Chemical Engineering PhD Symposium

Opening Lecture by Professor Liangfang Zhang, University of California, San Diego:
“Engineering biomimetic nanoparticles for drug delivery, detoxification and vaccination”

Monday 3 July 2017, 9.30-16.30h
Lecture Theatre 1, Department of Chemical Engineering (ACEX 250)

Poster Presentations in the Design Rooms,
Department of Chemical Engineering (ACEX 306-312)

The symposium will be followed by a drinks reception in the Design Rooms
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Acknowledgments

We are most grateful to our major sponsors for their financial support of the research in our Department.
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10.50-11.10 Claudia Menichini
Patient-specific prediction of false lumen thrombosis in Type B aortic dissection

11.10-11.30 Morning Break

11.30-11.50 Roberto Ibarra Hernandez
Flow structures in liquid-liquid pipe-flows using laser-based diagnostic techniques

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Building an adsorbent platform using boron nitride: insights into pore network design and impact on sorption

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Crystallisation of Macroscopic Hydrates and Investigation of Their Drying Behaviour

14.30-14.50 Alessandra Vichi
Chemical imaging of cultural heritage objects at the micro-scale: novel applications to study polymer degradation

14.50-15.10 Jeng Yi Chong
Into the transport mechanism in graphene oxide membranes

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15.30-15.50 Shiqi Wang
Synthesis and Characterisation of Smart Amino Acid-Based Polymeric Materials for Drug Delivery

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Assembly of polymer-nanoparticle capsules with tuneable shape, internal morphology and pulsed release via osmotic extraction and kinetic arrest

16.10-16.30 Gonzalo Bustos Turu
Integrated modelling for smart and sustainable urban energy systems

16.30-18.00 Drinks Reception and Announcement of Prize Winners (Design Rooms)
Engineering a marrow-mimetic environment for human blood production

Presenter: Mark Allenby
Supervisors: Athanasios Mantalaris, Nicki Panoskaltsis

Abstract:

Clinical red blood cell (RBC) transfusion in the UK requires 8000 blood donations per day at a cost of £2.25 billion per year (Blood & Transplant 2013). Current research investigating the laboratory production of RBCs seek to alleviate these demands, but remain more than 50-fold above clinically relevant costs, and lack the RBC production efficiency found within the human body (Rousseau et al. 2014).

Human RBC production occurs within the bone marrow: a macroporous sponge-like scaffolding filled with blood cells alongside many other supportive structural cells. Microporous blood vessels nourish this marrow scaffolding with oxygen and nutrients while filtering out marrow-produced RBCs into bodily circulation. Current research in understanding normal human blood production, optimising laboratory blood production, and devising treatment for abnormal blood production takes place within a homogenous liquid medium, neglecting the role of the complex structural environment during natural blood production.

To develop a physiologically relevant model to study and optimize human RBC production outside the body, we have engineered a marrow-mimetic bioreactor. This bioreactor consists of a porous polyurethane scaffold impregnated with ceramic hollow fibres and coated in collagen. When perfused, hollow fibre vasculature diffuses nutrients and growth factors into the surrounding cell-laden scaffold matrix and filters small RBC products out into collected media. To characterize this process, we have developed quantitative 3D image analysis algorithms to spatially assess bioreactor distributions of and associations between different cell types relevant to physiological blood production (Allenby et al. 2017).

Using these tools, we spatiotemporally mapped the bioreactor production of RBCs from NHS human umbilical cord cells. We found blood production occurred in dense clusters with structural cells which provided physical contact, secreted supportive hormones, and deposited structural proteins as occurs naturally in the marrow. The bioreactor was able to expand cells across 28 days at 1,000-fold higher cell densities with 10-fold fewer supplemented factors than current liquid methods while continuously harvesting red blood cell product. We further explored the capabilities of this bioreactor through the design of miniaturised, parallelised mini-bioreactors.

The bioreactors we have developed may represent more physiologically-relevant laboratory platforms to study normal blood production and generate RBCs for clinical transfusion, and to study abnormal blood production (e.g. cancerous or leukemic) as a platform for drug testing and drug discovery.

References:


Patient-specific prediction of false lumen thrombosis in Type B aortic dissection

Presenter: Claudia Menichini
Supervisors: Prof. Xiao Yun Xu

Abstract:
Type B aortic dissection is a critical clinical emergency caused by the rupture of the inner wall of the aorta, the main artery originating from the heart and supplying oxygenated blood to the entire body and organs. The formation of a tear allows blood to flow into the aortic wall layers, leading to the formation of a second blood filled region known as the “false lumen” (FL). This disease compromises blood supplies to the organs and can lead to complications such as aneurysm and rupture, with mortality rates increasing by 1-2% per hour if left untreated.

Although Type B aortic dissections are generally associated with high in-hospital survival rates, post-discharge prognosis is poor, with 5-year mortality rates varying between 48-82% [1]. Significant predictors for long term outcomes include the formation and extent of blood clotting (thrombosis) in the FL (i.e. non-thrombosed, partially or completely thrombosed false lumen). Partial FL thrombosis was identified as a significant predictor for late complications due to increased FL pressure and hence a high risk for aneurysm growth and rupture [1,2]. On the other hand, improved outcomes are associated with complete FL thrombosis, which can be achieved through endovascular repair (TEVAR). If it was possible to predict which patients would develop FL thrombosis and to what extent and how to improve the chances for complete FL thrombosis treatments could be significantly improved.

This study is concerned with the development and application of a novel computational model to predict FL thrombosis in medically treated and TEVAR patients under physiological conditions. Thrombus formation and growth are predicted through the evaluation of hemodynamic parameters and flow patterns [3]. The model has been applied to patient-specific geometries reconstructed from CT images and representing (i) medically treated patients with no thrombosis; (ii) medically treated patients with partial thrombosis; (iii) TEVAR patients with partial thrombosis; (iv) TEVAR patients with complete thrombosis [4]. All patients were kept under medical surveillance, and predictions of thrombus growth were compared with follow-up CT scans. Good agreement between predicted thrombosis and in vivo data was found in all cases. The model was able to predict how variations in morphology and flow led to different thrombus growth patterns, demonstrating its applicability to patient-specific prediction of FL thrombosis. This work could help identify key predictors of FL thrombosis and risk factors for incomplete FL thrombosis and late complications, which could help clinicians develop optimal treatment strategies.

References:
Flow structures in liquid-liquid pipe-flows using laser-based diagnostic techniques

Presenter: Roberto Ibarra
Supervisors: Prof Omar K. Matar and Dr Christos N. Markides

Abstract:

Liquid-liquid flows in pipes, which can be found in a large number of industrial applications, show complex hydrodynamic behaviour as result of the inherent physical properties and the characteristics of the pipe (e.g. material and inclination). Researchers have attempted to characterise the flow in terms of global parameters such as pressure gradient, phase fractions, and flow regimes (i.e. geometrical configurations of the phases in the pipe). However, detailed space- and time-resolve phase and velocity measurements must be obtained in order to understand the physics and fundamental behaviour of the flow. This can be achieved with the implementation of laser-based diagnostic techniques in which the flow is illuminated with a thin laser sheet at high frequencies, usually, in the vertical plane that passes through the centre-line of the pipe. The emitted and scatter light from fluorescent dyes and tracer particles in the flow is captured by high-speed cameras revealing instantaneous flow structures. The optical nature of these techniques suggests the use of refractive-index-matched pair of test fluids in order to avoid light refraction at the moving liquid-liquid interface. However, this can result in the selection of fluids with physical properties which may not represent actual applications of interest.

In this work, a novel two-line laser light sheet arrangement was used to obtain instantaneous spatio-temporally measurements in a non-matched-refractive-index pair of test fluids. Instantaneous vector velocity fields, mean velocity profiles, turbulence characteristics (i.e. velocity fluctuation and Reynolds stresses), and interface profiles are extracted from the laser-based measurements. Experimental data reveal complex flow structures and interaction between the liquid phases which are dependent on the fluid velocities and pipe inclination. These data aim to improve the development and validation of closure relationships and advanced computational flow models for the prediction of multiphase flow parameters.
Building an adsorbent platform using boron nitride: insights into pore network design and impact on sorption

**Presenter:** Sofia Marchesini  
**Supervisor:** Camille Petit

**Abstract:**

Porous boron nitride (BN) is an analogous polymorph to activated carbon, but with higher thermal stability and a “richer” chemistry owing to its bond polarity. These added properties make porous BN an excellent candidate for a range of applications such as molecular separation, drug delivery and catalysis. However, in order to achieve the desired performance for a given separation process, the porosity of BN needs to be finely tuned and the parameters that control it must be identified. Thus far, this has been difficult to achieve.

Herein, porous BN with a range of different pore structures and morphologies was produced via a simple template-free method. The properties of BN were studied from the macro- to the nano-scale with a variety of characterisation techniques and the mesopores were directly visualized using a state-of-the art 3D tomography technique. The surface area of BN was increased up to 1900 m$^2$/g and control over the micro- and mesopore volumes was achieved. Owing to their large porosity, the samples were tested for gas adsorption and surpassed or rivalled current benchmarks. To further evaluate the potential of the materials at scale, BN pellets were produced without the use of any binders and minimal reduction porosity was observed. This finding is unusual yet very promising from an application standpoint.
Raman-imaged CH$_4$-CO$_2$ hydrate exchange

Presenter: Hao Bian
Supervisors: Geoffrey C. Maitland, Klaus Hellgardt, Jerry Y.Y. Heng

Abstract:
Methane hydrates, in which CH$_4$ molecules are trapped inside polyhedral hydrogen-bonded water cage-like structures in soft mineral sediments, are a potential energy source that occur naturally in permafrost and along the continental shelves, with the capacity to supply a large component of the world’s future energy demands [1]. Furthermore the enhanced recovery of methane (CH$_4$) hydrates by carbon dioxide (CO$_2$) injection is a promising route for combining long-term storage of CO$_2$ with the production of methane from naturally occurring hydrates [2]. Some progress has been made in understanding the fundamental aspects of this process: for example, molecular exchange of hydrate guests has been found to be a diffusion-limited process, influenced by particle sizes, temperature-pressure conditions, and nature of the guest molecules. However, the microscopic exchange mechanism is still a subject of debate. There are discrepancies in the literature regarding the fraction of recoverable CH$_4$ and the CH$_4$-CO$_2$ exchange rate, even for measurements conducted at similar experimental conditions. Raman spectroscopy has been used previously in guest exchange studies to quantify hydration numbers and cage occupancy ratios but the method was limited to point measurements which are unable to observe the CO$_2$-CH$_4$ exchange efficiently at the crystal length-scale.

A high-pressure low-temperature optical reactor was designed, commissioned and applied to this problem. The cell accommodated samples over a temperature range of 288 K to 353 K and at pressures up to 50 MPa. Fast temperature response (up to 5 K/s), and stable temperature control (+/- 20 mK) were facilitated by using four Peltier elements. A large optical path allowed the acquisition of in-situ 3D Raman images to reveal the molecular structure and (CH$_4$-CO$_2$) exchange kinetics of gas hydrates in both single crystal and polycrystalline methane hydrates. An oscillating temperature dynamic method was used to form polycrystalline hydrates at pressures up to 20 MPa and by contrast single crystal hydrates were formed under a small thermal driving force (around 2K) at pressures up to 10 MPa. The polycrystalline hydrates exhibited a much faster CH$_4$-CO$_2$ exchange rate compared to the single crystal hydrates; defects and crystal imperfections also had a significant effect on this rate. The morphology of methane hydrates, hitherto ignored, hence plays a critical role in the exchange process, which helps to explain the discrepancy of exchange rates for similar conditions reported in the literature. These time-resolved Raman results indicated a diffusion-controlled guest molecule substitution process and molecular mechanisms are proposed. The Raman spectra were also used to quantify the exchange kinetics and the cage occupancy of the methane hydrates.

References:
Phase behaviour of (CO$_2$ + diluents) mixtures relevant to CCS and flue-gas applications

**Presenter:** Lorena dos Santos de Souza  
**Supervisor:** J. P. Martin Trusler

**Abstract:**
Understanding the phase behaviour of (CO$_2$ + diluent) mixtures is crucial in carbon capture, transport and storage (CCS) operations. For the design, optimisation and safe operation of these processes accurate equations of state (EOSs) are required to describe thermodynamic properties of the various mixtures of CO$_2$ with relevant substances, including H$_2$, N$_2$, CH$_4$, Ar, CO and O$_2$. A popular and potentially very-accurate approach is to use empirical multi-fluid multi-parameter EOS models. In order to adjust the interaction parameters in those models, reliable and accurate experimental phase equilibrium data are indispensable. Nevertheless, comprehensive reviews by Li et al. [1], Gernert et al. [2] and others, identify gaps and significant discrepancies in the literature reporting experimental VLE data for mixtures of CO$_2$ with substances relevant in CCS and flue-gas applications. Discrepancies between literature sources are particularly noticeable in the vicinity of critical points.

In the present study, new VLE measurements have been made on two relevant systems: (CO$_2$ + CH$_4$) and (CO$_2$ + CO). The measurements were carried out on isotherms at temperatures ranging from just above the triple-point to just below the critical point of CO$_2$ and at pressures from the vapor pressure of pure CO$_2$ up to approximately 15 MPa or, if lower, the mixture critical temperature. All measurements were performed using the low-temperature VLE apparatus described by Fandiño et al. [3], which is associated with low standard uncertainties of 0.006 K for temperature, 0.003 MPa for pressure and 10-2x(1 - x) for mole fraction x.

The new VLE data, together with earlier results from our laboratory on (CO$_2$ + H$_2$) and (CO$_2$ + N$_2$) [3], have been compared with the predictions of available thermodynamic models, including GERG-2008 [4] and EOS-CG [2]. Additionally, the data have been correlated with the Peng-Robinson EOS [5], generally incorporating a single temperature-dependent binary interaction parameter kij (T). EOS-CG showed significantly better agreement, especially close to the critical point, than found with the Peng-Robinson model.

The new experimental VLE data help to fill important knowledge gaps relating to the thermophysical properties of mixtures of CO$_2$ with substances relevant in CCS and flue-gas applications.

**References:**

**Acknowledgements**
We gratefully acknowledge the funding provided by of Science Without Border (Ciência Sem Fronteiras) and their permission to publish this research.
Crystallisation of Macroscopic Hydrates Using a Bioinspired Approach and Investigation of Their Drying Behaviour

Presenter: Efthychios Hadjittofis

Supervisors: Geoff G. Z. Zhang¹, Jerry Y. Y. Heng²

¹ Drug Product Development, Research and Development, AbbVie Inc., North Chicago, Illinois, USA
² Surfaces and Particle Engineering Laboratory, Chemical Engineering Department, Imperial College London, London, UK

Abstract:

A bioinspired approach for the growth of macroscopic Carbamazepine Dihydrate (CBZD) crystals was developed, based on the findings for the crystallisation of hemozoin in malaria parasites. Using water and organic solvents slightly miscible to water, a triphasic liquid-liquid-solid system was created. Macroscopic prismatic crystals were grown epitaxially on the interface between the two liquid phases. The chemical potential of the water dissolved in the organic solvent was found to be sufficient to sustain the nucleation and growth of CBZD, over any anhydrous polymorphs. Diffusion of water from the aqueous phase to the organic keeps the hydrate crystals stable. Even though CBZD crystals are usually needle-shaped, thus inadequate for further studies, the crystals obtained from this method are prismatic and hence further studies could be performed more easily.

Upon dehydration, at constant temperature and ambient pressure, CBZD crystals dehydrate to the Triclinic anhydrous polymorph of Carbamazepine. The dehydration is accompanied by the formation of cracks, appearing preferentially on the (020) facet of the crystal. The most profound of these cracks are associate with the water channels, accommodating stoichiometric water. Examination of partially dehydrated macroscopic crystals reveals that these cracks stem from inside the crystal, owe to the built up of vapour pressure caused by water evaporation.

The Triclinic polymorph appears, on all the crystal facets, in the form of whiskers. The density difference between the CBZD and Triclinic leads to a compressive stress, proportional to the chemical potential difference associated with the dehydration process. This is found to be the driving force for the whiskers’ growth.

Figure: Schematic of the whisker growth mechanism.

References:

Chemical imaging of cultural heritage objects at the micro-scale: novel applications to study polymer degradation

Presenter: Alessandra Vichi
Supervisor: Sergei G. Kazarian

Abstract:

The development and optimisation of non-destructive analytical techniques to study unique objects of our cultural heritage has become of increasing interest for conservation scientists. Understanding the causes of the physical-chemical degradation of these objects is of vital importance to develop methods to preserve them. In some cases, degradation can be so severe that the preservation of the object becomes a serious challenge. Numerous classes of both organic and inorganic materials, present in historic and artistic items, and their degradation can be studied by Fourier Transform Infrared (FTIR) spectroscopy. In addition, Attenuated Total Reflection (ATR) - FTIR spectroscopic imaging has recently emerged as a powerful set-up that combines the possibility of label free detection of these materials with the ability to study their spatial distribution at the micro-scale in an intrinsically non-destructive way.\(^1\,\text{2}\)

Natural and synthetic polymers, either present as original materials or introduced during conservation treatments, constitute a widespread class of organic materials commonly found in objects of museum collections. In this project, we apply ATR-FTIR spectroscopic imaging to analyse selected samples from degraded historic items made of synthetic polymers (cellulose nitrate (CN)-objects and polyvinyl chloride (PVC)-toys) and from collagen-based artefacts (parchment and leather book covers). The samples were provided by the Victoria & Albert Museum (UK), the British Library (UK) and the Matenadaran Institute of Ancient Manuscripts (Armenia). In addition, an innovative optical system of apertures was designed to fit a FTIR microscope. This system allows the angle with which IR light reaches the interface between the ATR crystal and the sample to be changed (Figure 1), allowing the depth at which the IR spectra are collected to be controlled.\(^3\) By probing a sample of CN from a mid-19th century handbag at different depths, we observed that hydration of the polymeric network can occur below the surface. Hence, the results from this study could help to establish improved conservation protocols for safeguarding irreplaceable items in museum collections.

\[ d_p = \frac{\lambda_0}{2m \sin^2 \theta_i - \left( \frac{n_2}{n_1} \right)^2} \]

Figure 1. A) Equation linking depth of penetration (\(d_p\)) to wavelength (\(\lambda_0\)), the indexes of refraction of the ATR crystal (\(n_i\)), the sample (\(n_s\)) and the angle of incidence (\(\theta_i\)). B) Schematic showing the use of apertures in the optical path of the micro ATR set-up: top no aperture; bottom with optical aperture selecting a smaller angle of incidence (aperture 1). C) Spectra at different depths of a cellulose nitrate sample from a mid-19th century handbag (Conservation Department, V&A, London) with ATR-FTIR spectroscopic imaging and the optical apertures.

References:
Into the transport mechanism in graphene oxide membranes

Presenter: Jeng Yi Chong

Supervisors: Prof. Kang Li, Dr. Cecilia Mattevi, Dr. Bo Wang

Abstract:
Graphene oxide (GO) membranes fabricated by stacking single-layer GO flakes have a well-defined interlayer space, showing excellent molecular sieve properties. GO membranes have been studied for pressure-driven nanofiltration to retain small molecules and multi-valent salts [1-3]. However, it is still puzzling that while many studies suggest fast liquid transport through the extremely tortuous transport path, contradictory observations have also been obtained. This presentation will discuss the water transport in GO membranes to understand the real water permeation flux of GO membranes. We reveal that GO membranes prepared by varied methods and on different substrates present severe reduction in water permeability due to the compaction of their original loose microstructure. The water flux dropped continuously from tens of LMH bar\(^{-1}\) down to the range < 0.1 LMH bar\(^{-1}\) after more than ten hours. This result demonstrates that the structures of GO membranes prepared by current approaches are far from the ideal laminar structure. The high water permeation observed in previous studies could arise from the disordered membrane microstructure. In addition, GO membranes showed a higher water permeation flux in pervaporation when vacuum was applied on the permeate side, due to the high capillary force in the membranes. With the understandings on the transport mechanism in GO membranes, we propose an alternative means of measuring the effective interfacial tension between water and miscible solvents such as ethanol. This simple measurement method will be a useful tool for studies such as viscous fingering and microfluidic processes where transient interfaces of miscible liquids may occur.

References:
Synthesis and Characterisation of Smart Amino Acid-Based Polymeric Materials for Drug Delivery

Presenter: Shiqi Wang
Supervisor: Dr. Rongjun Chen

Abstract:

The delivery of various therapeutics, particularly macrodrugs such as proteins and nucleic acids, is of great importance for modern therapy[1]. However, there are many different barriers in the complex bioenvironment, which significantly limited the drug availability and efficacy[2]. Herein, the aim of my project is to develop smart amino acid-based polymeric materials for drug delivery. Specifically, three drug delivery vehicles are reported, namely, dual-responsive hydrogels for colon-targeted delivery[3], membrane-active polymers for intracellular delivery[4], and nanogels which combine the advantages of the former two drug carriers to achieve intracellular delivery of drugs for colon cells.

1) Dual-responsive hydrogels were prepared by a facile one-pot reaction, with adjustable structure and mechanical behavior. With pH-responsive anionic pseudo-peptides as backbones and disulfide-containing L-cystine dimethyl ester as crosslinkers, these hydrogels were able to shrink and retain payloads in acidic stomach environment but degrade and release them in colon rapidly and completely. The high loading efficiency, rapid but complete triggered-release and good biocompatibility make these hydrogels promising candidates for colon-targeted oral delivery.

2) For intracellular delivery, a series of anionic, cell penetrating peptide (CPP)-mimicking, lysine-based hyperbranched polymers have been developed. To our knowledge, it is the first report of anionic, hyperbranched, CPP-mimicking polymers. These polymers caused complete membrane disruption at late endosomal pH while remained non-lytic at physiological pH. The pH-responsive conformational alterations and the multivalency effect of the hyperbranched structure were demonstrated to effectively facilitate their interaction with cell membranes, thus leading to significantly enhanced membrane-lytic activity compared with their linear counterpart. The unique structure and pH-responsive cell-penetrating abilities make the novel hyperbranched polymers promising candidates for cytoplasmic delivery of biomacromolecular payloads.

3) To intracellular delivery of drugs for colon cells, nano-sized hydrogels were prepared using membrane active polymers. The nanogels were designed to have pH-responsive swelling behaviour and controlled dissociation, thus retaining the colon-targeted property of the abovementioned hydrogels. After dissociation, the polymers could further facilitate the delivery of drugs into cells. Some preliminary results showed the nanogels had been successfully prepared and model drugs could be loaded and released as designed. The further intracellular delivery study is still on-going.

References:
Assembly of polymer-nanoparticle capsules with tuneable shape, internal morphology and pulsed release via osmotic extraction and kinetic arrest

Presenter: Christiana E. Udoh
Supervisors: João T. Cabral and Valeria Garbin

Abstract: Capsules are essential vehicles for the storage and delivery of drugs, biologically active species, surfactants and personal care formulations.\(^1\) The morphology of capsules has been shown to control their assembly and packing, flow, optical, magnetic and release properties.\(^2\) Polymer and nanoparticle-based capsules can be engineered to have high cargo capacity, biocompatibility and surface functionalities underpinning growing applications in pharmaceutical, biological and the energy industry. Recent advances in the field of droplet microfluidics have provided an attractive platform for high-throughput, single and multiple, emulsification and templating of droplets combining exceptional size and morphology control, and low polydispersity. However, to date the formation of composite capsules from polymer-nanoparticles mixtures has not been explored, despite the rich phase behaviour of these mixtures.\(^3\) The precise and facile encapsulation and delivery of nanoparticles could have a major impact in fields as diverse as pharmaceutical sciences and catalysis. Here we establish a general approach for polymer-nanoparticle capsule design, with tuneable morphologies, and high cargo capacity, mapping accessible shapes and morphologies, with expected impact on their dissolution behaviour.

We report the assembly of polymer-nanoparticle composite capsules obtained from both nucleation and spinodal demixing, modulated by radial concentration gradients that originate during solvent extraction. We demonstrate a range of internal morphologies, including bicontinuous microstructures, as well as isotropic and non-isotropic external shapes. We propose a robust morphology diagram in terms of the concentrations of polymer and nanoparticles, which were polyelectrolyte sodium poly(styrene sulfonate) and 22-nm silica nanoparticles in this work. Upon immersion in water, we find that capsules formed with either neat polymer or neat nanoparticles dissolve rapidly and isotropically, while bicontinuous, hierarchical, composite capsules dissolve via directional bursts of nanoparticle clusters, without disrupting the particle scaffold. The time scales for release are generally long and can be tuned through pH. The versatility, facile assembly, and response of these nanocomposite capsules thus shows great promise in precision delivery.

![Figure 1: Scanning electron microscope images of microcapsules obtained by selective solvent extraction, showing internal and external morphology](image)

References:

5. Udoh, C.E; Cabral, J.T; Garbin, V (in preparation)
Integrated modelling for smart and sustainable urban energy systems

Presenter: Gonzalo Bustos-Turu
Supervisor: Professor Nilay Shah

Abstract:

Local and global environmental concerns, as well as a fast urbanisation, are making cities to change the way energy is consumed, distributed and generated. In the next decades, cities will have to adapt their energy infrastructure to integrate a new set of low carbon technologies in their energy infrastructure. And this integration presents challenges in the design, planning and operation of energy networks. This PhD project is focused on the development of a simulation and optimisation modelling framework to assess different energy management strategies in urban energy systems. This modelling framework is tested in two case studies. The first one is focused on transport electrification and the integration of electric vehicles through smart charging strategies. In the second case study, focused on heat electrification, the coordination of a group of heat pumps is analysed. These case studies highlight the importance of the spatial and temporal characterisation of the energy demand, considering the level of flexibility users can provide to the system. Trade-offs between the environmental and economic performances of smart energy management strategies are also assessed within the proposed modelling framework.
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