalysts which add to the cost of the operation as a result of downstream removal of the catalyst. Thus, to reduce the cost of the esters synthesis, heterogeneous acid catalysts and effective multi-phase mixing devices are imperative. In this study, carboxylic acid esterification was investigated using hexanoic acid esterification with methanol as a case study. The reaction was heterogeneously catalysed by sulphonic acid functionalised divinylbenzene/styrene copolymer (Amberlyst^{TM} 70, Dow Chemical Company). An oscillatory baffled mesoreactor was selected for the reactions. This reactor has been designed particularly for screening of reactions because of its effectiveness in multi-phase mixing, and small volume which reduces the amount of reagents required and wastes generated (Zheng et al, 2007). The hexanoic acid esterification was screened continuously at multi-steady states and dynamic modes, across 1:1 – 30:1 methanol to hexanoic acid molar ratios and reaction times of 1 – 20mins residence times, at reactions temperature of 60 °C and oscillatory condition of 4.5Hz frequency and 8mm amplitude.

The results showed that steady states were achieved at all the residence times for the multi-steady states screening. These results were indicative of the high degree of plug flow regime inside the oscillatory baffled mesoreactor, which are in agreement with the residence time distribution (RTD) tests on the reactor. The induction (time to achieve steady state) times for the various steady states achieved were in the range of 1.2 – 1.4 residence times. The hexanoic acid conversions increased with both methanol molar ratio and the reaction time, for instance about 55% was obtained at 2.5min, and 96% at 20min, for the reactions at 30:1 methanol to hexanoic acid molar ratio. There was consistency in the hexanoic acid conversion at every residence time for the multi-steady states reactions, showing that the Amberlyst^{TM} 70 catalyst was stable; there was no leaching or deactivation. Our findings indicate that 95 – 99% conversion of the hexanoic acid was possible at less that 30mins reaction time, as compared to a couple of hours required to carry out this chemical transformation in a conventional homogeneous batch esterification processes. Hexanoic acid conversions at the dynamic and multi-steady states screening of the esterification process were found to be similar, which suggests that process development time could be greatly reduced by screening of reactions in dynamic mode.

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Zheng, M., Skelton, R. L., Mackley, M. R. (2007) *Biodiesel reaction screening using oscillatory flow meso reactors.* Process Safety and Environmental Protection 85, pp 365-371.

Algal FAME production with a novel surfactant based catalyst in a reactive extraction

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Reactive extraction (*In situ* transesterification) of FAME (Fatty acid methyl ester) from microalgae is an intensified process of producing FAME by directly contacting the biomass with methanol containing a catalyst. This approach is simpler and potentially more cost-effective, because of its elimination of the solvent extraction steps. The current study involved development of a novel surfactant catalyst (ZDS; zirconium dodecyl sulphate) for usage in the “reactive extraction” of FAME from *Chlorella* and *Nannochloropsis* . Additionally, the FAME yield produced when using sodium dodecyl sulphate (SDS) and H_2SO_4 catalyst was investigated. Microalgae was also characterised before and after the reactive extraction in terms of carbohydrate and protein content. Water tolerance of the process at low methanol lipid molar ratio for *Nannochloropsis* species was also evaluated and the result is shown in fig2.The maximum FAME yield as well as initial and final algal biochemical compositions are shown in fig 2. In conclusion, the inclusion of sodium dodecyl sulphate in H_2SO_4 significantly improved the FAME yields obtained from the microalgae. The process is tolerant to water within the specified process conditions but the low methanol lipid molar ratio significantly reduced the FAME yield. Zirconium dodecyl sulphate catalyst performed better with *Nannochloropsis* than in *Chlorella*. The microalgae maintains almost all the protein content and some of the carbohydrate after the *in situ* transesterification. The reaction time and yields were significant function of algae strain and catalyst.

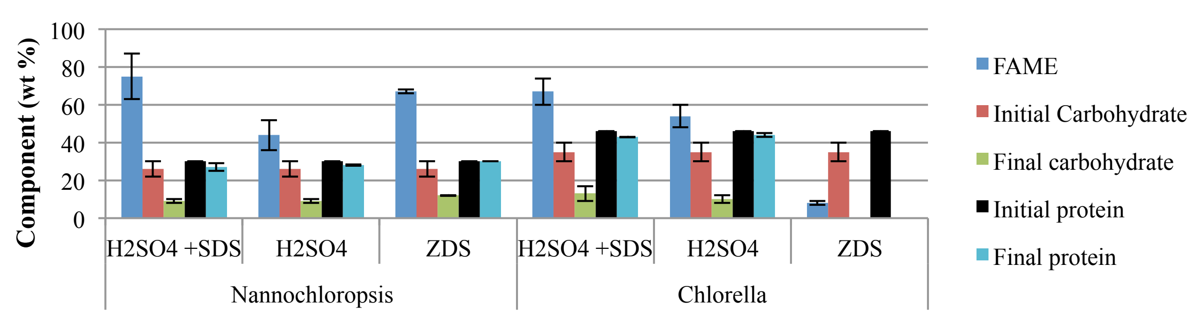

Fig1: Compositions of the microalgae before reactive extraction and at Maximum FAME yield

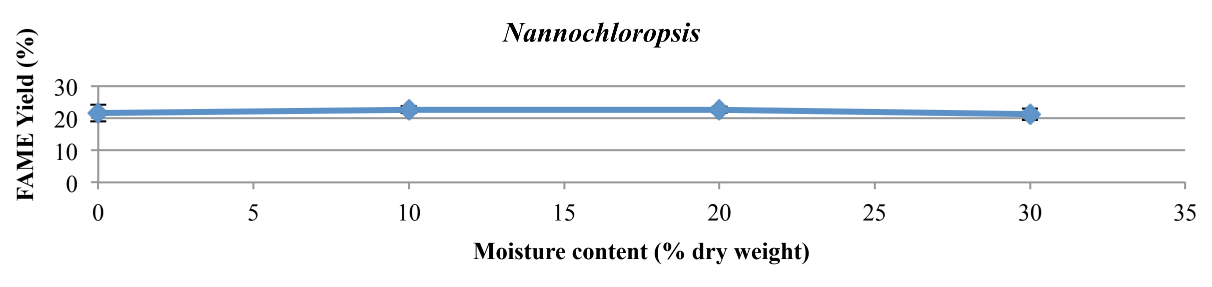

Fig2: Reactive extracted FAME yield from a wet *Nannochloropsis* at methanol/lipid ratio (=300)

Velasquez-Orta S. B., Lee, J. G. M. and Harvey, A. (2012). "Alkaline *in situ* transesterification of *Chlorella* vulgaris." *Fuel*, 94, 544-550.

Catalytic hydrothermal processing of different vegetable oils using HZSM5

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Hydrothermal liquefaction is a promising route to process biomass into fuels; especially it has been popular for the upgrading of microalgae because no prior drying was required (Biller et al, 2011) (Duan et al, 2010). Lipids can be extracted from different sources of plant based oil seed crops (sunflower oil, rapeseed etc) and from microalgae, and they can potentially be upgraded into diesel-like fuels using HZSM5 zeolites. Tryglycerides are hydrolysed into fatty acids above 300°C and a pressure around 15bar (King et al, 1999). Watanabe et al, (2006) and Fu et al (2010) have observed that the conversion of fatty acids under subcritical and subcritical water were low. The additions of catalyst (metal oxide or Pt/C) have improved the selectivity toward the production of aliphatic compounds.

During this work, sunflower oil and other vegetable oils including soya oil, linseed oil and sunflower oil; (which contain mainly polysaturated fatty acids), jatropha oil (monosaturated fatty acids) and palm oil (saturated fatty acid) have been processed at 350°C in subcritical water alone and with HZSM5. The resulting product has been analysed using a variety of methods, including size exclusion chromatography, boiling point distribution (using thermogravimetric analysis) and GC-MS.

The starting plant oils and hydrothermal oils are also analysed by GC-MS following conversion of existing fatty acids to FAME. It was determined that during hydrothermal liquefaction of sunflower oil with a high content of linoleic acid, (absence of catalyst) the majority of the triglyceride was hydrolysed into fatty acids. Furthermore, FAME analysis indicated that the C18:2 linoleic acid has been reduced into C18:1 or C18:0 or smaller fractions. Using HZSM5 triglycerides were upgraded into smaller molecules including alkenes and aromatics. Most of the linoleic acid was converted into smaller molecules and the main fatty acid remaining is C16:0.

In this work, the impact of different degrees of unsaturation has been investigated using different vegetable oils and at different temperatures (250-300°C), in order to understand the mechanism with and without the zeolite catalysts.

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Process Intensification: Nanoparticle production in Spinning Disc Reactor

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In recent years, the spinning disc reactors (SDRs) have been developed as process intensification equipment, where rapid mass and heat transfer rates can be obtained from the thin film of liquid produced due to centrifugal acceleration of rotating disc. In developing these characteristics, the SDR is considered a tool of process intensification due to its compactness, flexibility (as an inherently safe and continuous reactor technology) and capability to deliver better product quality. SDR is an attractive and viable technology for drug manufacture and crystallization. Crystallization processes in the pharmaceutical industries intend to achieve crystals with controlled size, shape, purity, and polymorphic form. A Plug flow crystallizer provides impressively productive crystallization methodology and consistent product can only be achieved in plug flows. An imperfect crystallization is caused by less intensive mixing, so fast processes, like nucleation in crystallization, are typically highly dependent on mixing. The purpose of this experimental study is to determine the feasibility of producing nanoparticles of titanium dioxide (TiO2) in a continuous spinning disc reactor (SDR) as an example of a process intensification technology. Acidified distilled water and TTIP (titanium tetra isopropoxied) were introduced into the centre of the disc at different molar ratio and flowrate and the disc was rotated at different speed. It has been seen that at the same ratio of Water/ TTIP, applying higher flowrate provides more uniform and smaller nanoparticles. It has been found that the higher the flowrate and rotational speed, the smaller the particle size and narrower particle the size distribution (PSD). studies showed that the important advantage of the SDR technology is the increased number of particles with controlled size, shape and size distribution that reach quality requirements.

Keywords: process intensification, spinning disc reactor, nanoparticle, titanium dioxide

On the investigation of nucleation mechanism in an oscillatory baffled crystallizer

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This presentation reports the outcome of the examination of the effect of mixing intensity on the nucleation mechanism of seeded crystallization of sodium chlorate in various configurations of stirred tank crystallizer (STC) and oscillatory baffled crystallizer (OBC). The results show that for the STC, an un-scraped system always yielded crystals of the same enantiomorphism as the seed crystal. The introduction of scraping to the STC resulted in product crystals of the opposite enantiomorphism to the seed being formed (Callahan and Ni, 2012), however changing the rate of stirring (RPM) had no influence over the percentage similarity to the seed crystal. For the OBC, scraping always gave a product crystal crop with less than 100 % similarity to the seed. Similarly, this was unaffected by altering the frequency of oscillation. Removing the scraping effect brought an increase of the similarity to the seed but the product crystals never reached 100 % similarity to the seed enantiomorphism. For both scraped and un-scraped OBCs, reduction of the oscillation amplitude did increase the similarity of the products to the seed and 100 % similarity to the seed was achieved at the lowest operating amplitude. These findings provide some scientific insights as to why the fluid regime in the OBC has the ability to promote nucleation while such an ability is unlikely in the STC..

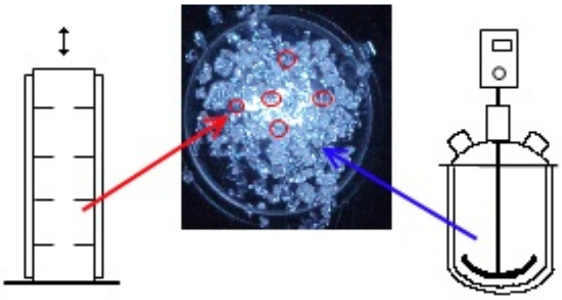

Figure 1. OBC (left) produces crystals of opposite enantiomorphism to the seed crystal. STC (right) produced crystals exclusively of the seed enantiomorphism.

Callahan, C.J. and Ni, X. (2012), *Probing into Nucleation Mechanisms of Cooling Crystallization of Sodium Chlorate in a Stirred Tank Crystallizer and an Oscillatory Baffled Crystallizer*, Crystal Growth & Design 12, pp 2525- 2532.

Reversed Crystal Growth of ZnO Microdisks.

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Hexagonal microdisks of zinc oxide (Figure 1a) have been synthesized via a hydrothermal method where the central part can be selectively dissolved by ethylenediamine to form microstadium shaped particles (Figure 1b). Nanocones and nanorods of ZnO can be grown on the outer and inner walls of the microstadiums via a further hydrothermal step creating so-called 'decorated microstadiums' which show improved efficiencies in water photolysis due to their high surface area. A reversed crystal growth mechanism (Chen et al, 2007) was revealed for the microdisks by analysing specimens across a range of time intervals using X-ray diffraction, scanning and transmission electron microscopies. It was found that initially the precursor materials aggregate into disordered quasi spherical particles on the glass substrate and then undergo surface crystallization to form a very thin single-crystalline hexagonal cup with a non-crystalline base located at the interface between the particle and the substrate (Figure 1c). As more precursor materials joins at the base of the particles, another quasi spherical aggregate forms, which then also undergoes surface crystallization. When the reaction time was increased, the crystallization extended from the surface towards the core (Self et al, 2013). The exterior of the one dimensional stacking of blocks of the hexagonal ZnO microdisks is similar to the mysterious appearance of the stone pillars we see at the Giant's Causeway, Northern Ireland.

We, and others in our group, are currently investigating the non-classical crystal growth mechanisms of other materials such as $CaCO_3$, zeolites and metal organic frameworks etc.

We would like to thank Ryan Tian and Huajun Zhou of the University of Arkansas and Heather Greer and Ross Blackley of the University of St Andrews for their assistance with this research.

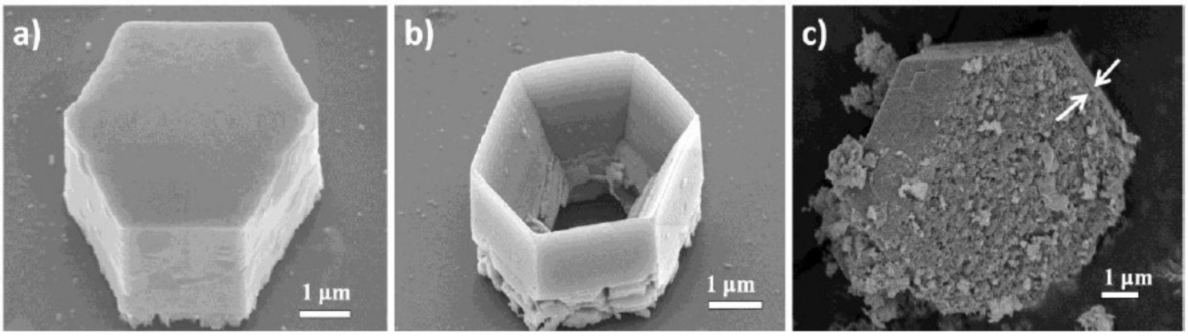

Figure 1. SEM images of novel ZnO morphologies. (a) Hexagonal microdisk grown on a glass substrate, (b) microstadium particle after selective dissolution and (c) a broken ZnO microdisk revealing the core-shell structure. The arrows in (c) indicate the thin single crystalline shell.

Chen, X. Y. Qiao, M. H. Xie, S. H. Fan, K. N. Zhou, W. Z. and He, H. Y. (2007) *Self-Construction of Core-Shell and Hollow Zeolite Analcime Icositetrahedra: A Reversed Crystal Growth Process via Oriented Aggregation of Nanocrystallites and Recrystallization from Surface to Core*, J. Am. Chem. Soc. 129, 13305.

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Preparation of biodegradable polymer nanoparticles for pharmaceutical applications in co-flow microfluidic devices

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In this study, a new microfluidic method for the production of biodegradable nanoparticles of tunable sizes was developed. The method is based on micromixing / direct nanoprecipitation in co-flowing streams of two miscible liquids. Polycaprolactone (PCL) was chosen for particle fabrication, because it is a biodegradable and bioresorbable polymer (Vert et al, 1992) commonly applied in pharmaceutical industry, while tetrahydrofuran (THF) was used as a water-miscible volatile solvent (Okada, 2002). The experimental set-up is depicted in Figure 1. The organic phase (a mixture of PCL and THF) was injected through the inner glass capillary with a tapered cross section culminated in a narrow orifice. Microfluidic devices with five different orifice diameters (60, 150, 200, 300, and 400 µm) were fabricated and the particle generation process for each orifice size was investigated using five different aqueous to organic phase ratios, Q_{aq}/Q_{or} (1.5, 3.0, 4.5, 7.0, and 10.0). The smallest nanoparticles with a mean size of 398–544 nm were produced using an orifice size of 60 µm. The position of liquid/liquid interface at different Q_{aq}/Q_{or} values, as recorded by a high-speed video camera, is shown in Figure 2. The higher the aqueous to organic phase volume ratio, the higher the dilution factor and the smaller the nanoparticles formed in the device.

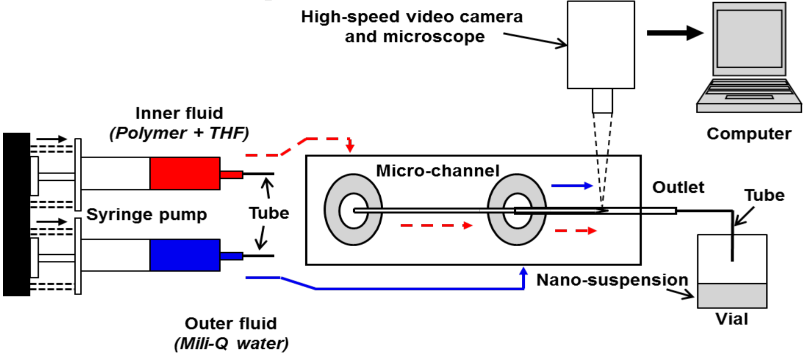

Figure 1. Schematic diagram of the experimental setup used in this work.

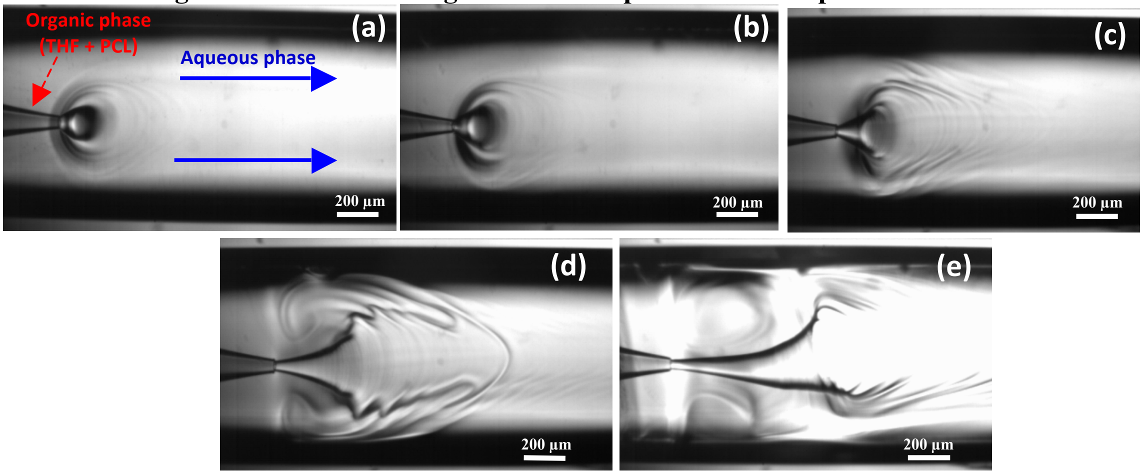

Figure 2. The position of liquid/liquid interface in a microfluidic device at the orifice size of 60 µm under (a) Q_{aq}/Q_{or}=10, (b) Q_{aq}/Q_{or}=7, (c) Q_{aq}/Q_{or}=4.5, (d) Q_{aq}/Q_{or}=3, (e) Q_{aq}/Q_{or}=1.5.

Vert, M. Li, SM. Spenlehauer, G. Guerin, P. (1992) *Bioresorbability and Biocompatibility of Aliphatic Polyesters,* J Mater Sci Mater Med 3, pp 432–46.

Okada, M. (2002) *Chemical Syntheses of Biodegradable Polymers*, Progr Polym Sci 27, pp 87–133.

Development of Non-esterified fatty acid electrochemical biosensor

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Approximately 10% of the annual NHS budget (~£9billion), is spent on treating diabetes and its subsequent complications. With an increase in people being diagnosed with type 2 diabetes (T2D), there is a high demand in biosensors that can monitor not only the blood glucose levels but also the other biomarkers associated with T2D. Non-esterified fatty acid (NEFA) is a biomarker for T2D development. Scheme 1 highlights the two important steps in NEFA detection (Shimizu et al., 1980).

$$\textbf{Step 1}\quad \text{NEFA + Coenzyme A + ATP} \xrightarrow{\text{Acyl-Coenzyme A synthetase (ACS)}} \text{Acyl-Coenzyme A + AMP + pyrophosphate}$$

$$\textbf{Step 2}\quad \text{Acyl-CoenzymeA} + O_2 \xrightarrow{\text{Acyl-Coenzyme A oxidase (ACOD)}} \text{enoyl-CoA} + H_2O_2$$

Scheme 1: Enzyme's involved in the different methods for detection of NEFA

The fatty acids investigated were palmitic acid and oleic acid, both are one of the most abundant plasma NEFA's. As H_2O_2 production is proportional to the concentration of NEFA, H_2O_2 was electrochemical detected. Cyclic voltammetry, linear sweep voltammetry and chronoamperometry were carried out based on the reactions in steps 1 and 2. Oxidation of H_2O_2 was subsequently detected in solution using different types of screen printed electrodes (SPE's). Current response showed linearity up to 3.00 mM NEFA concentrations (Figure 1). The enzymes were then immobilized on the working electrode of the SPE by layer-by-layer technique. Current response showed linearity up to 0.90 mM NEFA concentrations.

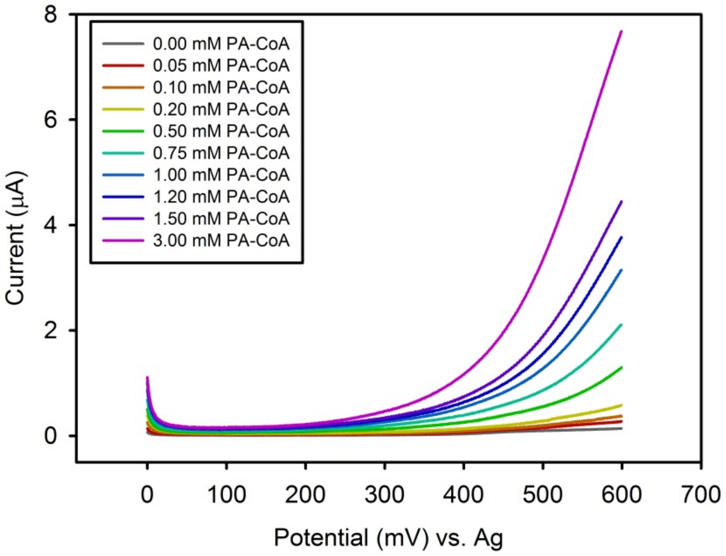

Figure 1: Linear Sweep voltammogram from the enzyme reaction (step 2 in Scheme 1) at different PA-CoA concentrations using Carbon SPE. The Scan rate was at 1 mVs.

Shimizu, S., Tani, Y., Yamada, H., Tabata, M. and Murachi, T. (1980) 'Enzymatic determination of serum-free fatty acids: A colorimetric method', *Analytical Biochemistry,* 107, (1), pp. 193-198.

Improving Yield and OEE of Filling Unit Operation within the Manufacturing Process for Multi Dose Powder Inhalers

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Powders are multiphase discontinua, comprising of solids, liquids and gases. In bulk, powders can exhibit features of all three phases when subjected to different conditions. Powder bulk characteristics are affected by a combination of the physical properties of the powder and external variables such as consolidation, aeration and moisture. There are too many combinations of permutations of properties and external variables to mathematically predict how a powder will behave under different conditions. This makes processing powders difficult and expensive as a lack of understanding of how bulk powder characteristics affect processes causes product and time to be lost.

There are three product strengths used in the manufacture of the Diskus inhaler, each with a varying concentration of active pharmaceutical ingredient. The difference in strength affects the powder properties and therefore the processing of each product. This is not reflected in the standard operating procedures for the three main controlling parameters. Yield and operational equipment effectiveness is lost as a result due to long machine start-up optimisation and filling weight failures during operation. In order to improve the performance of the filling unit operation, a series of experiments is proposed to determine the optimum filling machine parameter settings depending on the bulk powder characteristics of each batch.

An initial machine characterisation exercise using a Response Surface Methodology approach has been performed. The experiment used a single batch which enabled an initial model to be fitted to the dose weight performance for three parameters including interaction and quadratic terms. While this is only valid for that specific batch, further experimentation taking into account the product strength as an input category will enable a general model for each product strength to be fitted. The initial result of the machine characterisation yielded a better understanding of how the key parameters affected the performance of the filling machine.

Further work will utilise powder characterisation techniques as input parameters to a filling unit operation performance model. This will enable optimisation of machine parameters taking into account variation in batches of the same product strength. The nature of powder characterisation techniques means that a multivariate approach will be required to create a model. Investigations into the utilisation of powder characterisation parameters to be used in modelling to predict responses related to critical product performance indicators extra to the dose weight will also be performed.

An Investigation on Cake Permeability Measurement and Prediction

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Permeability is an important parameter in modelling the behaviour of fluid transport in porous media or packings, since it is used to predict the fluid flow through the material for a given pressure difference. However, there are various methods and models to predict permeability. The Kozeny-Carman (K-C) and Happel-Brenner (H-B) models are the most successful for analysing permeability but with limitations (Rushton et al. 2000 and Mauran et al. 2001). The main objectives of this work are: to measure and predict permeabilities of different materials under various conditions. After that compares the experimental results with the modelling ones using K-C and H-B models in order to investigate the lowest value of error between both methods under these conditions. Later on is to create and find a new computing model to investigate particle permeability under the same conditions using Artificial Neural Network approach in MATLAB Software. In order to study various separation processes the particle permeabilities were measured using two different experimental ways: high and low shear. Furthermore, number of solids was used in order to study porous media with different particle characterizations such as size, size distribution, shape and particle concentration. In the experiment, water was used as the permeated fluid.

The results show that, although, the largest permeability value and cluster size of particles were found in sedimentation, the lowest was found in filtration process where shear and pressure is high (Fig. 1). Also, the deduced cluster size during filtration was close to the value obtained by laser diffraction under conditions of high energy input. Cluster formations play an important role in determining permeability and, therefore, filtration rates (Di-Giovanni et al. 2012). The conventional approach is to use constant pressure (CP) laboratory tests, however, the results demonstrate that constant rate (CR) filtration is a more reliable method for data acquisition, especially when determining the filter medium resistance. The calculated specific resistance, from the particle size distribution data and the Kozeny-Carman equation is one order of magnitude lower than that measured, even though the solids were robustly characterised, see Fig. 2 (Mahdi and Holdich 2013). However, a complete and straightforward methodology is presented for investigating this and the significance, or otherwise, of medium resistance on the later stages of the filtration. Hence, further work is being performed on the use of an Artificial Neural Network (ANN) to predict permeability (and cake resistance) from particle characterisation data. It is found that, to use ANN both material and processes characterization need to be full understand in order to find the most effective variables on permeability values, which will be used as input parameters (Mahdi 2011).

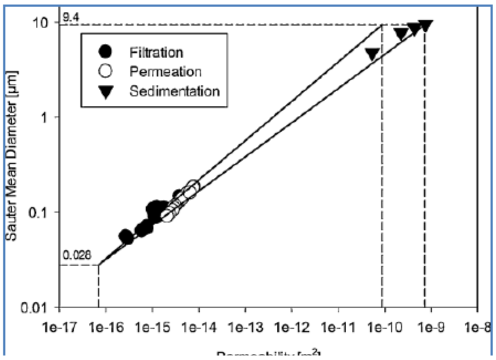

Fig. 1: Results deduced from experimental readings and the predicted operating envelope based on particle characterisation.

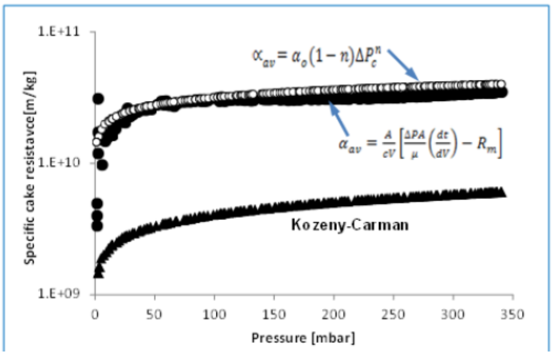

Fig. 2: The pressure effect during CR test on the specific cake resistance [*21% v/v feed solids at 10 rpm*] and theoretical resistance by K-C- Eq.

Di Giovanni B.A., Mahdi F.M., Starov V.M., Holdich R.G., (2012) *Chem. Eng. Res. Des.*, Part (A) **90**
Mahdi F.M., Holdich R.G., (2013) *Chem. Eng. Res. Des.*, **91**- CHERD-1129 (in press)
Mahdi F. M. (2012), *UKPTF, IChemE*, Loughborough
Mauran S., Rigaud L., Coudevylle O., (2001), *Transport in Porous Media* **43**, pp.355-376
Rushton A., Ward A.S., Holdich R.G., (2000) *VCH, Verlagsgesellschaft mbH*, Weinheim, Germany

Hydrogen Energy – Development Of Non-Noble Catalysts For Hydrogen And Oxygen Evolution In Alkaline Polymer Electrolyte Membrane Electrolysis

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The development of hydrogen production through electrolysis is hindered by the high costs associated with the technology, specifically the ion exchange membranes and electrocatalysts that are employed in the membrane electrode assemblies in electrolysers. The development of non-noble catalysts suitable for hydrogen and oxygen evolution in alkaline electrolysis is critical for successful industrial application.

Synthesis of NiO was achieved through thermal decomposition, chemical bath deposition and solution growth techniques. A mixed metal oxide, $NiCo_2O_4$, was synthesized through thermal decomposition of metal nitrate salts. Cyclic voltammetry and steady state electrochemical experiments on the electrodes were conducted in an electrochemical half cell. A thin film of pure NiO was formed onto a titanium substrate through chemical bath deposition followed by thermal decomposition. The performance of the electrode, relative to the mass of the catalyst loading, produced 0.25 A cm^{-2} mg^{-1} in 1 M NaOH at 25°C (IrO_2 produced 0.44 A cm^{-2} mg-1 in the same electrolyser). The electrode's performance is attributed to the nanoporous structure of the catalyst film (20 – 200 nm pore diameters), which was formed from the chemical bath deposition method used to prepare the catalyst films, although the procedure has a limited film thicknesses so higher loadings and current densities could not be achieved.

Higher loadings of other catalysts were made possible with addition of a PVDF binder to the catalyst film. Physical analysis through XRD was performed on the most promising catalysts for the oxygen evolution reaction to confirm their composition. A blend of α-$Ni(OH)_2$ and $4Ni(OH)_2 \bullet NiOOH \bullet xH_2O$ formed through the chemical bath deposition technique produced higher current densities (104 mA cm^{-2} at 0.8 V vs. Hg/HgO) than another non-noble metal catalyst, $NiCo_2O_4$ (97 mA cm^{-2}) in 1 M NaOH at 25°C. An alkaline polymer electrolyser free from noble metals was developed with a membrane electrode assembly that utilised a partially fluorinated membrane, a PVBC/PVC ionomer in the catalyst layers, 1.0 mg $NiMoO_4$ cm^{-2} in the cathode and 0.7 mg $NiCo_2O_4$ cm^{-2} in the anode. It produced 0.4 A cm^{-2} in 1 M KOH at 25°C at a potential of 1.9 V.

Poster Presentations

Product Driven Process Development of Emulsion Systems

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High energy rotor-stator devices are commonly used for the manufacture of emulsions across process industries. However, despite the growing number of applications [for examples, in foods, home and personal care, cosmetics, health care products, fine chemicals and pharmaceuticals] for such emulsions and the recognised impact that manufacturing processes have on their physical properties and performance characteristics, the open literature reveals few design parameters which provide clear linkages between such processes, as determined by equipment design and operation, and those physical properties and performance characteristics, as determined by constituent type, dispersed phase droplet size and the droplet size distribution.

Now, an important and emerging class of such rotor-stator devices comprises the Fluid Dynamic Mixer [FDM], a proprietary device of Maelstrom APT Limited. That device builds on the highly successful cavity transfer mixing technology which emerged in the 1980s. This poster considers the emulsification of a model O/W emulsion system subject to changes in order of ingredient addition. The droplet size distribution was analysed using a Malvern Mastersizer 2000 (Malvern Instruments Ltd, Malvern). In this study, results indicate that the most effective means of facilitating droplet break-up is via the staged addition of the surfactant solution to an oil rich system [Process 3].

Figure 1: Fluid Division Mixer (1)

Process #	1	2	3	4
D_{32} (µm)	5.805	5.538	2.359	7.231
D_{43} (µm)	6.562	6.403	3.020	8.424

Table 1: Effect of Order of Addition to Droplet Break-up

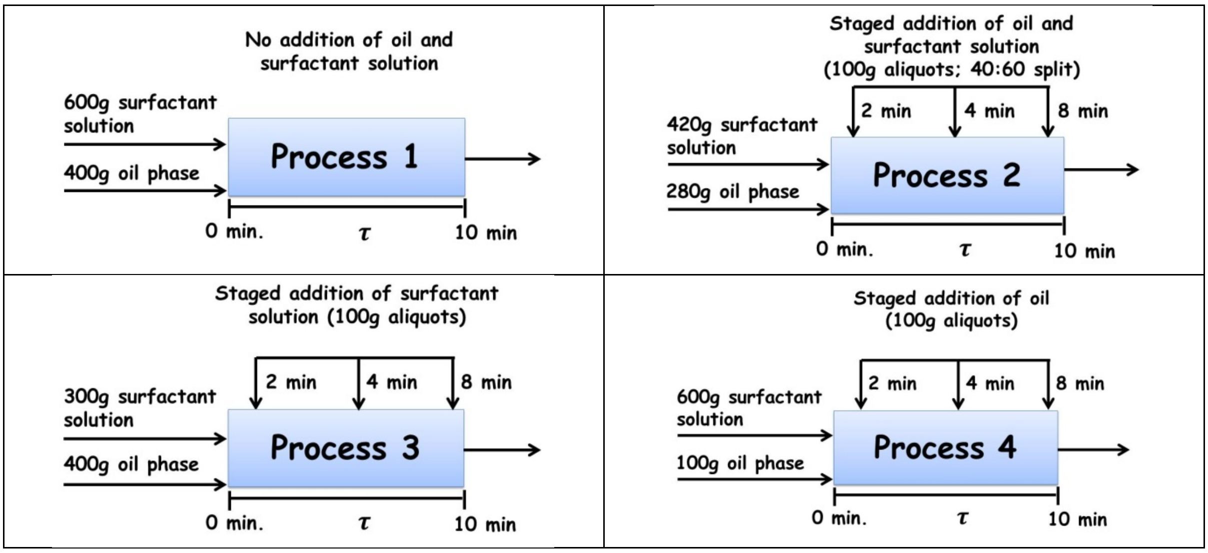

Figure 2: Order of Ingredient Addition – Process 1 to 4

(1) Maelstrom APT Limited. FDM DB75-200 product data sheet. http://www.maelstrom-apt.com/wp-content/themes/maelstrom/imgDoc/productDocuments/DB75-200.pdf

Dynamic Process Monitoring Using Partial Least Squares and Extensions

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* Corresponding author. Email bothinah.altaf@newcastle.ac.uk

Multivariate statistical process monitoring (MSPM) plays an important role in competitive industrial world. It helps to attain an enhanced understanding of industrial processes and ensures the satisfactory performance and production in term of safety, quality and economic requirements. By detecting the abnormal events, one can eliminate the root causes and hence, improves process efficiency and quality products. As most of industrial processes are generally dynamic in nature, the traditional MSPM methods such as Principal Component Analysis (PCA) and Partial Least Squares (PLS), which assume that processes are operated under steady state, show unsatisfactory performance. This is because they do not consider the complex dynamic characteristics of modern industrial processes and hence, increase the false alarm rate and decrease the effectiveness of the monitoring system. Therefore, a dynamic version of the MSPM method was developed.

The rapid development of automated data acquisition systems increases the number of measured variables. Hence, an advanced MSPM method is required to improve the interpretability of the process behaviour. Consequently, multiblock dynamic PLS (MBDPLS) was proposed to monitor the whole process and the individual units. This approach is extended to adaptive multiblock dynamic PLS (AMBDPLS) for process monitoring in real time basis. The main challenge with the AMBDPLS based monitoring scheme is the impact of outlying samples as the model will incorrectly adapt to these. Therefore, robust AMBDPLS is proposed which is resistance to outlying samples. In addition, it enables to monitor the whole process as well as individual units.

The proposed methods were tested and compared using the data generated from a simulation of Tennessee Eastman Process (TEP). This is widely accepted as a realistic application for process monitoring and fault diagnoses studies among both academic and industrial practitioners. Further, the TEP (Figure 1) is complex dynamic, nonlinear and multiple units process (Downs and Vogel, 1993). Application of the proposed method showed a superior performance compared to the MBDPLS and AMBDPLS. Robust AMBDPLS can be considered as a combined monitoring system of MBDPLS and AMBDPLS. This approach decreases the false alarm rate in comparison with MBDPLS and increases the fault detection rate in comparison with AMBDPLS. In addition, fault propagation in continuous processes can also be studied using the proposed approach.

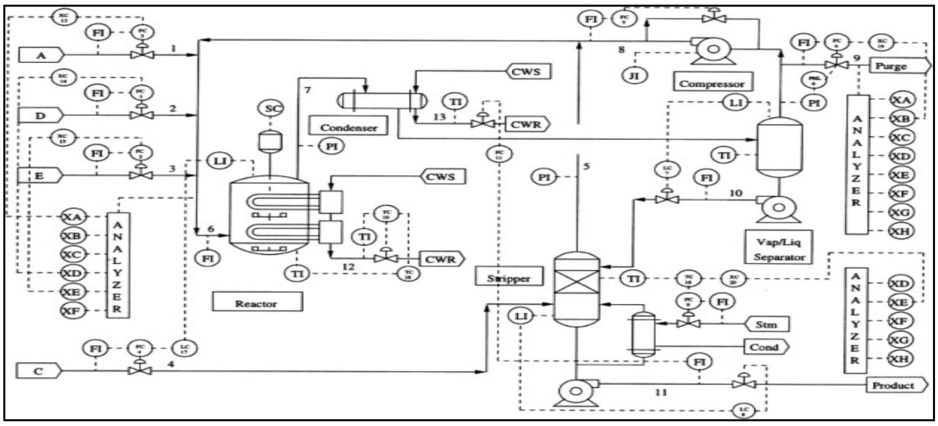

Figure 1. Tennessee eastman process (Downs and Vogel, 1993)

Downs, J. J. and Vogel, E. F. (1993) 'A plant-wide industrial process control problem', *Computers & Chemical Engineering,* 17, (3), pp. 245-255.

Harnessing Stranded and Flared Associated Natural Gas: The Role of Heat Transfer in Combined Micro-Channel reactors/Heat Exchangers

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Counter-currently pairing endothermic and exothermic reactions, side-by-side in auto-thermal, micro-channel reactors/heat exchangers is well established. The Fischer Tropsch process (for converting natural gas to synthetic crude) has been adapted to be carried out on in this manner, with the benefit of intensification including accelerating the process by between 10 and 1000 times. However, operational issues such as flow mal-distribution change in feed stock (natural gas) composition and pressure, etc. lead to the development of hotspots within the reactor; a phenomenon which has deleterious ramifications on the catalyst and overall reliability of the system. Two possible means of effectively combating this challenge are proposed.

The concept of hybrid cooling is imported from micro-electronics i.e. the synergistic combination of micro-channel and jet impingement schemes. This is to be done with a view to overcoming the drawbacks of either technique. The impingement is simulated by feeding the air for combustion through small jets along the reactor length. The effects of jet diameters and pressure drop on achieving near-isothermal conditions within the reactor are to be investigated experimentally. Results from preliminary numerical modelling of this hybrid system show that the desired isothermal conditions are attainable. Future work will look to validate these results experimentally.

It is also suggested that a layer of phase change material (PCM) be placed within the plate separating either reaction. This has the potential of acting as an energy storage buffer, the phase changing cycle which occurs with latent heat exchange at constant temperature acts a "thermal flywheel". This flywheel effect created within the reactor is able to control temperature excursions brought about fluctuations in feedstock quality. The problem in hand thus becomes one of optimisation, including choice and optimum thickness of PCM, statistically detecting temperature and feedstock composition disturbances, etc.

Hierarchical Growth of ZnO Crystals Hydrothermally from Zinc Acetate

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The hydrothermal synthesis technique is a popular means of preparing metal oxide particles due to its ability to produce crystalline particles directly from solution, with minimal agglomeration, (Baruah and Dutta, 2009). Hydrothermal synthesis of ZnO results in multiple crystal morphologies, depending on process conditions, (Wang et al, 1998; Yu and Yu, 2008). The material is of technological interest due to its wide band gap (~3.37 eV), high exiton binding energy (60 meV) and ultraviolet absorbance resulting in applications in opto-electronics, acoustics, solar cell devices, gas sensing, and cosmetics, (Wang, 2004).

Despite intense research, there continues to be a lack of understanding of the hydrothermal growth mechanisms resulting in ZnO microrods, (Wang et al, 2011). This presentation reports results of a study into the growth of ZnO hexagonal microrods from the hydrothermal reaction of zinc acetate and sodium hydroxide. Particles have been produced for different dwell times at a reaction temperature of 120 °C. Characterisation by scanning and transmission electron microscopy reveals that growth proceeds by the assembly of primary ZnO nanoparticles into pseudo hexagonal layers, which stack together to produce hexagonal rods, from which further crystallisation occurs resulting in well-developed hexagonal rods, Figure 1. Details of each stage of the hierarchical growth process will be illustrated and described.

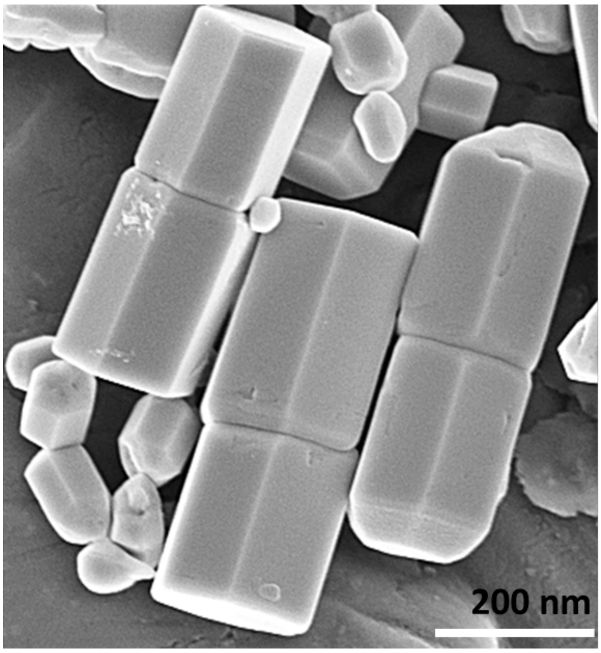

Figure 1. Hydrothermal ZnO Microrods

Baruah, S. Dutta, J. (2009) *Hydrothermal growth of ZnO nanostructures*, Sci. Technol. Adv. Mater. 10 pp 1 – 18

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Wang, M. Zhou, Y. Zhang, Y. Hahn S. H. Kim, E. J. (2011) *From $Zn(OH)_2$ to ZnO: a study of mechanism of phase transformation*, CrstEngComm, 2011, 13, 6024 – 6026

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Modelling of Waste recovery via pyrolysis

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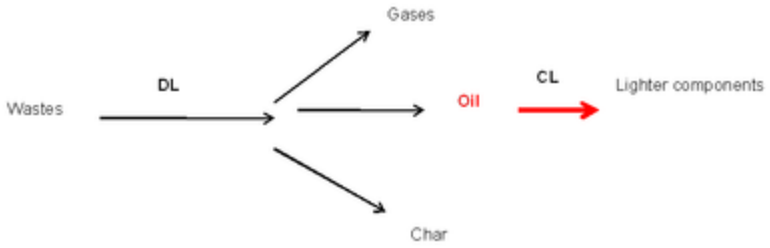
Pyrolysis is a process increasingly employed for thermochemical conversion of wastes and recovery of lower molecular weight hydrocarbon products to be used as fuel or chemical feedstock. The optimisation of the process demands knowledge and control of the kinetics of pyrolysis for accurate predictions of the products' distribution.

The lumping kinetics approach (e.g., Astarita, G and R Ocone, AIChE Journal, 34, 129, 1988) is applied to model the pyrolysis of wastes and successive fractionation of the liquid products. The schematic of the process is as follows:



A discrete lumping methodology is applied to the three lumps formed by the gases, the oil and the char resulting from the pyrolysis of wastes. The fractionation of the oil is described through the continuum lumping approach. The "lump" represented by the oil, obtained through the application of the discrete lumping (DL) model represents the feedstock for the continuum lumping (CL) model to furnish the composition of the fractioned products. The work presents a number of scientific challenges: firstly, the kinetics of plastics pyrolysis must be elucidated; additionally, the fractionation of the bio-oil would present an "apparent" kinetics of the multi-component mixture which is not simply explicable through the kinetics of each single reaction.

G. Astarita and R. Ocone (1988). "Lumping nonlinear kinetics." AIChE Journal 34(8): 1299-1309.

Organic Matter Transformation in Sewer Processes

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Sewer network is a system that collected wastewater from water supply of a community and also runoff water that results from precipitation. Sewer can be categorized into sanitary sewers, storm sewers and combine sewer. Sanitary sewers deal with wastewater from residential, commercial area and industries. Storm sewers are constructed for collection and transport of runoff water and combined sewer are combination of sanitary and storm sewers. There is lots of process that happen inside a sewer, as that is the reason a sewer is considered as a reactor for microbial processes (Hvitved-Jacobsen, 2002). A sewer consists of wastewater, biofilms and sediments. My research will be focusing on the biofilm of combine sewer. Biofilm can be aerobic, anoxic, anaerobic or any combination of them. I will be researching on the growth of the biofilms (Madigan, 2009), the process of biofilm attachment and detachment (Simões,2007), factors that influencing the process, roles and transformation of organic matter in the process, characterizing microbial growth on different substrates, and results obtained from the experiment will be compared with results from the real sewers.

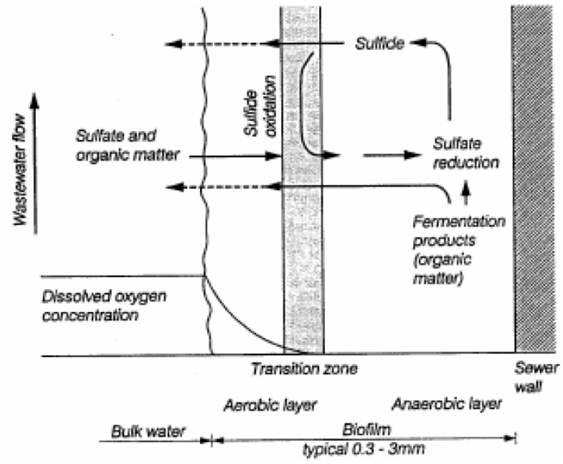

Figure 1. Aerobic and anaerobic process interactions in a biofilm (Ashley, 2004)

Hvitved-Jacobsen, T., Vollertsen, J. and Haaning Nielson, A. (2002) *Sewer Processes: Microbial and Chemical Process Engineering of Sewer Networks*. Boca Raton, Fla.: CRC Press.

Madigan, M., Madigan, M. and Brock, T. (2009) *Brock biology of microorganisms*. San Francisco, CA: Pearson/Benjamin Cummings.

Ashley, R. (2004) *Solids in sewers*. London: IWA.

Simões, M., Cleto, S., Pereira, M.O., Vieira, M.J. (2007) Influence of biofilm composition on the resistance to detachment. *Water Science and Technology*, 55(8-9), 473-480.

Investigations into Parameters Affecting Purity in Oscillatory Baffled Crystalliser and Stirred Tank Crystalliser

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School of Engineering and Physical Sciences, Heriot Watt University, Edinburgh EH14 1AS; Email: hrm2@hw.ac.uk

Crystallization is a unit operation, often used for purification; therefore obtaining the highest possible purity of product is of paramount importance. In cooling crystallization the general trend is that the purity of product decreases as the cooling rate or mixing intensity of the system is increased (Givand et al, 1999). Confidential results obtained elsewhere (NiTech) show that the crystals produced in an oscillatory baffled crystallizer (OBC) had a higher purity than those produced in the traditional stirred tank crystallizer (STC) at the same operating conditions with identical compounds. Finding the scientific explanations behind this difference and exploring ways of improving purity is the main focus of this research.

Using urea as the model compound, this poster will present experimental data on purity obtained at various conditions, which agree with these unpublished data for all conditions tested. Three possible hypotheses are currently being investigated to account for possible reasons for the purity differences:
(1) the effects of cooling rate and the related heat transfer differences within the vessels;
(2) the different mixing mechanisms between the OBC and STC;
(3) or the combined effect of the cooling rate and the mixing mechanism.

We will also show the purity data to testify the first two hypotheses that are partly responsible for the differences to a varying degree. Future work involves the addition of known impurity into the systems; this would further cast insights into this matter.

Givand, J.C., A.S. Teja, and R. W. Rousseau, *Manipulating crystallization variables to enhance crystal purity.* Journal of Crystal Growth, 1999. **198-199, Part 2**(0): p. 1340-1344.
Clients trials data from NiTech Solutions Ltd

Development of Algal Biodiesel via synthetic biology

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Metabolic engineering and synthetic biology approaches provide the possibility to improve biofuel production from various microorganisms. Microalgae species store high amounts of lipid, which can be further processed into biodiesel. Biological improvement of microalgae lipid yields will help for a promising future for algal biodiesel generation.

This project seeks to increase algal lipid yield by manipulation of microalgae metabolic pathways, such as promoting lipid production and photosynthetic activities or preventing the storage of starch. To achieve this goal, biological mechanisms and protein and gene identity must first be understood. Algal growth, lipid level/composition, photosynthetic activities, energy flux as well we other metabolic factors will be observed and compared under different light intensities, nutrient concentrations as well as other conditions. Microalgae are known to accumulate lipids under nutrient stress, however, with a reduction of growth and overall yield (Longworth et al., 2012). Further more, proteomics methods will be applied to understand the mechanisms such as how the stress induces lipid production and what pathways are involved in this process.

Currently, the algae species *C. reinhardtii* wild type CCAP 11/32C, *C. reinhardtii* starchless strain and *C. reinhardtii* cell wall deficient mutant are cultured in a series growth medium containing different concentrations of sulphur. Growth observations, Nile Red neutral lipid analysis, GC analysis of lipid composition, spectrophotometer analysis of carbohydrate and chlorophyll, HPLC separation and MS identification of proteins will be carried out in this project.

Longworth, J., Noirel, J., Pandhal, J., Wright, P.C., and Vaidyanathan, S. (2012). *HILIC- and SCX-Based Quantitative Proteomics of Chlamydomonas reinhardtii during Nitrogen Starvation Induced Lipid and Carbohydrate Accumulation.* J. Proteome Res. *11*, 5959–5971.

Iron for Nitrobenzene Reduction

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Nitrobenzene, a common contaminant used in industry, has received increased public concern as a result of its toxicity. Iron powder has proven promising in various types of contamination remediation including nitro-aromatic removal. This research aims to investigate the degradation of nitrobenzene using iron powder. A series of experiments were carried out, using iron powder supplied by Alfa Aesar, to study the kinetics of reduction and the effect of shaking speed, iron loading, initial concentration and pH of nitrobenzene solution on the rate of nitrobenzene reduction. The results demonstrate that nitrobenzene is reduced in the presence of iron powder and the rate of nitrobenzene reduction increases with shaking speed and iron loading in the system. In contrast, the rate of nitrobenzene reduction decreased with increasing initial solution pH. In addition, the rate of nitrobenzene reduction was influenced by initial nitrobenzene concentration with nitrobenzene reduction following a pseudo-first order kinetic model for all experimental systems used in this study.

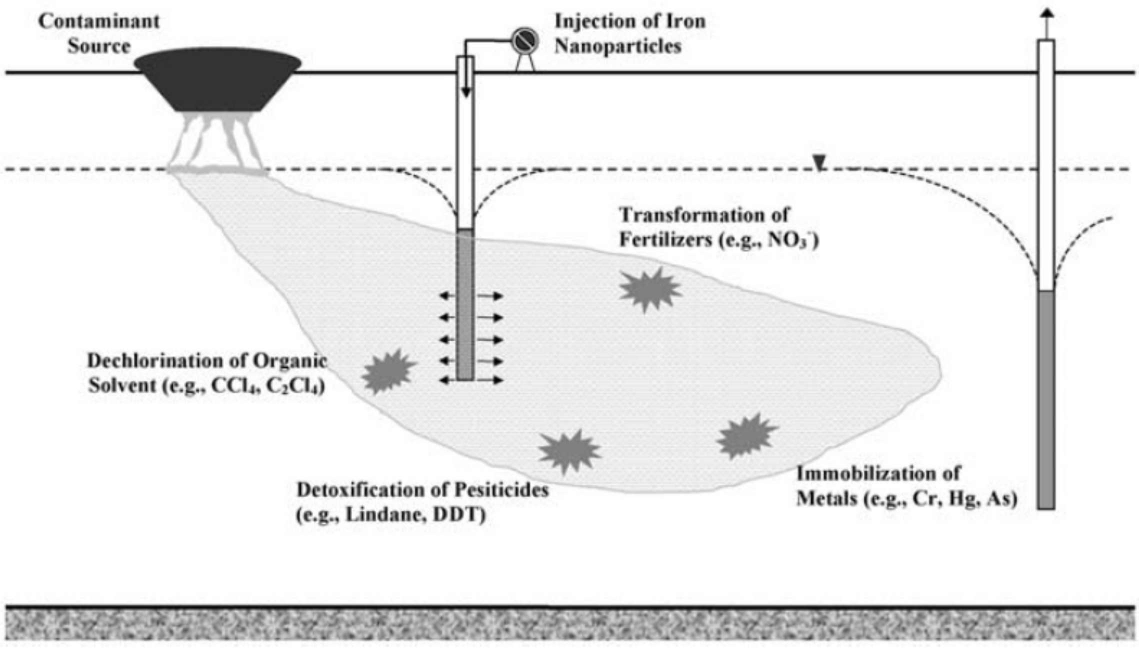

Figure 1 In situ groundwater remediation technology (Zhang, W.X., 2003)

Zhang, Wei-Xian (2003) *Nanoscale iron particles for environmental remediation: An overview*), Journal of Nanoparticle Research 5, pp 323-332.

Production of microparticles for drug delivery in flow focussing microfluidic devices

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Monodisperse biodegradable poly(lactic acid) (PLA) and polycaprolactone (PCL) microparticles of different size and morphology (porous and coherent) were produced using a novel approach based on emulsification in a 3D (axisymmetric) flow focusing glass capillary device (Chu et al, 2007). In a 3D flow focusing device, the dispersed phase is completely surrounded by the continuous phase during droplet formation process, owing to a circular cross section of the entry orifice, and wetting of the channel wall can be avoided (Vladisavljević et al, 2012). In this work, the dispersed phase was either a single-phase liquid (a mixture of PLA or PCL and a volatile organic solvent) or water-in-oil emulsion and the continuous phase was 5% aqueous solution of polyvinyl alcohol. As shown in Fig. 1, the continuous and dispersed phases were pumped to the device counter-currently using separate syringe pumps. The droplets were collected through a collection capillary with a tapered cross section and vacuum evaporated to form particles. The drop generation process was recorded using a high-speed camera attached to an inverted microscope (Figure 2). When a hydrophilic drug, lidocaine hydrochloride, was dissolved in the inner water phase, encapsulation efficiencies above 70% were achieved. Although glass capillary devices cannot easily be replicated as those made from mouldable polymers such as polydimethylsiloxane (PDMS), they are more chemically and mechanically robust than PDMS devices, do not swell, and the size of entry orifice can be precisely controlled by a micropipette puller to produce droplets of tunable size (Fig. 2).

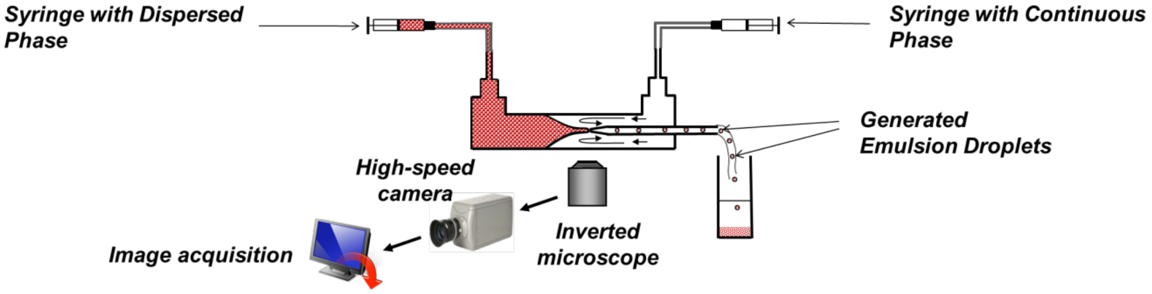

Figure 1. Apparatus setup of microfluidic device for the production and monitoring of emulsions.

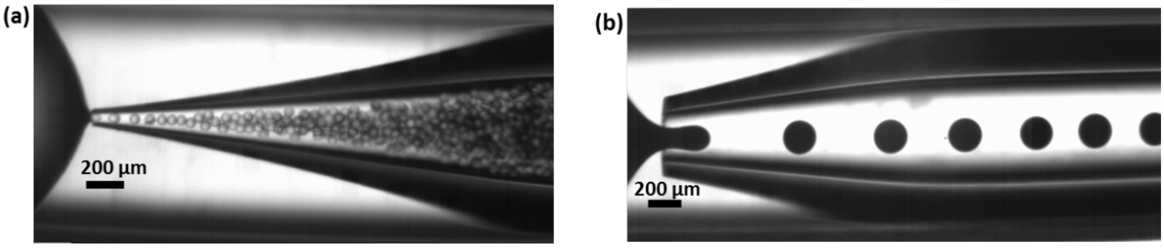

Figure 2. Generation of uniform droplets with adjustable sizes in flow focusing glass capillary devices: (a) Single emulsion (Q_c= 0.5 ml/h, Q_d = 0.2 ml/h , $d_{orifice}$ = 53 µm, $D_{droplet}$= 51 µm) (b) Double emulsion (Q_c= 0.6 ml/h, Q_d = 0.4 ml/h, $d_{orifice}$ = 300 µm, $D_{droplet}$= 202 µm).

Chu, L., Utada, A., Shah, R., Kim, J. & Weitz, D. (2007) *Controllable Monodisperse Multiple Emulsions*, Angewandte Chemie International Edition, 46(47), pp. 8970-8974.

Vladisavljević, G.T., Kobayashi, I. & Nakajima, M. (2012) *Production of Uniform Droplets Using Membrane, Microchannel and Microfluidic Emulsification Devices*, Microfluidics and Nanofluidics, 13(1), pp. 151-178.

Novel amine functionalised silica based adsorbent for CO_2 capture

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Inspired by the ability of diatoms to grow well defined and complex silica skeleton under green conditions, previous studies have shown that specific amine containing compounds have the ability to condense silica from a silica precursor solution[1]. In this study, a bio-inspired approach for synthesizing amine modified silica for CO_2 capture has been investigated. Both functionalised and un-functionalised silica were synthesised using a bio-inspired route. Sodium metasilicate pentahydrate was used as the silica precursor while diethylenetriamine (DETA) as the amine source. The synthesized sorbents are then characterized using infrared spectroscopy (IR), N_2 adsorption, elemental analysis, thermogravimetric analysis (TGA) and CO_2 adsorption analysis to investigate the effect of functionalization on the adsorption properties of the as synthesized sorbents. Results obtained have shown that functionalization of these sorbents greatly enhanced their adsorption capacities. Under static adsorption conditions, capacities of up to 57.2 $mgCO_2/g$ sorbent has been achieved. Although this is short of the 88 $mgco_2/g$ sorbent recommended for commercial applications, there is a positive indication that the prospect of a bio-inspired methods for synthesis of amine functionalised silicas as sorbents for CO_2 capture is promising, cost effective, regenerable and a greener means for CO_2 capture.

1. *Begum, G., et al., Bioinspired silicification of functional materials: fluorescent monodisperse mesostructure silica nanospheres. Chemistry of Materials, 2009. 22(2): p. 551-556.*

Characterisation of High Shear Rotor Stator Devices.

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High Shear Rotor Stator devices (H.S.R.S.) are commonly used for the manufacture of structured liquids (such as emulsions) across many process industries (i.e. foods, home and personal care, cosmetics, healthcare, fine chemicals and pharmaceutical industries). However despite the growing number of applications for such liquids and hence H.S.R.S. there is almost no fundamental understanding (in the open literature) of how these devices interact with these structured fluids (Atiemo-Obeng & Calabrese, 2004).

Effective process scale up of H.S.R.S. from the laboratory environment to factory scale is thus of crucial importance for the process industries. Hence comparison of H.S.R.S. at different scales and operating conditions is needed.

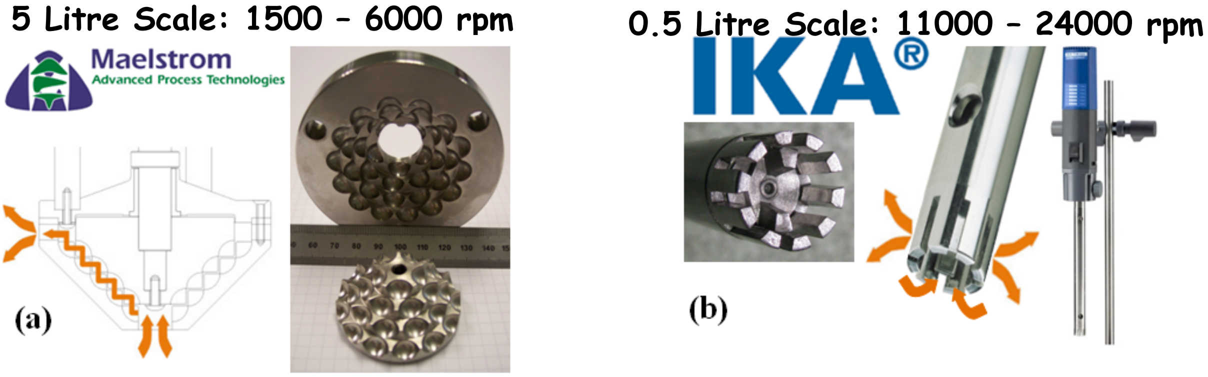

Figure 1: (a) Fluid Division Mixer (F.D.M.) DB50-4-4-15 (b) IKA ULTRA TURRAX T18 fitted with a S 25 N – 18 dispersing unit.

This work reports the comparison of two commercially available (and geometrically dissimilar) H.S.R.S. devices shown in Figure 1 that operate at different scales. The devices are compared using several literature correlations (tip speed, shear rate, energy dissipation and Weber number) for a model emulsion system and their applicability discussed.

Atiemo-Obeng, V.A. & Calabrese, R.V. (2004) Rotor-Stator Mixing Devices, In: Handbook of Industrial Mixing, E. L. Paul, V.A. Atiemo-Obeng and S. M. Kresta, Eds., John Wiley & Sons, Inc., New York, pp. 479-505.

Feasibility of the Microwave Regeneration of adsorbents for CO_2 capture

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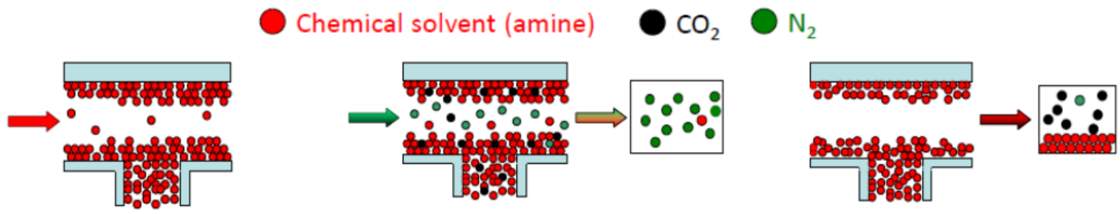
New ideas for carbon capture are urgently needed to combat climate change. A novel concept has been suggested concerning the 'Wetting Layer Absorption' (WLA) process[1-3] in which a porous material is used to support liquid-like regions of absorbing solvent, which in turn absorb carbon dioxide.



Step 1: Absorbent loading

Step 2: CO2 Capture

Step 3: CO2 Recovery

Figure 1. WLA Process

Another novel aspect of this work is the investigation of microwave regeneration for the recovery of CO_2. Microwave-swing processes can operate at lower temperatures, and be much faster and more efficient than conventional heating processes which are responsible for most of the energy penalty for carbon capture.

To assess the feasibility of the microwave-driven recovery of CO_2 we study the dielectric properties of relevant fluids using molecular dynamics simulations. The dielectric spectra of different solvents of particular interest for this application will be determined using Explicit Hydrogen and United Atom force fields, and the possible influence of temperature will be assessed. The results will show whether the studied models, which were developed for the prediction of a particular set of properties, show a good performance in the estimation of dielectric properties.

[1] Sweatman, M. B. (2010) *Equilibrium behaviour of a novel gas separation process, with application to carbon capture*, Chemical Engineering Science 65, pp 3907-3913.

[2] Sweatman, M. B. (2011) *Improving the equilibrium performance of active carbons for separation processes by co-adsorption with low pressure solvent: application to carbon capture*, Adsorption 17, pp 723-737.

[3] EPSRC grants **EP/F061285/1** and **EP/J019704/1.**

Nucleation of Cystals under Controlled Flow Conditions.

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Crystal nucleation is a puzzling phenomenon whereby supposedly disordered liquid solutions become locally ordered to a sufficient extent that they form a stable region (nucleus) of a new crystalline phase. The new crystalline phase then grows by the addition of further molecules from solution, to form a macroscopic crystal.

Going beyond the basic science of nucleation is particularly challenging for designing industrial processes because processes typically involve flow and mixing. This makes controlling nucleation much more complex due to the interplay of the phase transition (nucleation of solid phase from supersaturated liquid solution) with the flow and mixing conditions.

My research involves using optical based measurements to study the effect of flow on nucleation. Supersaturated solutions of the amino acid glycine are subjected to controlled flow conditions, resulting in the shearing of the solutions. The sheared solutions are then monitored using a purpose built instrument that allows turbidity and scattering to be simultaneously monitored.

The work carried out so far suggests that shear has a profound effect on crystallisation by significantly increasing nucleation rates. The findings have the potential to impact the design and control of manufacturing processes involving crystallisation.

Physicochemical Characterisation Of A Solid Torrefied Biomass

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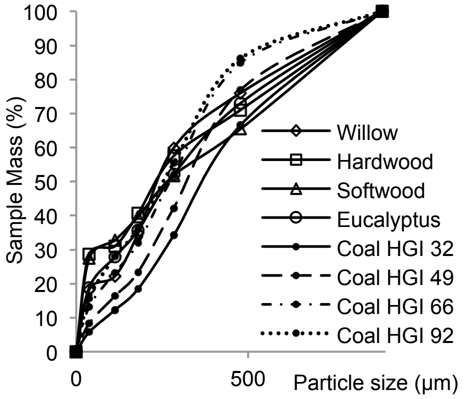

Figure 1. Particle size distribution curves for biomass torrefied at 270-290°C with a residence time of 40-50 mins alongside four standard reference coals of HGI 32, 49, 66 and 92.

Biomass has become the world's fourth largest source of energy and in order to make it increasingly beneficial towards a more sustainable environment, the application of torrefaction can be feasible. Torrefaction is a mild pyrolysis treatment under inert atmosphere that has the ability to improve the physical and chemical properties of a biomass[1]. There have been a number of studies that examined the modifications in terms of proximate, ultimate, mass and energy yields[2,3]. In this study, several wood fuels: (willow, eucalyptus, a mixture of hardwoods (oak and birch) and a mixture of softwoods (pine, larch and spruce)) were torrefied at 270 – 290ºC and 290 – 310ºC with two residence times (40 – 50 mins and 70 – 80 mins). This paper presents a more thorough look into the properties of these four torrefied biomass. Grindability, density, hydrophobicity and surface area were investigated, as well as the morphology and composition. Information from microscopic and spectrometric studies, namely Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), Fourier Transform Infrared Spectroscopy (FTIR) and X-ray Photoelectron Spectroscopy (XPS) is also discussed here. An increase in the severity of the torrefaction conditions greatly improved the physical characteristics of a torrefied biomass. Figure 1 illustrates the improved grinding behaviour after torrefaction. XPS and FTIR are able to follow a change in the chemical properties of the torrefied biomass compared to the raw biomass. However, the TEM and surface area data did not show much difference after torrefaction in terms of porosity. Briefly, temperature plays a major role during torrefaction. Choosing an optimum condition is fundamental to attaining an efficient high energy yield. Treatment at a medium temperature at a short residence time seemed to be the ideal condition to achieve good physical properties and high energy yield. A mixture of pine, spruce and larch, containing the least amount of hemicellulose yielded the most amount of energy (95%), followed by a mixture of oak and birch (80%), willow (79%) and eucalyptus (75%).

1. D. Medic, M. Darr, A. Shah, B. Potter, J. Zimmerman. (2012). *Effects of torrefaction process parameters on biomass feedstock upgrading*, Fuel 91, pp 147-154.
2. T.G. Bridgeman, J.M. Jones, I. Shield, P.T. Williams. (2008). *Torrefaction of reed canary grass, wheat straw and willow to enhance solid fuel qualities and combustion properties*, Fuel 87, pp 844-856.
3. M.J. Prins, K.J. Ptasinski, J.J.G. Janssen. (2006). *Torrefaction of wood: Part 2. Analysis of products*, Journal of Analytical and Applied Pyrolysis 77, pp. 35-40.

Bio-inspired Silica nanoparticles: Optimisation for Delivery Applications and Understanding Biological Safety.

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In recent years there has been much interest in the use of silica nanoparticles for drug delivery. Several varieties of mesoporous silica nanoparticles (MSN) have been developed and have been shown to have desirable hold and release profiles for a variety of small drugs (e.g. ibuprofen) and large proteins (e.g. albumin). MSNs are manufactured using harsh chemicals and extremes of pH and temperature and so any drug must be loaded in a separate step. Therefore, a process which occurs under benign conditions where the drug can be loaded in situ, is clearly more favourable and environmentally friendly. Bio-inspired silica nanoparticles are the focus of this project and were inspired by benign silica condensation observed in diatoms (a type of algae). We aim to first characterise the particles and understand the chemistry of altering their key properties (e.g. size and pore size) and then investigate their ability to have both small and large molecules loaded and released from them (i.e. act as a drug delivery system). Finally we must investigate the particles cytotoxicity on a variety of different cell types, as any drug delivery system must be benign to normal human tissues to be even considered an effective drug delivery system.

Characterisation of Spatially Resolved Spectroscopic Measurements for Use in Monitoring Pharmaceutical Fermentation

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Process analytical techniques are important for efficient and safe manufacturing of pharmaceutical products. They hinge on the development of robust measurement and calibration methodologies for on-line implementation. NIR sensors are capable of rapid physical and chemical composition of process streams, however for fermentation processes this application potential has not been fully realised.

Near infrared (NIR) light is commonly used in optical devices as it is able to travel to a further depth in a system than visible light (Fabbri et al, 2003). NIR measurements can be used to obtain both chemical and physical properties of a system and is cheaper than other technology that is of comparable accuracy.

The research from this PhD is based on spatially resolved measurements. Spatially and angularly resolved systems involve collecting light from an optical probe at varying distances and angles from the light emitting fibre to obtain the spatially and angularly resolved reflectance measurements.

The novel spatially and angularly resolved system used in this research is able to collect data from the NIR wavelength range 890-2125nm and the UV wavelength range 330-1050nm. The system is based around a fibre probe constructed with multiple fibres. These fibres include source fibres; which emit light from a light source at set angles, and collect reflected light at four set distances from the source.

Prior to developing measurement and calibration methodologies the NIR probe system was required to be characterised. Using a light scattering medium called intralipid of varying concentrations, necessary information of the fibre probe system was determined. These limits included ensuring a signal was obtained from the least concentrated sample, and also a noise analysis. The noise analysis was essential as it allowed the systematic errors to be quantified from each fibre.

Further experimental work included building PLS models to correlate results between the experimental obtained spatially resolved measurements and a reference measurement to determine the accuracy of the spatially resolved to collect reflectance. This involved looking into pre-processing of the spatially resolved reflectance signal to obtain the best PLS result possible.

Francesco Fabbri, Maria Angela Franceschini, and Sergio Fantini. Characterisation of the spatial and temporal variations in the optical properties of tissuelike media with diffuse reflectance imaging. **.** *Applied Opics, 2003, Vol. 42 pg 3063-3072*

Software Framework For A Holistic Approach To The Analysis And Reduction Of Environmental Burden In Food Production

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A software framework is being developed applying a holistic approach to the evaluation of environmental burden of processes and systems. Within this work, consideration is being given to providing a solution capable of meeting the needs of a wide audience of potential users. Through the use of open tools and a modular structure, the tool will provide a platform for collaborative research whilst retaining consideration for less technical users and the communication of data.

Within the research being conducted, the tool will be applied to the analysis and optimisation of food processing, which within the UK accounts for 14% of total energy use, 10% of industrial water use (DEFRA 2006) and globally 12% of greenhouse gas emissions (IPCC 2007). In addition to this, inefficiencies are reported through 16% (Lee and Willis 2010) of produce being wasted during production. Through use of the framework, software modules will be constructed to represent specific unit operations used in food production, simulating and optimising both existing techniques and novel approaches to improve the overall resource efficiency.

The poster examines the approach being taken, detailing the high level design of the platform and the way in which multiple user requirements are being considered.

Department for Environment Food and Rural Affairs (DEFRA). 2006. 'Food Industry Sustainability Strategy'.

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Lee, Peter, and Peter Willis. 2010. Waste Arisings in the Supply of Food and Drink to Households in the UK. WRAP.

Complex Flow of Concentrated Suspensions.

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Colloidal systems, such as concentrated particles suspended in a liquid or gas, are very common in nature and industry. Examples are diverse, ranging from soil and sediments in geology, to powder flow and slurries in chemical processes. The flow of concentrated suspensions has many complicated features that can cause problems in industry and have significant consequences in natural phenomena.

Work carried out so far has involved designing and constructing a rotating cylinder shear cell geometry to allow the effects of Couette flow on colloidal suspensions to be investigated. The shear cell has been designed so that it can be placed under an optical microscope, therefore allowing samples to be viewed while undergoing shear. This will allow fast optical tracking to be performed on samples, and this should lead to a better insight into the complex flow of concentrated suspensions.

Efficiency of steam generation and waste utilisation in a spirits plant.

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The food and drink processing industries are worldwide large consumers of thermal energy and due to usually fairly low efficiencies, there are huge opportunities to improve its utilisation. In this study a medium scale spirit plant situated in China was audited. Based on the data obtained, energy and mass balances were performed in order to determine efficiency of thermal energy use, the potential of cost effective reduction of energy consumption, recovery and assess potential use of waste heat to lower the fossil fuel consumption and CO2 emission. The study focus on the steam generation and utilisation within the process. The steam is generated using coal as a fuel in a boiler and then it's sent to the process where there are only two steps which require energy input but currently present high inefficiencies. All of the operations are manual and currently there isn't any implementation for energy efficiency measures.

Fermented grains are used for the spirit production and even though they are re utilised during the process at the end are disposed as biological waste consisting mainly of wet distillers grains (WDG). The feasibility of using the waste either as fuel for co-combustion for the steam generation, as well as the opportunity to use it as feed for an Anaerobic Digestion system to provide biogas as fuel for the process will be studied and evaluated. Both measures will reduce the amount of coal that is used at the moment, leading to a more sustainable operation.

Development of a Potential Immunocontraceptive Nanomaterial using Molecular Dynamics Simulations

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With an ever increasing world population the need for contraceptives is also increasing. However, there is a significant proportion of people whose contraceptive needs are not being met and the number of unplanned pregnancies is continuing to rise (Garside et al, 2012). One possible method of contraception would be through the use of conjugating an anti-fertility peptide onto nanoparticles. As a model antigen, we are examining the neuropeptide mammalian gonadotrophin releasing hormone (GnRH-I), which is known to control fertility. By examining the potential interactions of GnRH-I and its analogues with a nanoparticle surface, we can determine the optimal orientation for triggering an immunological response to the GnRH-coated nanoparticles.

While are primary aim is to examine the interactions of GnRH-I, we are also interested in GnRH-II and GnRH-III decapeptides, which may also have roles in fertility, since these peptides vary only between amino acids 5-8 from GnRH-I (Khan et al, 2007). Computer simulations using molecular dynamics have been used to investigate how these decapeptides behave and interact with an inorganic nanoparticle surface in a neutral aqueous environment. The interactions at this step can allow the optimum design of the nanoparticle with surface peptides that are free to interact with the surrounding environment, thus having the desired potential to invoke a biological response. Furthermore, the interactions between the three decapeptides and MUC-1 (the protein that makes the majority of the uterine mucosal layer, DeSouza et al, 1999) are also being investigated.

Garside, D.A; Gebril, A; Nimmo, N; Alsaadi, M; Mullen, A.B; Ferro, V.A., "An Update on Developments in Female Hormonal Contraception"., *Current Women's Health Reviews,* 2012, **8,** 276-288.

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De Souza, M.M; Surveyor, G.A; Price, R.E; Julian, J.A; Kardon, R; Zhou, X; Gendler, S; Hilkens, J; Carson, D.D., "MUC1/episialin: a critical barrier in the female reproductive tract"., *Journal of Reproductive Immunology,* 1999, **45,** 127-158.

Optimising conical inline filter design by manufacturing using additive technology.

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Additive Manufacturing (AM) is compared with conventional manufacturing (CM), in building conical in-line filter support with fluid dynamically improved design and low material wastage in the manufacturing process. CM comprises of sheetmetal bending, punching and welding. The methodology adopted compares the difference in material consumed in the manufacturing process, the difference in the pressure drop and the difference in friction factor across the filters, with and without the filter mesh. These three issues were considered to address the freedom of design, cost effective manufacturing and environmental benefits that could be achieved using AM. The height of the AM filter and CM filter are 120mm and 160mm, the bottom and top diameters of both the conical in-line filters are 76mm and 25mm. Filter meshes for the skeletons were fabricated accordingly. The tests were conducted using a test rig in the industrial collaborator's site. From the build method it was found that the material consumed for AM filter is reduced by 50% when compared to CM filter. The results with no mesh around the filters showed that the pressure drop and friction factor were lower for AM filter when compared to the CM filter. The use of mesh in the tests showed that the pressure drop across the AM filter is lower than the CM filter. However the friction factor of the AM filter is higher when compared to that of the CM filters, which is unfavourable.

A Novel Procedure in Ambient Pressure Dried Silica Aerogels

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Aerogels have been researched in many fields of applications due to their advanced properties like low density and good heat insulation. The development of aerogels is limited by the high standard requirements of supercritical drying equipment. Hence in recent years, some studies of ambient pressure drying (APD) approaches have been carried out through a solvent exchange for reducing the surface tension on the interface of nano-pores. According to the conventional APD requires a large amount of specific solvent which has extremely low surface tension, and a heat treatment after drying procedure, thus APD needs to be further improved to achieve a lower cost and environmental requirement.

In this experiment, the synthesis of the silica wet-gels followed a hydrolysis process with a tetraethylsilicate-based precursor. However, unlike supercritical drying or conventional APD process, a novel procedure of soaking silica gels in carbonic acid to prevent drying shrinkage was successfully applied to fabricate silica aerogels by drying at low temperatures. A mechanism was suggested to explain the phase transformation in pores positively maintained the net-structure of silica gels during an APD process.

The resulting silica aerogels were characterised by scanning electron microscopy (SEM) and BET surface area test. The aerogels dried with ethanol had a density of $\approx 0.31 \mathrm{g/cm^3}$ and the BET surface area was $681 \mathrm{m^2/g}$. The novel approach was combined with the conventional ambient pressure drying method (hexane was used as solvent) in attempt to further reduce surface tension. This yielded a silica aerogel with a density of $\approx 0.30 \mathrm{g/cm^3}$ and a BET surface of $563 \mathrm{m^2/g}$.

Keywords: silica aerogels, ambient pressure drying, carbonic acid

Modelling of Waste recovery via pyrolysis

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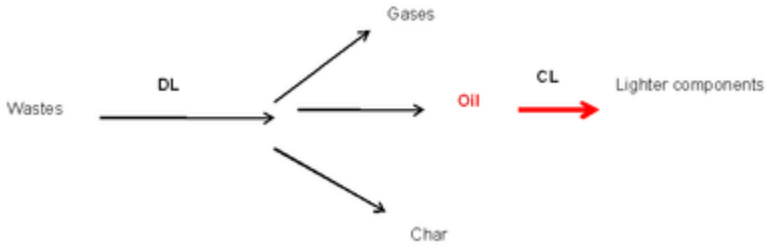
Pyrolysis is a process increasingly employed for thermochemical conversion of wastes and recovery of lower molecular weight hydrocarbon products to be used as fuel or chemical feedstock. The optimisation of the process demands knowledge and control of the kinetics of pyrolysis for accurate predictions of the products' distribution.

The lumping kinetics approach (e.g., Astarita, G and R Ocone, AIChE Journal, 34, 129, 1988) is applied to model the pyrolysis of wastes and successive fractionation of the liquid products. The schematic of the process is as follows:



A discrete lumping methodology is applied to the three lumps formed by the gases, the oil and the char resulting from the pyrolysis of wastes. The fractionation of the oil is described through the continuum lumping approach. The "lump" represented by the oil, obtained through the application of the discrete lumping (DL) model represents the feedstock for the continuum lumping (CL) model to furnish the composition of the fractioned products. The work presents a number of scientific challenges: firstly, the kinetics of plastics pyrolysis must be elucidated; additionally, the fractionation of the bio-oil would present an "apparent" kinetics of the multi-component mixture which is not simply explicable through the kinetics of each single reaction.

G. Astarita and R. Ocone (1988). "Lumping nonlinear kinetics." AIChE Journal 34(8): 1299-1309.

A Generic Selction Criterion For Three Phase Separators

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Oil and gas surface production needs separation equipment in order to meet the requirements of refineries and oil transmission networks for single-phase fluids.

Historically, engineering considerations were the major drivers for separation of reservoir fluids at oil production sites. Recent popular concern about the environment and sustainable production of the diminishing reserves of fossil fuels has led to a refocusing of separation requirements to meet increasingly more stringent legal emission levels in produced water. This has prompted the need for modelling and optimization of separators to meet these demands (James et al, 2007).

The first step to a better and successful design of a three phase separator, is to appropriately select the best type of separator to be used for a given reservoir composition. At the moment, this selection of the best type of separator (horizontal, vertical or spherical) is done mainly on the experience of the design engineer and is usually specific to the company involved. Using the rules proposed in this work will help to select an appropriate separator that will help to achieve proper separation and reduce the amount of hydrocarbons in effluent water.

There are no standard selection criteria available in the literature to guide the engineer to select the most appropriate separator for a given duty. Therefore five simple heuristic rules, have been devised which are to be applied sequentially.

Rule 1: Decide on the purpose for which the equipment will be used A pilot scale knock-out- vessel will have a different configuration and dimension to a full scale production knock-out-vessel.

Rule 2: Consider the application to which the separator will be applied, this criterion should be considered simultaneously to the first rule.

Rule 3: Consider the pressure of the reservoir fluid to be separated; the operating pressure at which the separator will be used determines the type of vessel to use.

Rule 4: Consider the number of phases to be separated, if the separator will handle liquid-liquid mixture, Gas-liquid mixture or Gas-liquid-liquid mixture.

Rule 5: Consider the composition of the well stream and how well extraneous materials such as sand, paraffin and mud will be handled.

Conclusion

A set of heuristics for separation selection have been proposed in this work, and it is believed that this will serve as a decision support tool for the design engineer to choose an appropriate separator. Once this is done, the next step is to provide a complete computer simulator for the three phase separator to ensure the system chosen meets the requirements without undue over-design and additional cost.

James , H. T., Atalla, F. Sayda. (2007). 'Modeling and Control of Three-Phase Gravity Separators in Oil Production Facilities'. Proceedings of the 2007 American Control Conference (pp. 4847-4853). New York City: IEEE

Comparison of nano-inorganic catalyst for reversible hydration of carbon dioxide

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The gradual increase in the amount of CO_2 in the atmosphere to do industrialization has led to the concern of global warming. Thus a need is there to safely store CO_2 in the lithosphere, leading to the international consciences to carbon capture and storage (CCS). Storage of CO_2 in mineral form is considered as one of the safest modes of storage, but the process is limited by the hydration of CO_2 to carbonic acid. Carbonic Anhydrase (CA) enzyme promotes the conversion of carbon dioxide to carbonic acid is a promising candidate but has several limitations (Bhaduri and Siller, 2013). Recently the use of nickel nanoparticles (NiNPs) was reported for the catalytic enhancement of CO_2 hydration (Bhaduri and Siller, 2013). The surface chemistry of the hydration process catalyzed by NiNPs was discussed and was observed is caused due to the formation of hydroxide groups on the NiNPs surface upon suspension in water. It was also found that Fe_2O_3 nanoparticles (Fe_2O_3 NPs) also have similar hydroxides generated on their surface when treated with water (Baltrusaitis and Grassian, 2005; Baltrusaitis et al., 2007). Thus the current study was undertaken to test the catalytic activity of Fe_2O_3 NP for reversible hydration of CO_2 and compare with that of NiNPs. From the results it was observed that Fe_2O_3 NPs do not have any considerable effect on the hydration reaction even though they show similar surface chemistry. The uptake enhancement of CO_2 uptake of Fe_2O_3 NPs is less than that of the NiNPs.

Keywords: Carbon capture and storage, CO_2, hydration reaction, NiNPs, Fe_2O_3 NPs, catalysis.

Baltrusaitis, J., Grassian, V.H., 2005. Surface reactions of carbon dioxide at the adsorbed water-iron oxide interface. Journal of Physical Chemistry B 109, 12227-12230.

Baltrusaitis, J., Schuttlefield, J.D., Zeitler, E., Jensen, J.H., Grassian, V.H., 2007. Surface reactions of carbon dioxide at the adsorbed water-oxide interface. Journal of Physical Chemistry C 111, 14870-14880.

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Continuous Screening of an Imine Synthesis Reaction using Mesoscale Oscillatory Baffled Reactor

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A mesoscale oscillatory baffled reactor (mesoscale-OBR) of 350mm length and 5.0 mm internal diameter, giving a total volume of the reactor of approximately 5.5ml was developed as a platform to conduct process screening or preliminary feasibility studies at laboratory scale. The reactor has been assessed with various baffle designs for various applications (solid-liquid and liquid-liquid reactions etc.). Uniform mixing inside the reactor is achieved by the interaction of the oscillatory flow (superimposed upon a net flow) and the baffle geometry.

In this study, the mesoscale-OBR was used to rapidly obtain and logically process data such as optimal conditions and kinetic parameters of a chemical reaction in a continuous mode. Its purposes were to reduce process development time, the amount of chemicals required and waste generated. Reactions of several aldehydes with primary amines to form imines were chosen to demonstrate the ability of the mesoscale-OBR.

Experiments were conducted at ‘steady-state’ and ‘dynamic’ screening modes. Both methods allow more than one variable to be manipulated, e.g. residence times and ratios of the reagents etc. A clear step-change in conversions between residence times (reaction times) was observed, which indicated that a high degree of plug flow was achieved in the mesoscale-OBR. Experimental results obtained from the two methods were identical but the latter could provide data in only 10% the time. The consistency in experimental results and rapid responses to the changes of the input lend the mesoscale-OBR to further processing developments, e.g. introducing additional reagents into the flow stream to generate further reactions/products etc. The rapid data generation coupled with modelling provides full understanding mechanisms of reactions and allows results, e.g. kinetic parameters, to be determined more rapidly and easily. Generally, the advantages of using the meso-OBR for continuous screening processes were fourfold:

- The process development time when using dynamic screening was reduced by 25% compared to the steady state method and by 50% compared to batch screening using beakers
- Each data point at a given steady state was equivalent to one batch reaction. Hence, more data is produced per volume of reactants used.
- The ability of screening through experimental space with two or more variables allows more data to be collected. This eliminates multiple reactions that need to be conducted in batch to obtained similar data points.
- Data was reproducible, e.g. rate constant for 1-butanamine, N-phenylmethylene synthesis was obtained with a standard deviation of 6.0 x 10^{-3} $mol^{-0.9}L^{0.9}s^{-1}$, compared to 2.0 x 10^{-2} $mol^{-0.9}L^{0.9}s^{-1}$ for similar experiments in typical batch beakers.

A Novel Modelling Approach to the Mixing Process in Twin-Screw Extruders.

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In this research, we propose and experimentally validate theoretical models for the mixing process in plasticating co-rotating twin screw extruders using a combination of statistical techniques and mechanistic modelling. A predictive model for the global residence time distribution was developed using a continuous exponential distribution model by examining the local contributions. Parameters such as the mean residence time, mean time delay, degree of fill, local drag and volumetric flow rates were obtained using mechanistic modelling by mathematically modelling the flow dynamics in the extruder. Predictive models of the mean residence time and time delay were subsequently developed. The effect of input conditions such as feed rate and screw speed on the shape of the residence time distribution curve and the degree of mixing were also evaluated by analysing the variance in this distribution.

Increase in feed rate at constant screw speed and vice versa results in narrowing the shape of the residence time distribution curve, with the feed rate having a higher sensitivity. The mean residence time and time delay was observed to drop with an increase in the feed rate. With an increase in the screw speed at constant feed rate, a reduction in the mean residence time was observed at the expense of an increased time delay. This has been validated against the experimental results.

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Pyrolytic characteristics and kinetics of microalgae (*Chlorella vulgaris* and *Nannochloropsis oculata*) using thermo gravimetric analyser

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Pyrolysis and kinetic studies of two microalgae species (*Chlorella vulgaris* and *Nannochloropsis oculata*) were investigated using a thermogravimetric analyser from 50 to 800 ^{o}C in a nitrogen flow rate of 30ml^{-1}. The microalgae have been characterised for proximate and ultimate analysis while the thermogravimetric experiment was carried out at the heating rates of 5, 15, 30 and 50 ^{o}C. The parameters of the reaction kinetics were determined using iso-conversional methods.

Keywords: Microalgae, Chlorella vulgaris, Nannochloropsis oculata, Pyrolysis, Thermogravimetric analysis

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