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Welcome to the 2014–2015 CPSE Annual Report
Professor Nilay Shah
CPSE Director

“It has been a great pleasure to see CPSE grow in size and breadth, while continuing to excel in both fundamentals and applications.”
**Understanding the Performance of Complex Systems**

We have a sense that the words we use to describe the complexity of the modern world provide only a superficial understanding of the underlying mechanisms of the processes upon which we depend. In 1989, Professor Roger Sargent gathered together a group of engineers, mathematicians and molecular scientists and established the Centre for Process Systems Engineering to define and quantify the components that make up complex industrial chemical processes in order to optimize performance.

Since then our field of work has expanded to encompass many other critical industrial and biological systems and has led to the development of algorithms and computer simulations that describe individual processes, from the molecular to macroscopic scale, that combine to define, for example: a bacterial cell’s ability to produce a synthetic oil; the design of an optimized urban energy system and the economics of a commodity supply chain. Statistical routines have been developed to model the performance of complex systems even in the absence of full descriptions of all the contributory components.

**CPSE History**

**International Research Leader in Process Systems Engineering**

The Centre for Process Systems Engineering (CPSE) is a multi-institutional research centre. It was inaugurated in August 1989 by Professor Roger W.H. Sargent and involves Imperial College London and University College London.

A report by a panel of external, international experts to the EPSRC research council described CPSE as being “one of the major centres of excellence in its area of expertise in the world and is seen as the benchmark against which other world centres are judged”.

Innovative and dynamic in its approach to research and development, CPSE’s accomplishments include the Queens Prize for Higher Education, presented in 2003 for research excellence and technology transfer.
The CPSE continues to deliver a unique multi-disciplinary approach to Process Systems Engineering. The number of academic staff has expanded to over 30 to meet the growing demand for research and education in this critically important subject.

The group has an annual research income portfolio of £30M. Since it was founded in 1989, CPSE has used its expertise in Process and Product Design, Operations and Control and Modelling and Model Solution tools to investigate a wide range of technically and commercially important issues. The scope of CPSE continues to evolve and adjust to changes in technology and commercial needs with work underway, for example, in new areas such as 'Environmental Systems' and "Computational Optimisation and Machine Learning."

During 2014 and 2015, the number of academics grew following the affiliation of eight new members from both Imperial College London and University College London: Dr Marc Deisenroth, Lecturer in Statistical Machine Learning, Department of Computing; Dr Adam Hawkes, Senior Lecturer in Energy Systems; Dr Federico Galvanin, Lecturer, Department of Chemical Engineering; Dr Gonzalo Guillén-Gosálbez, Reader in Process Systems Engineering; Dr Alexandros Kiparissides, Lecturer in the Department of Biochemical Engineering; Dr Niall Mac Dowell, Lecturer in Energy and Environmental Technology and Policy; Dr Ruth Misener, Royal Academy of Engineering Fellow, Lecturer, Department of Computing; Dr Wolfram Wiesemann, Assistant Professor, Business School.

Former CPSE Director, Professor Stratos Pistikopoulos left Imperial College to join Texas A&M University. Professor Pistikopoulos was a great supporter of CPSE, having led the Centre for seven years (2002-2009). Professor Pistikopoulos will continue to be a member of CPSE as Visiting Professor.

The CPSE's acclaimed leadership in Process Systems Engineering is highlighted by the number of papers in prestigious publications. In the last two years, there have been over 300 publications. Many papers by CPSE researchers have been recognised for their originality, significance and influence.

A paper co-authored by Professor George Jackson on the Statistical Associating Fluid Theory (SAFT), was selected as one of the 'All Time Greats' in the history of *Industry & Engineering Chemistry Research (I&ECR)*. The paper, "New Reference Equation of State for Associating Liquids" by Walter G. Chapman, Keith E. Gubbins, George Jackson, and Maciej Radosz, *I&ECR* 29, 1709, (1990), describes an approach which permits scientists to make precise predictions about the behaviour of a broad range of liquids including solutions of polymers and surfactants.

A paper by the Molecular Systems Engineering Group was listed as "one of the most accessed in 2014" from The Journal of Chemical Physics. The paper is entitled "Accurate statistical associating fluid theory for chain molecules formed from Mie segments", by Thomas Lafitte, Anastasia Apostolakou, Carlos Avendaño, Amparo Galindo, Claire S. Adjiman, Erich A. Müller and George Jackson, J. Chem. Phys. 139, 154504 (2013).

Another paper from the Molecular Systems Engineering Group was selected as "one of the 12 most notable papers", out of 425 papers, published in the proceedings of the 12th International Symposium on Process Systems Engineering held in Copenhagen. The paper is entitled "Deterministic global optimization and transition states", by Claire Adjiman and Dimitrios Nerantzis, Elsevier, Amsterdam, 851–856 (2015).

Further endorsement was received for a book, "Distillation: 1. Fundamentals and Principles, 2. Operations and Applications, 3. Equipment and Processes" which won the 2015 PROSE Chemistry & Physics Award. Professor Andrzej Górk, Editor of Chemical Engineering and Processing: Process Intensification and Professor Eva Sørensen, Editor in Chief of Chemical Engineering Research and Design as well as their co-authors (Hartmut Schoenmakers and Zarko Oljic) received the award at the Association of American Publishers' (AAP) Professional and Scholarly Publishing (PSP) Annual Conference in Washington, DC. Awarded for the best in professional and scholarly publishing, the book addresses important current research on industrial distillation, process design, operation and control aspects, and conceptual design.
Academic Distinctions and Awards

The Centre’s reputation is further enhanced by the prestigious national and international awards received by CPSE academics. CPSE academics are international leaders in their fields and have multi-disciplinary backgrounds, including: chemical engineering, mathematics, physics and chemistry. Their expertise has been recognised by numerous awards.

IChemE honoured CPSE’s founding father Professor Roger Sargent, considered the "Pioneer of Process Systems Engineering." by creating a new medal in his name, called the Sargent Medal for research in computer-aided product and process engineering. The IChemE established the medal in recognition of the work of members of the chemical engineering academic community who have contributed significantly to the advancement of the profession and society. Professor Costas Pantelides was the recipient of the Sargent Medal for 2015.

Two CPSE academics were amongst the 2014 IChemE winners. Professor George Jackson won the Guggenheim Medal for research excellence in thermodynamics and/or complex fluids. Dr Niall Mac Dowell won the Nicklin Medal for exceptional contribution to the process sciences by an author who has graduated within the last ten years.

Professor Nilay Shah and Professor Claire Adjiman were elected Fellows of the Royal Academy of Engineering. The Academy’s Fellowship represents “the nation’s best engineering researchers, innovators, entrepreneurs, business and industry leaders.” Election to the Academy is by invitation only.

Professor Eva Sørensen won the highly prestigious Inspiration Award for Women which supports Breakthrough Breast Cancer. Professor Sørensen featured on a list of luminaries which included J.K. Rowling and Maya Angelou. Professor Sørensen was nominated for the Inspirational Teacher Award but was instead awarded an Inspiration Award for her outstanding contributions to education at University College London and further afield.

Dr Benoît Chachuat and Dr Ruth Misener each won an AIChE Computing & Systems Technology Division (CAST) Award. Dr Benoît Chachuat received the CAST Outstanding Young

Professor Geoffrey Maitland was inaugurated the 74th President of IChemE. Immediately after becoming president, Professor Maitland launched the ChemEng365 blog. The daily blog catalogues 365 chemical engineering successes and achievements.

Dr Wolfram Wiesemann become a Fellow of the new KPMG Centre for Advanced Data Analytics. The centre is funded by KPMG with £10m directly (£20m total). The Centre will focus on five core areas of research: Capital, Growth, People, Operations and Resilience. The focus will be on ground-breaking analytics techniques and algorithms that will put the UK at the forefront of data science.

Professor Costas Pantelides was awarded the Imperial College President’s Medal for Excellence in Innovation and Entrepreneurship.
Student Distinctions and Awards

Once again, all of our graduates who were applying for jobs were successful. Below are examples of some of the awards they have won.

Thapanar Suwanmajo (supervisor Dr J Krishnan) and Pongsathorn Dechatiwongse (supervisor Professor Geoffrey Maitland) won the 2014 Anglo-Thai Education Awards in the Engineering/Technology category. The Award for Excellence is given to Thai postgraduate students studying in the UK who have exceptional academic achievements.

Ioscani Jiménez Del Val (supervisor Dr Cleo Kontoravdi) won the Dudley Newitt Prize for Computational/Theoretical Excellence.

Susie Sou (supervisor Dr Cleo Kontoravdi) won the best poster prize at the UK Meeting of the European Society for Animal Cell Technology in Nottingham.

María Fuentes Gari (supervisor Professor Sakis Mantalaris) won second prize at the 2nd Young Entrepreneur Award Competition (YEA). YEA is an international business plan competition organized by the Fourth Valley Concierge Corporation and Asia Innovators’ Initiative. President, Nobuyuki Iide, Former CEO of Sony Corporation presented the award.

Aiman Alam-Nazki (supervisor Dr J Krishnan) won an EPSRC Prize Fellowship. The Prize Fellowship is a scheme intended to help universities attract and retain the very best newly qualified PhD graduates, who have been supported by the EPSRC. Aiman Alam-Nazki also won the Dudley-Newitt Prize for Theoretical/Computational Excellence, an award given annually to the best thesis in the Chemical Engineering Department at Imperial in this category.

CPSE students dominated the awards at the Qatar Energy R&D Award for two years running, 2014, Tareq Al-Ansari (co-supervisor Professor Nilay Shah) and in 2015, Ibrahim Daher (co-supervised by Professor Geoff Maitland and Dr John Crawshaw) won the Qatar Energy R&D Award. Tareq and Ibrahim were recognised as rising stars in the Gulf State of Qatar winning the award for their outstanding PhD research which could have a major impact on industry in Qatar.

Post Doctorate Distinctions and Awards

Yun-Bo Zhao (supervisor Dr J Krishnan) was selected in the 1000Plan programme for young talent. The initiative aims to recruit, and provide financial support for outstanding scientists and leading experts who will work in China and play a leading role in the development of high-tech industries or new fields of study in the nation’s major innovation projects, key programmes of study or laboratories, central enterprises or state-owned financial institutions, or high-tech development zones or industrial parks.

High Profile Events

President of the Republic of Singapore’s Visit
In October 2014, the President of the Republic of Singapore, Tony Tan Keng Yam was hosted and given a tour of the Carbon Capture Pilot Plant by Professor Nilay Shah (CPSE Director) and Professor Alice Gast (Imperial President).

17th British-French-German Conference
A number of CPSE academics, students and researchers were part of the team that organised the 17th British-French-German Conference on Optimisation. The conference was 17th of the series of French-German meetings which started in Oberwolfach, Germany in 1980. Since 1998, the conference has been organised under the participation of a third European country. This time it was jointly organized with Britain and took place at Imperial College London. The conference consisted of invited plenary talks, parallel invited and contributed sessions. The conference was organised by Imperial College London, the Department of Computing, the Centre for Process Systems Engineering and the Imperial College Business School.

Enhancing Education

The CPSE continued to expand and develop education in Process Systems Engineering.

New Courses

Optimisation Courses
The CPSE identified the need for technical training in optimisation and to address this created two new courses. In April 2015, the first course took place with participants from CPSE Industrial Company Members and PhD students.
• The Introduction to Optimisation Course provides an introduction to concepts in problem formulation and solution methods for linear, nonlinear and mixed-integer problems, focusing on local optimisation methods, with a brief introduction to global optimisation.

• The Advanced Optimisation Course builds on the introductory course and focuses on concepts in global optimisation, bilevel optimisation, dynamic optimisation, optimisation under uncertainty.

Detailed information on the courses is available on the CPSE website.

Part-time MSc in Process Automation

The new Part-time MSc in Process Automation, Instrumentation and Control was launched in December 2014. The aim of the programme is to broaden and deepen the expertise and experience of personnel employed in process automation, either in the design and development of control and related systems, in their application, or in their operation and management. A highlight of the year has been accreditation of the programme by IChemE, IET and the Institution of Measurement and Control.

New Institutions

CPSE has been instrumental in the creation of two new institutes.

Sustainable Gas Institute (SGI)
Professor Nigel Brandon (Director) and Dr Adam Hawkes (Deputy Director) launched the Sustainable Gas Institute (SGI) in May 2014. The Institute is a unique academic-industry partnership and a ground-breaking collaboration between the United Kingdom and Brazil. Their role is to lead research and define innovative technologies that enable natural gas to play a key role in a low-carbon world. The Institute is a multi-disciplinary organisation operating on a ‘hub and spoke’ model, with their international research hub at Imperial College London and spokes in development at leading research universities around the world. Campaigns to build on these key relationships with Brazil have led to the creation of the Sustainable Gas Institute in Brazil, and in 2016 CPSE will be working to launch the Institute in China.

Institute for Molecular Science and Engineering (IMSE)
Professor Claire Adjiman (Co-Director) and Professor Nicholas Harrison (Co-Director) established the Institute for Molecular Science and Engineering (IMSE) in August 2015. IMSE is one of Imperial College London’s Global Institutes, drawing on the strength of its four faculties to address some of the grand challenges facing the world today. The Institute’s activities are focused on tackling problems where molecular innovation plays an important role. The Institute brings together researchers from a diverse range of specialisms to network, communicate and collaborate. The institute also connects these researchers with a wide spectrum of stakeholders including industrialists, interested individuals, government representatives, and researchers from other academic institutions, to enhance discovery and innovation within the molecular field.

Lectures and Seminars

Lectures
Annual Professor Roger W. H. Sargent Lecture
On the first Thursday in December, CPSE annually celebrates its founding Academic Father Professor Roger Sargent through the Professor Roger W. H. Sargent Lecture. This tribute to Professor Sargent celebrates his legacy in the field of Process Systems Engineering. Recent eminent speakers who delivered the lectures are:


2014 Professor Stratos Pistikopoulos FREng, CPSE, Imperial College London. “Multi-Parametric Programming & Control 25 years later: what is next?”

Seminars
CPSE has been running a successful Seminar Series for many years and each year we invite distinguished national and international experts to the Centre. For over six years Dr J Krishnan has been organising the CPSE Seminar Series. From 2015, Dr Ruth Misener and Dr Panos Parpas have taken on the tradition of hand-picking speakers from around the world. CPSE Industrial Consortium members are all welcome to attend these seminars.

2014 CPSE Seminar Series
Professor Arthur D. Lander, University of California, Irvine, CA
Professor Nick Sahinidis, Carnegie Mellon University
Professor L. N. Trefethen, University of Oxford

2014 Special Seminars
Professor Julio Banga, CSIC, Spain
Professor Ambros Gleixner, Zuse Institute Berlin
Professor Ignacio E. Grossmann, Carnegie Mellon University
Professor Jay H. Lee, Daegjeon, Korea
Mr Hernan Leovey, Humboldt University
Dr Mark Peters, UNISA
Professor B. Erik Ydstie, Carnegie Mellon University

2015 CPSE Seminar Series
Professor Ana Barbosa-Póvoa, Técnicó Lisboa, Portugal
Professor Robert Bixby, Gurobi, USA
Professor Leo Liberti, École Polytechnique ParisTech, France
Professor Alexander Mitsos, RWTH Aachen
Professor Kim Chuan Toh, National University of Singapore
Professor Philippe Toint, Université de Namur, Belgium

This is my last Annual Report publication as the Director of CPSE. I will be stepping down and passing on the reins to Claire Adjiman on 1st August 2016 and moving to the post of Head of Department of Chemical Engineering at Imperial College London. It has been a great pleasure to see CPSE grow in size and breadth, while continuing to excel in both fundamentals and applications. I leave it in the capable hands of Claire, however, I will remain part of CPSE. Professor Nilay Shah, CPSE Director.
“Members of the Industrial Consortium can scope out opportunities for optimising their interaction with CPSE through company-specific workshops and one-to-one interaction with leading academics across a broad range of disciplines.”
Companies have increasing pressures to stay ahead of their competitors. They need to be innovative, continuously launch new products and improve existing products and processes. In today's global market companies are faced with additional pressures to make their operations more energy efficient, safe and environmentally benign. Science and Engineering play a vital role in underpinning the success of the majority of today's commercial businesses. The CPSE Industrial Consortium provides "a one-stop-shop" for companies seeking solutions to improve their products and operations. Member companies are invited to become involved in the specification, development, validation and final commercial implementation of algorithms, software tools and methodologies derived from leading-edge generic research performed in the Centre. Our members also have opportunities to guide our research and development resources through joint programmes and MSc projects. They are able to access and review technology in one or half-day workshops designed in conjunction with individual members, as well as, participating in additional technology focus briefings for specific sectors. We also hold an annual meeting hosted by CPSE at Imperial College. This includes the annual Roger Sargent lecture, short lectures by research students, guest lectures by consortium members, research updates by academic staff and opportunities for informal social and technical meetings.

Our members join the CPSE Industrial Consortium to gain

- Privileged access to world-class academics from two top universities. CPSE academics between them have over 500 years of research experience. They come from many disciplinary areas including: chemical engineering, mathematics, physics and chemistry and are leaders in their fields.
- Access to well-trained PhD students and Post Doctoral researchers. The Consortium provides opportunities for members to interact with the Centre at many levels. Members are able to evaluate and recruit high calibre PhD students and Researchers from around the world.
- The opportunity to exploit and develop research and resources. Members have the opportunity to guide research development and resources towards their own business needs and have access to all the non-confidential reports of work carried out by the Centre.
- Partnerships: Membership opens the opportunity for the creation of partnerships. Some consortium members have recognized the need to develop in-depth and long-term research relationships with CPSE and have opted to establish Partnerships.
- Links to other Imperial College and UCL Departments. Imperial College and UCL have many other world-class departments which can be accessed through consortium membership. Members will be directed to key academics in both universities.
- Access to worldwide networking with major companies. The consortium provides a neutral platform for intercompany networking and benchmarking with some of the largest multinational companies.
- Staff training: the consortium provides an opportunity for company employees to attend courses on optimisation.
- A member of academic staff ("friend") as a liaison point for your company

We offer:

- At least one active collaborative research project
- Interns for flexible internship projects
- An annual, company-specific workshops to scope out opportunities
- A warm welcome to company staff to secondments in CPSE
- The CPSE Newsletter
- A one-stop-shop for systems engineering technology and solutions to problems
- Access to facilities and expert assistance for cutting edge software evaluation
- The provision of opportunities for inter-company networking and benchmarking
- A credible, world-class partner for joint proposal development and joint projects
- Opportunities for member companies to interact with the Centre at a range of levels
- Access to an exclusive members-only website

Industrial Consortium Company Members

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“Research carried out over the last few years has shown that the modelling techniques developed for the process industries by CPSE can deepen our understanding of a wide range of complex systems from the chemical processes within living cells to national energy supply chains.”
A new competence area has been created called Computational Optimisation and Machine Learning to focus on developing in a rapidly evolving area.
“The CPSE offers a unique experience to graduates, including the opportunity to work with internationally renowned academics and some of the biggest industrial companies in the world.”
CPSE research in Product and Process Design tackles the constraints and objectives imposed by today's business environment, in particular, in the field of sustainable development.

We take into account the economic, environmental, safety and health aspects and use systematic model-based methodologies for the rational design of processes encompassing a growing range of scales, such as:
- Nano-scale models for materials selection
- Meso-scale models for design of specific processes
- Overall process models for integrated plant design

There are several themes within Product and Process Design, however, the areas that we are concerned with are: Materials design for process synthesis such as development of methodologies property prediction techniques; the design problems with a large number of degrees of freedom (molecular structure, microstructure, formulation variables etc.) Another theme is the design of novel manufacturing processes. Here we are interested in the development of models and techniques for design of state-of-the-art processes, with a particular emphasis on fine chemicals and pharmaceuticals. We also look at the integrated process synthesis and the development of tools for the analysis of interactions between design and operability. Technology transfer is also an interesting theme which still requires more study. In particular, the facilitation of more mature technologies to industrial partners still remains a challenge.

Traditionally, the water industry relied on civil engineering to solve its challenges but the expertise in the chemical-engineering field is being increasingly relied upon. Chemical engineers can play a vital role in reducing water losses by transferring knowledge from the process industry to the provision and distribution of potable water. The objective of the work in CPSE focuses on the development of predictive mathematical models based on first principles and the application of optimisation techniques to provide an optimal process flowsheet.

Figure 1: Drinking water is a limited resource

Water Treatment – Predictive modelling of conventional clean water treatment
Eva Sørensen
A major challenge currently facing a sustainable future is the ever increasing demand for clean water of adequate quality and quantity.

Currently, work within the clean-water industry relies heavily on empirical/hydraulic models. This is due to the clean-water industry being quite traditional in the way it approaches its problems. However, it is slowly realising the importance of maintaining a competitive edge. Our research looks at deriving individual unit models and validating and combining units and considering plant-wide operation. By incorporating the use of mathematical models that can describe the processes, we believe industry can develop its understanding of a unit and be able to find more cost-effective solutions.

To create a model representation of water treatment processes and their interactions to mitigate risk

- Each unit is derived and validated separately and then uses a plug flow reactor (PFR) model to represent the distance the water has to travel between various process units
- The process flowsheet is used to reflect the units operated, chemical additive processes and the physical processes that can be modelled using first principles to deepen the understanding of how each unit operation works.

Figure 2: Creating a model representation of water treatment processes and their interactions to mitigate risk
Figure 3: Optimisation of WTW based on superstructures

The advantage of having a dynamic model of a clean water treatment process is invaluable. To demonstrate the applicability of the overall plant model, a sensitivity analysis can be performed by considering the impact of a disturbance propagating through the process for an illustrative case study, where the concentration for source of raw water inlet changes. The case study is implemented in gPROMS. The results produced are reflective of how a system would react to a change like this.

There are various different processing units available for each specific process type. For example, coagulation and flocculation can occur in a CSTR or the chemical coagulant can be injected at one point and allowed to flow through different chambers creating a turbulent flow. There can be multiple units of the same process in parallel as well as for different water sources; some unit configurations work better.

Rational mixture design: optimisation-based approaches
Claire S Adjiman and Suela Jonuzaj

The formulation of mixtures offers a potential route to enhanced performance across a wide range of chemical engineering applications, from separation processes to product design. However, mixture design can be very challenging because it requires finding the optimal number, identities and compositions of mixture components and using nonlinear property models, which results in complex nonlinear problems with a large combinatorial space. Thus, a restricted version of the problem is usually posed, where the number of mixture ingredients is fixed in advance, before other design decisions are made. This restricts our ability to identify the optimal mixture.

In view of these challenges, our work focuses on developing a comprehensive and systematic methodology within the Computer-Aided Mixture/blend Design framework by combining mathematical modelling, optimisation and chemical engineering insights to formulate the general mixture problem. Within this approach, the optimal number of components in a mixture, their identities and compositions are determined simultaneously. A logic-based methodology, Generalised Disjunctive Programming, is used to express the general mixture problem within a mathematical framework and formulate the discrete choices inherent in the problem.

The novel framework proposed has been applied successfully to the design of solvent mixtures for separation processes, including crystallisation and liquid-liquid extraction. Significant benefits can accrue by employing this approach in product design, especially as the number of desirable mixture components increases: the explicit evaluation of every choice of the number of components is avoided, making it possible to consider larger design spaces.

The work has been published in Jonuzaj et al. (2016) and Jonuzaj and Adjiman (2016), and will be presented as a keynote at the 26th European Symposium on Computer Aided Process Engineering (http://escape26.umsi.si).


**Competence Area**

**Operations and Control**

**Process Operations** uses mathematical models that capture the underlying science of a process and adopts an optimization approach to give improved operation in terms of product quality, energy usage, environmental impact and sustainability. The research within the Centre covers optimization of the operations of existing plants, optimal designs for new plants that take account of dynamic operation at the design stage, management of supply chains and of batch processing.

**Process control** covers the theory and practice of advanced automation and control applied to a wide variety of processes including reaction, adsorption, granulation and polymerization carried out within a spectrum of manufacturing industries including oil & gas. Competencies feeding into applications include: integration of design; operation and decision making; multi-scale modelling; integrated monitoring of processes; electrical and mechanical equipment; and theoretical advances in robust parametric control. A special feature of the programme is the ability to move new theory rapidly towards practical realisation and thus to help the process control sector take early advantage of new developments.

**A selection from the activities in the past year includes:**

**Multi-parametric NCO-tracking controllers for linear dynamic systems**

Driven by the need to improve performance and reduce economic costs in industrial processes, on-line optimization and real-time control have been receiving a lot of attention. The strategy employed in classical model predictive control (MPC) is to solve the optimization problem in a receding horizon manner. This is often a rather computationally demanding task that may cause serious delays especially for systems with fast dynamics, leading to suboptimal performance or even infeasibility. In the multi-parametric programming paradigm, the optimization is performed off-line, resulting in a priori explicit mapping of the solutions, effectively control strategies as a function of measurable quantities. Likewise, NCO tracking is a measurement-based optimization approach to enforcing optimality in the presence of uncertainty, via tracking of the necessary conditions for optimality (NCO).

This project is concerned with a methodology for combining multi-parametric programming and NCO tracking into a unified framework for model predictive control, for which we coined the name “multi-parametric NCO-tracking control”. Such a combination is especially promising in that using feedback laws tracking the optimality conditions inside a multi-parametric controller has the potential to dramatically reduce the number of critical regions compared with classical mp-MPC controllers based on time discretization. Moreover, multi-parametric programming provides a means for relaxing the fixed switching structure assumption in NCO-tracking, thereby paving the way towards a theoretical justification for NCO-tracking too. Our initial focus has been on constrained linear dynamic systems, and extensions to the general nonlinear case are now being investigated.

**Figure 1:** Comparison between the critical regions in a mp-NCO-tracking controller (top plot; 11 regions) and a mp-MPC controller over 50 stages (bottom plot; 1687 regions) for a constrained FCC unit operated in partial combustion mode.
Robust MPC using set-based methods

Classical MPC control is based on a certainty-equivalence principle, whereby the future of the system is optimized as if neither external disturbances nor model mismatch were present. Although these uncertainties are the main reason why feedback is needed in the first place, the main advantage of certainty-equivalence in MPC is that the resulting optimization problems can often be solved efficiently, in real time. Moreover, this approach works well in many practical applications, and it often exhibits a certain robustness due its inherent ability to reject disturbances. However, the constraints may become violated when large disturbances occur, since uncertainty is not taken into account in optimizing the predicted state trajectories. In such cases, robust MPC schemes may be used to mitigate these optimistic predictions.

Our focus in this project is on robust MPC schemes using set-based methods, known collectively under the name tube-based MPC. The predicted trajectory is replaced by a robust forward invariant tube (RFIT) in the state-space, namely a tube that encloses all possible state trajectories under a given feedback control law, which is independent of the uncertainty realization. In contrast to existing methods which parameterize the control law, our approach introduces a min-max differential inequality exploiting the properties on the boundary of RFITs. These min-max differential inequalities provide sufficient conditions for a time-varying convex-set-valued function to be an RFIT, for an inclusive class of input-affine nonlinear control systems. We also derive practical implementations of tube-based MPC based on ellipsoidal calculus, which (i) scale linearly with the length of the prediction horizon, and (ii) do not rely on a particular parameterization of the control law. In principle, this approach can achieve arbitrary precision insofar as the tubes are represented with sufficient accuracy. The construction of robust MPC controllers with such properties is unprecedented for nonlinear input-affine systems.

This work is a collaboration with ShanghaiTech (Dr. Houska) and the University of Freiburg (Prof. Diehl).

**Figure 2:** Ellipsoidal RFIT for robust MPC control of a constrained spring-mass-damper system, along with three uncertainty realizations (dashed blue lines).

Process Automation Research Programme

Worldwide, there is a huge inventory of currently installed process plants and our research finds ways of helping these to run efficiently and smoothly. This is achieved by optimizing the operation of the process and equipment by detection and diagnosis of the root causes of process inefficiencies. The methods make use of all available information, not only measurements from operating processes but also qualitative and connectivity information from process schematics and drawings, plus reasoning from scientific first principles.

Process plants depend upon mechanical and electrical equipment. We are looking at measurements from the mechanical and electrical sub-systems to understand the whole picture and are also exploring the interactions between a.c. transmission grids and process plants which are large electrical consumers. The work is being undertaken by Imperial researchers, industrial research engineers on secondment and PhD students sharing their time between Imperial and industrial placements with collaborating companies. More information on Process Automation is available at:

http://www3.imperial.ac.uk/processautomation

**Detection of Disturbances**

The process automation group develops methods for detection and diagnosis of process disturbances. Recently, the work has examined transient disturbances in multi-rate systems. The motivation for these developments is that there is an increasing industrial requirement for the analysis of data sets comprising measurements from industrial processes together with their associated electrical and mechanical equipment. These systems are increasingly affected by transient disturbances, and their measurements are commonly sampled at different rates. Progress with these objectives is illustrated in Figure 3.

The methods are based on nearest-neighbours techniques, meaning that they identify occurrences of similar patterns in the time trends. They build a vector of anomaly indices which are high for the period with the transient disturbance. The general applicability of the above methods is well illustrated by case studies from oil and gas plants and from an experimental compressor rig where process measurements are treated together with electrical measurements from the variable speed drive.

Recently the same methods have been used for automated detection of transient events in an electrical transmission grid as measured by instruments called Phasor Measurement Units. Power system disturbances generally result from the penetration of heavy or light loads, sudden changes in the operation conditions, and faults.

The timescale is much faster than that of events in a process system. Detection of power-system disturbances is a difficult task because of system complexity, diversity of operating conditions and interference from noise. It places high demands on reliable, sensitive and real-time implementation. The successful results show that methods can be adapted across time scales.
The work has received financial support from the Portuguese Foundation for Science and Technology (FCT) under Fellowship SFRH/BD/61384/2009, from the Marie Curie FP7-IAPP project “Using real-time measurements for monitoring and management of power transmission dynamics for the Smart Grid – REALSMART”, Contract No: PIAP-GA-2009-251304, and from EPSRC EP/L014343/1 “Stability and Control of Power Networks with Energy Storage (STABLE-NET)”. Multi-criterion manufacturability indices for ranking high-concentration monoclonal antibody formulations

The need for high-concentration formulations for subcutaneous delivery of therapeutic monoclonal antibodies (mAbs) can present manufacturability challenges for the final ultrafiltration/diafiltration (UF/DF) step. Viscosity levels and the propensity to aggregate are key considerations for high-concentration formulations.

This project created a novel framework for deriving a set of manufacturability indices related to viscosity and thermostability to rank high-concentration mAb formulation conditions in terms of their ease of manufacture. This is illustrated by analysing published high-throughput biophysical screening data that explores the influence of different formulation conditions (pH, ions and excipients) on the solution viscosity and product thermostability.

The project used a decision-tree classification method, CART (Classification and Regression Tree) to identify the critical formulation conditions that influence the viscosity and thermostability. The ultimate industrial deliverable from the work was a set of stress maps which show viscosity and thermostability as functions of the formulation conditions and time profiles during UF/DF.

The framework helped to identify the optimal formulation conditions that minimize the potential for both viscosity and aggregation issues during UF/DF.

The work is a sub-project of the EPSRC Centre for Innovative Manufacturing in Emergent Macromolecular Therapies led with UCL. It is sponsored by EPSRC and pharmaceutical companies including GE Healthcare, GlaxoSmithKline, Pfizer and MedImmune.

**Operations and Control – Highlighted project**

**Supercritical gas recycle for surge control of CO2 centrifugal compressors**

The highlighted project concerns computer-based design and analysis of control systems for centrifugal compressors when the operating fluid is supercritical CO\textsubscript{2}. The work has implemented a non-linear dynamic model including a main forward compression line together with hot and cold recycles. The work is based on a validated model of a CO\textsubscript{2} compressor station in collaboration with the industrial partner.

Industrial compressor trains typically use both hot and cold gas recycle for the purposes of surge avoidance. The idea is that the operating fluid is recycled back to the compressor inlet if the flow rate reduces such that the operating point of the compressor approaches the surge line. Hot recycling feeds fluid back to the compressor inlet directly through the recycle valve, while cold recycling also cools the fluid. Ideally recycling would be avoided since recycling of already-compressed fluid represents a waste of energy. On the other hand, the compressor must be protected from surge, and at the same time must fulfill delivery of the operating fluid to the downstream processes or pipeline in the right thermodynamic state. The analysis in this project has provided some insights into the dynamics and control of the two configurations.

The work demonstrated that compared to the hot recycle, the process configuration including a cold gas recycle has better overall stability, but higher power consumption and lower values for the control performance indicators. Moreover it compares subcritical and supercritical compression during surge prevention and highlights the importance of the selection of the gas recycle configuration when full recycle is needed. The key findings are outlined in the table on the right.

**References**


<table>
<thead>
<tr>
<th>Cold recycle</th>
<th>Hot recycle</th>
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<tbody>
<tr>
<td>Advantages: No issues of overheating since the recycled gas is cooled. No loss of machine integrity if the machine runs continuously in recycle mode.</td>
<td>Disadvantages: Repeated opening and closing of the recycle valve occurs because the inlet pressure increases when recycled fluid is fed back. This causes interaction between the surge control system and the pressure control system. Higher overall power consumption and lower pressure control performance.</td>
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<tr>
<th>Recycle of subcritical CO₂</th>
<th>Recycle of supercritical CO₂</th>
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<tbody>
<tr>
<td>Cold recycle circulates 23% more gas than hot recycle and hence equipment sizing will be similar. Designs may be based on considerations outlined above in this table.</td>
<td>Cold recycle circulates 82% more gas than hot recycle due to the change of state from supercritical to subcritical. Therefore cold recycle may be more effective for supercritical CO₂ surge protection.</td>
</tr>
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</table>

The work was funded by the Marie Curie Marie Curie FP7-ITN project “Energy savings from smart operation of electrical, process and mechanical equipment – ENERGY SMARTOPS”, PITN-GA-2010-264940, and by EPSRC EP/J020788/1 Gas-FACTS: Gas – Future Advanced Capture. Thank you also to ESD Simulation Training for their encouragement, advice and technical support for the project.

**References**


Competence Area
Modelling and Model Solution Tools

The development of new and improved Modelling and Model Solution tools is a key factor in maintaining the excellence of CPSE’s academic research and has led to many of the software packages in this area that are now the accepted standards in industry.

The models and solution tools in use and under development in CPSE focus on different spatial and temporal scales across a wide range of process systems engineering problems. Four recent examples are described below:

Zacros
Zacros is a Kinetic Monte Carlo software package written in Fortran and developed at UCL for simulating molecular phenomena on catalytic surfaces. The tool enables researchers in the areas of Computational Catalysis and Surface Science to perform dynamic modelling of adsorption, desorption, surface diffusion, and reaction processes on heterogeneous catalysts. The rates of these elementary processes are typically computed from ab initio simulations, thereby enabling the prediction of catalytic performance metrics (such as activity and selectivity) from first principles, and the detailed validation of hypothesised kinetic mechanisms against experimental data.

The package employs the Graph-Theoretical KMC methodology coupled with cluster expansion Hamiltonians and Bronsted-Evans-Polanyi relations, which can naturally capture: steric exclusion effects for species that bind in more than one catalytic site; complex reaction patterns involving adsorbates in specific binding configurations and neighbouring patterns; spatial correlations and ordering arising from adsorbate lateral interactions that involve many-body contributions; changes in the activation energies of elementary events, influenced by the energetic interactions of reactants with neighbouring spectator species.

The software was commercialised by UCL Business in Nov-2013, and has a dedicated website [http://zacros.org] with documentation, tutorials, list of publications and links to e-Lucid, the UCL online licensing portal from where users can obtain Zacros from. The code can be obtained free of charge by academics, and since inception it has been distributed more than 70 users in 25 countries worldwide. For more information about Zacros please contact Michail Stamatakis [m.stamatakis@ucl.ac.uk].

Global Sensitivity Analysis (GSA)
GSA is used to identify key parameters whose uncertainty most affects the output. This information can then be used to rank variables, fix unessential variables and decrease problem dimensionality. Over the last decade GSA has gained acceptance among practitioners in the process of model development, calibration and validation, analysis of problem structure, reliability and robustness analysis, decision-making under uncertainty, quality-assurance, and complexity reduction. The variance-based method of global sensitivity indices (SI) developed by Sobol’ has become the method of choice among practitioners due to its efficiency and ease of interpretation. However, there is an important class of practical design problems involving inequality constraints imposing structural dependences between model variables in addition to potential correlations between them.

The development of efficient computational approaches for constrained GSA (cGSA) is challenging because the feasible domain of the model variables’ variation may have an arbitrary shape including non-convex or disconnected (as opposed to hyperrectangular spaces considered within conventional GSA).

We have proposed a novel concept of constrained Global Sensitivity Analysis which adds the ability to analyse model output variance in such domains. The advantage of the presented formulations is that no prior knowledge of conditional or marginal distributions is assumed. All the required dependences are derived from the joint p.d.f. and, furthermore, in the presence of constraints it is sufficient to know the joint p.d.f. corresponding to the unconstrained formulation.

Grid cubature and Monte Carlo estimates have been proposed for the evaluation of main and total effect indices. The new approach amounts to greatly expanding the scope of GSA to a wide range of situations of practical importance involving inequality constraints.

For more information about GSA please contact S. Kucherenko and O.V. Klymenko.
Set-Valued Integration of Uncertain Dynamic Systems

Many engineering design and control problems can be formulated, analyzed and solved in a set-based framework. When it comes to designing a control system for instance, the constraints, uncertainties and design specifications are described naturally in terms of sets. In measuring the effect of a disturbance on a system’s response or in bounding the error of an estimation algorithm likewise, sets play a central role. A number of key set-theoretic concepts were proposed in the early 1970s, but their systematic application was not possible until enough computational capability became widely available. Today, many such methods and tools are available for the estimation and control of linear systems, but it is less so for nonlinear systems.

The development of set-valued integration algorithms for uncertain dynamic systems has been an on-going research area in Dr Chachuat’s group for over 10 years. Central to these approaches is the ability to compute tight enclosures of the range of multivariate systems, e.g., using ellipsoidal calculus or higher-order inclusion techniques based on multivariate polynomials. In recent years, we have developed efficient methods, both continuous-time and discretized approaches, capable of propagating generic set-parameterizations in order to yield tight enclosures on the reachable set of an uncertain ODE or DAE system. Moreover, sufficient conditions that guarantee stability of the bounding system have been identified for the first time.

For more information on set-valued integration please contact Benoît Chachuat.

Simulation of long-term global energy transitions

The 5th Assessment Report of Working Group 3 of the Intergovernmental Panel on Climate Change was released at the end of 2014, setting out approaches to climate-change mitigation. A number of models were used to support this study, each being global in scope, with long time horizons to capture the dynamics of climate change, and particularly to explore approaches to limiting average surface temperature rise to less than 2°C. The importance of these models has increased as a result of the Paris Agreement, further pushing the ambition to limit temperature rise to 1.5°C.

The Sustainable Gas Institute is developing a new energy systems simulation environment. Instead of using intertemporal optimisation like many other models, it strives to simulate investment and activity in each sector of the global economy (split into roughly 30 regions) in a way that is appropriate for each sector. The model is bottom-up, including engineering detail and basic economic characteristics for thousands of technologies. It is built on the principles of simplicity and transparency, and the modelling framework will ultimately be made open source. For further information about global energy systems modelling please contact Adam Hawkes.
The Computational Optimisation Group has a 30-year track record of research in decision-making under uncertainty, stochastic and robust optimisation. Current interests of the group include representing uncertainty in optimisation models, designing numerical optimisation algorithms and computational software frameworks, and applying these algorithms to energy production, capacity planning, manufacturing and distribution models under uncertainty, financial engineering and risk management. The Statistical Machine Learning Group focuses on Bayesian methods. Application areas include autonomous systems, robotics, time series analysis, reinforcement learning, and brain-machine interfaces. Several other groups within CPSE also have strands of research in computational optimisation.

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<th>Area</th>
<th>Academic</th>
<th>Expertise</th>
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<td>Deisenroth, Misener</td>
<td>Algorithm design, Optimisation for machine learning, Parameter estimation</td>
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<td><strong>Optimisation-based Control</strong></td>
<td>Bogle, Chachuat, Deisenroth, Dua</td>
<td>Dynamic optimisation, Multiparametric programming, Optimal Control</td>
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<tr>
<td><strong>Implementations &amp; Software</strong></td>
<td>Adjiman, Chachuat, Fraga, Kucherenko, Misener</td>
<td>Deterministic global optimisation, Global sensitivity analysis, Set-membership estimation, Mixed-integer nonlinear optimisation, Multi-objective optimisation</td>
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<td><strong>Large-Scale Convex Optimisation</strong></td>
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<td><strong>Mixed-Integer Nonlinear Optimisation</strong></td>
<td>Adjiman, Chachuat, Misener</td>
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<td><strong>Signal Processing</strong></td>
<td>Deisenroth</td>
<td>Bayesian state estimation, System identification, Inference and learning in nonlinear dynamical systems</td>
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Highlighted Project
Bayesian Optimisation with Dimension Scheduling: Application to Biological Systems

Highlighted Project Authors: Doniyor Ulmasov, Caroline Baroukh (INRA, France), Benoît Chachuat, Marc Peter Deisenroth, Ruth Misener.

Bayesian Optimisation (BO) is a data-efficient, global black-box optimisation method optimising an expensive-to-evaluate fitness function; BO uses Gaussian Processes (GPs) to describe a posterior distribution over fitness functions from available experiments. Similar to experimental design, an acquisition function is applied to the GP posterior distribution over fitness functions to suggest the next (optimal) experiment.

Dynamic models of biological processes allow us to test biological hypotheses while running fewer costly, real-world experiments. We consider estimating biological parameters (e.g., reaction rate kinetics) by minimising the squared error between model and experimental data points. Specifically, we propose BO for efficient parameter estimation of a dynamic microalgae metabolism model (Baroukh et al., 2014). The forcing function is based on light exposure and nitrate input; experimental data have been collected for measurable outputs including lipids, carbohydrates, carbon organic biomass, nitrogen organic biomass and chlorophyll. Our method is general and may be applied to any process model.

There are several timescales for collecting microalgae metabolism data: an experiment may take 10 days while each model simulation of Baroukh et al. (2014) runs in a fraction of a second. BO is traditionally applied to functions with expensive evaluation costs, e.g., running a 10 day experiment, but the objective of this paper is testing biological hypotheses; we are specifically interested in running the simulation model many times for parameter estimation.

In biological parameter estimation, BO is challenging because the parameters interact nonlinearly and the broad parameter bounds result in a huge search space. Due to the high problem dimensionality (in this context, 10 parameters), balancing exploration versus exploitation becomes more intricate and traditional Bayesian methods do not scale well. Therefore, we introduce a new Dimension Scheduling Algorithm (DSA) to deal with high dimensional models. The DSA optimises the fitness function only along a limited set of dimensions at each iteration. In each iteration, a random set of dimensions is selected to be optimised. This reduces the necessary computation time, and allows the dimension scheduling method to find good solutions faster than the traditional method. The increased computational speed stems from the reduced number of data points per GP and the reduced input dimensions in the GP; GPs scale linearly in the number of dimensions but cubically in the number data points. Additionally, considering a limited number of dimensions at each node allows us to easily parallelise the algorithm.

Compared to commercial parameter estimation for biological models and a traditional Bayesian Optimisation algorithm, our approach achieves strong performance in significantly fewer experiments and a reduced computation time. We also design and provide a graphical user interface (GUI), which allows untrained users to optimise any model that can be invoked through a command line. The framework removes the barrier of programming language by providing the user with a straightforward user interface to set BO parameters, observe the optimisation as the code runs, and examine the GP after the experiment has been completed.

Figure 1: Convergence of branch-and-lift for a bioreactor control problem (right plot), and illustration of limited clustering occurring when lifting the search space dimension M (left plot)

Highlighted Project References:
Dynamic optimisation of dynamic systems subject to uncertainty (Carlos Perez-Galvan, David Bogle – CONACyT)

Many process engineering problems have critical bounds (quality, safety or environmental) that must be satisfied at all times. These methods are desirable in applications such as guaranteed parameter estimation, optimal control, and safe critical applications where critical variables such as safety or environmental performance are an issue. In a dynamic optimisation algorithm guaranteed bounds on the dynamic variables of the models that describe processes are needed in order to solve the problem to global optimality in a rigorous way. Hence, verified bounds are a key step in the optimisation algorithm (Focus on first box of Figure 1). However, the construction of tight bounds is still an issue for practical applications. This project focuses on obtaining bounds that tightly enclose the representation of the reachable set.

Dynamic simulation
Verified methods of initial value problems (IVP) for ordinary differential equations (ODE) provide enclosures which are guaranteed to contain all the possible solutions of a problem (possibly subject to an uncertain value). The bounding method used in this project consists of two stages. The first stage is the validation of existence and uniqueness of a solution in which also a suitable a priori enclosure and a time step are obtained. The second stage involves the computation of a tighter enclosure in which a high order Taylor series is used to refine the solution obtained in the first stage.

Reduction of the overestimation
The major challenge in these methods is the reduction of the overestimation generated in the integration process which is mainly caused by the dependency and wrapping effect problems. This project addresses the reduction of the overestimation and the novel part of the method is the implementation of non-linear interval contractors such as Krawczyk, Newton/ Gauss-Seidel and Forward-Backward.

Figure 1 represents the construction of bounds for an exothermic batch reactor using the interval Taylor series method with different interval contractor implementations, namely, no contractor (NC), Newton and Krawczyk (K) contractors. The grey lines represent the reachable set; they have been constructed using Monte Carlo simulations (2000 samples).

Figure 2. Bounds constructed by interval Taylor series method without contractors (NC) and with Newton (N) and Krawczyk (K) contractors.

\[ \dot{X}(t) = k_0(1 - X(t))e^{\frac{E_a}{RT(t)}} \]

\[ \dot{T}(t) = \frac{UA}{C_40VCP}(T_a - T(t)) - \frac{\Delta H_R}{C_p}k_0(1 - X(t))e^{\frac{E_a}{RT(t)}} \]
**Global optimisation**

The algorithms with the Newton and Krawczyk contractors have been implemented in a global optimisation algorithm. The algorithm consists of a branch-and-bound tree, the node on which to branch was the one with the least lower bound. At each node, the variable with the greatest diameter (distance between its upper and lower bound) was selected for branching. The first order sensitivity calculations were included in order to discard regions not containing zero in its gradient.

\[
\begin{align*}
\min_u \phi &= -x_2(t_f) \\
\text{s.t.} & \\
\dot{x}_1 &= -k_1x_1 - (k_3 + k_4 + k_5)x_1x_2 \\
\dot{x}_2 &= k_1x_1 - k_2x_2 + k_3x_1x_2 \\
k_i &= a_i e^{-rac{698.15 + 50u}{R}}, \quad i = 1, \ldots, 5 \\
x_0 &= ([0.99, 1.01], 0) \\
t &\in [t_0, t_f] = [0, 10] \\
u &\in [0, 1]
\end{align*}
\]

**Figure 3.** Global optimisation subject to uncertainty of the oil shale pyrolysis process

Figure 3 shows a graph of an oil shale pyrolysis example in which the black line represents the optimal profile and the rest of the lines represent suboptimal trajectories. The algorithm which makes use of the interval Taylor series with contractors is able to obtain upper and lower bounds on the global optimum of this problem.
“CPSE researchers are taking Process Systems Engineering research into new domains such as nanotechnology, healthcare and sustainability. This is leading to powerful new methods applicable for solving an even wider range of challenges facing chemical engineers in industry.”
Application Domain
Chemical Manufacturing Systems

Many of the fundamental tools developed in the four competence areas of Product & Process design, Operations & Control, Modelling and Model Solution Tools, and Optimization & Machine Learning are motivated by the challenges arising from chemical manufacturing systems. This application domain explores the need for new technologies, more effective use of new tools of analysis, and improved integration of all elements of manufacturing operations, including machines, information and humans. Through this domain, CPSE serves several process industries such as bulk chemicals (including petrochemical and oil & gas), pharmaceuticals & agrochemicals, specialty chemicals, and biofuels.

Integrated Water Networks for Freshwater Minimization
Cheng Seong Khor, Benoît Chachuat, Nilay Shah
Due to the high demand for freshwater by the process industries, together with the drive for achieving sustainable development, water network synthesis problems have received increasing attention in the PSE community. For the objective of minimizing freshwater use and wastewater generation, water can be reused by channeling the effluent from a water-using operation to other operations, and possibly recycled to the operations where it was generated. In further reducing freshwater and wastewater flowrates after exhausting recovery opportunities via direct reuse/recycle, water regeneration can be considered, which involves performing partial treatment on the effluent by using water treatment and purification units such as membranes and steam stripping prior to reuse/recycle.

CPSE is investigating the synthesis of optimal water networks in the ‘environomic’ sense – that is, maximizing economic profit and meeting certain environmental sustainability criteria at the same time – while complying with constraints on the water users and/or final discharge limits to the environment. Our focus has been on using superstructure optimization together with realistic regenerator models, which leads to challenging, nonconvex MINLP models. Industrial case studies of water networks in petroleum refineries with a large number of wastewater sources and sinks as well as multiple regenerators have revealed that state-of-the-art global optimization technology can be applied to tackle these problems rigorously, leading in certain cases to more than 50% annual savings in freshwater use. Our recent work has investigated the problem of integrated water network synthesis under uncertainty, with risk management using the Conditional Value-at-Risk (CVaR) metric. It has been established that rigorous, risk-averse solutions can be computed in reasonable time too, which could make them the solution of choice in planning and decision making.

Figure 1: Principle of two-stage stochastic methodology for water network synthesis under uncertainty.

Figure 2: Histograms comparing the projected total annual cost distributions of risk neutral and risk-averse solutions for a water network consisting of 7 water-using operations, 3 sources and 3 sinks; the regeneration technologies considered for abatement of oil & grease and suspended solids are carbon filter and reverse osmosis.
Towards Membrane Cascades for Isothermal Refining
Vincentius Surya Kurnia Adi, Marcus Cook, Ludmila Peeva, Andrew Livingston, Benoît Chachuat

Crude oil refining is the second most energy-intensive industry after the chemical industry in advanced economies. Current refinery technology is based on distillation, which typically accounts for over half of the total energy consumption due to vaporization (phase change) and the need for reflux. Membrane technology offers a promising alternative for separating mixtures without the need to employ energy intensive operations based on phase change. In particular, organic solvent nanofiltration (OSN) provides a means for separating organic-organic mixtures such as crude oil. In many cases, a mixture separation may not be achieved through a single membrane pass because OSN membranes are not selective enough between the different constituents. Instead, the mixture can be processed through multiple membranes and/or using multiple passes, namely a membrane cascade arrangement.

Given the recent advances in the development of membranes for organic mixtures and their applications in membrane cascades, this project is concerned with the possible use of membranes for hydrocarbon mixtures. We are developing a superstructure optimization approach based on mixed-integer nonlinear programming (MINLP) to determine the most promising cascade configurations. The aim of the optimization is to determine the cascade design and operating conditions maximizing product purity, for a given composition of the inlet stream. Our initial focus is on a binary system of heptane and hexadecane to mimic the light-key and heavy-key in the multicomponent environment of a representative petrochemical/hydrocarbon feed stream while simplifying the analysis.

Economically Optimal Integrated Process and MPC Control Design
Flávio Strutzel; David Bogle, CAPES

The use of MPC (Model Predictive Control) is nowadays ubiquitous in the chemical industry and offers great advantages. The zone constrained MPC with economic optimization capabilities is today’s standard in the chemical industry. MPC reduces process variability and enables operation with lower quality giveaway, increasing output of high value added products and decreasing by-product output. However, new chemical processes are being projected without taking into account how design choices affect the MPC’s ability to deliver better control and optimization. Therefore, a methodology to determine if a certain design option favours or hinders MPC performance is desirable.

This project develops the “economic MPC optimization index”, whose intended use is to provide a procedure to compare different designs for a given process, assessing how well a given flowsheet interacts with a generic MPC package. This index is impacted by process controllability, control resilience, control requirements and restrictions of a given plant. It quantifies the economic optimization benefits available and how well the plant performs under MPC control, thereby providing a monetization measure of expected control performance.

This approach assumes the availability of a linear state-space model valid within the control zone defined by the upper and lower bounds of each controlled and manipulated variable. Process economics provides the basis for the analysis as the index needs to be minimised in order to find the most profitable steady state within the zone constraints towards which the MPC is expected to direct the process. Special attention is paid to the effect of model uncertainty and/or disturbances on the index, which may reduce profitability by restricting the ability of a MPC to reach dynamic equilibrium near process restrictions, thus increasing product quality giveaway and costs in turn. This approach has been demonstrated the case study of a realistically sized crude oil atmospheric distillation plant consisting of four alternative designs.
Figure 5: Illustration of the ‘economic MPC optimization index’ methodology for comparison of alternative process designs.
Application Domain
Molecular Systems Engineering

The Molecular Systems Engineering (MSE) group has over 30 staff and students and, since its inception, has published close to 200 papers many of which have received large numbers of citations in the academic press. The team has expertise in both molecular modelling and thermodynamics and process systems engineering. Their modelling work covers all scales from sub-atomic (quantum) to macroscopic. The group has a website (http://molecularsystemsengineering.com) where it is possible to access recent papers and results.

MSE research is underpinned by a £1.8M Platform Grant (EPSRC) which supports the next generation of post-doctoral researchers and has the support of BMS, Chemistry Innovation, GSK, P and G and Syngenta. The programme is entitled ‘Molecular systems Engineering of High-Value Structured and Formulated products’. The aim is to advance the tools of molecular systems engineering to tackle some of the key molecular challenges to improving the productivity of drug discovery and processing by improving our predictive capability of the relevant physical properties.

MSE collaborates with industry across a broad range of sectors from pharmaceuticals to oil and gas. The following highlights some of our recent publications and progress.

SAFT developments

Two recent papers highlight advances in developing intermolecular potential models for use with the SAFT-VR Mie equation of state and development of force-field parameters from the SAFT-γ Equation of State for use in course-grained molecular simulations.

Developing intermolecular-potential models for use with the SAFT-VR Mie equation of state

A major advance in the statistical associating fluid theory for potentials of variable range (SAFT-VR) has recently been made with the incorporation of the Mie (generalized Lennard–Jones [LJ]) interaction between the segments comprising the molecules in the fluid (Lafitte et al. J. Chem. Phys. 2013;139:154504). The Mie potential offers greater versatility in allowing one to describe the softness/hardness of the repulsive interactions and the range of the attractions, which govern fine details of the fluid-phase equilibria and thermodynamic derivative properties of the system. In our current work, the SAFT-VR Mie equation of state is employed to develop models for a number of prototypical fluids, including some of direct relevance to the oil and gas industry: methane, carbon dioxide and other light gases, alkanes, alkyl benzenes, and perfluorinated compounds. A complication with the use of more-generic force fields such as the Mie potential is the additional number of parameters that have to be considered to specify the interactions between the model molecules, leading to a degree of degeneracy in the parameter space. A formal methodology to isolate intermolecular-potential models and assess the adequacy of the description of the thermodynamic properties in terms of the complex parameter space is developed. Fluid-phase equilibrium properties (vapour pressure and saturated-liquid density) are chosen as the target properties in the refinement of the force fields; the predictive capability for other properties such as the enthalpy of vaporization, single-phase density, speed of sound, isobaric heat capacity, and Joule–Thomson coefficient, is appraised. It is found that an overall improvement of the representations of the thermophysical properties of the fluids is obtained using the more-generic Mie form of interaction; in all but the simplest of fluids, one finds that the LJ interaction is not the most appropriate. An update of our work in this area is found in Dufal et al. AIChE J 61 2891 (2015) and Sadeqzadeh et al., Fluid Phase Equilib. 407, 39 (2016).

Figure 1: Statistical associated fluid theory (SAFT) is fundamental to the group’s work.
**Force-Field Parameters from the SAFT-Equation of State for Use in Coarse-Grained Molecular Simulations**

A description of fluid systems with molecular-based algebraic equations of state (EoSs) and by direct molecular simulation is common practice in chemical engineering and the physical sciences, but the two approaches are rarely closely coupled. The key for an integrated representation is through a well-defined force field and Hamiltonian at the molecular level. In developing coarse-grained intermolecular potential functions for the fluid state, one typically starts with a detailed, bottom-up quantum-mechanical or atomic-level description and then integrates out the unwanted degrees of freedom using a variety of techniques; an iterative heuristic simulation procedure is then used to refine the parameters of the model. By contrast, with a top-down technique, one can use an accurate EoS to link the macroscopic properties of the fluid and the force-field parameters. We discuss the latest developments in a top-down representation of fluids, with a particular focus on a group-contribution formulation of the statistical associating fluid theory (SAFT-γ). The accurate SAFT-γ EoS is used to estimate the parameters of the Mie force field, which can then be used with confidence in direct molecular simulations to obtain thermodynamic, structural, interfacial, and dynamical properties that are otherwise inaccessible from the EoS. This year we have advanced in this area, presenting coarse grained (CG) for water (Lobanova et al., *Molecular Physics* 113, 1228 (2015); natural gases and condensates Herdes et al., *Fluid Phase Equilibria* 406, 91 (2015); suprespreading surfactants (Theodorakis et al., *Soft Matter* 11, 9254 (2015)).

**Applications**

- **Solvent design for separation**
  The group has carried out a series of studies on, in particular, the separation of carbon dioxide from methane.

- **A Hierarchical Method to Integrated Solvent and Process Design of Physical CO₂ Absorption Using the SAFT-γ Mie Approach**
  Molecular-level decisions are increasingly recognized as an integral part of process design. Finding the optimal process performance requires the integrated optimization of process and solvent chemical structure, leading to a challenging mixed-integer nonlinear programming (MINLP) problem. The formulation of such problems when using a group-contribution version of the statistical associating fluid theory, SAFT-γ Mie, to predict the physical properties of the relevant mixtures reliably over process conditions is challenging. To solve the challenging MINLP, a novel hierarchical methodology for integrated process and solvent design (hierarchical optimization) is presented. Reduced models of the process units are developed and used to generate a set of initial guesses for the MINLP solution. The methodology is applied to the design of a physical absorption process to separate carbon dioxide from methane, using a broad selection of ethers as the molecular design space. The solvents with best process performance are found to be poly(oxy)methylene)dimethylethers. A review of the results is presented in J. Bruger et al. AIChE J6,1 3249 (2015). The separation of carbon dioxide from gas streams is of significant importance in many energy development schemes. Further information is included in the Energy Systems Engineering section of this report.

- **Pharma – partitioning of APIs between solvents**
  Many APIs have low solubility in both water and other solvents and it is also difficult to predict partitioning between two solvents. Good progress has been made at modelling some of these systems. The figure shows the actual and the calculated solubility of ibuprofen and ketoprofen in water and acetone and shows that the models can achieve good agreement with measured values.

**Figure 2: Solvent design for separations and reactions**

When looking at systems where there are large numbers of potential solvents and extremely large numbers of potential solvent mixtures, computing time becomes a key factor for modelling. This can be managed by developing generic mathematical formulations of the mixture design challenge and then investigating the most effective solution strategies. Systems that have been studied include mixtures of solvents to maximise ibuprofen solubility and mixtures of solvents that give best performance for the extraction of acetic acid from water.

Similar issues occur when looking at how solvent selection can be used to maximise the reaction rate constant. To optimise it is essential to be able to consider a wide range of solvents (through Computer Aided design techniques), be able to make reliable predictions of kinetics using Quantum mechanics and, finally, integrate within process design by use of Mixed Integer Nonlinear Programming.

In an example case it was possible to increase the rate constant by 126% for the Menshutkin reaction of phenacyl bromide and pyridine and to verify this result experimentally.
Application Domain
Biological Systems Engineering

Biological Systems Engineering at CPSE is concerned with the elucidation and control of biological systems at multiple scales ranging from the molecular to the cellular to the tissue to the organ level and beyond. A range of approaches is developed and deployed for this purpose including different kinds of mathematical modelling, analysis, design, optimization and control, and experiments and their integration. The applications of this work span biomedical engineering, biotechnology and systems and synthetic biology. Snapshots of the work in biological systems engineering are presented below, revealing multiple facets of the work in this area.

Dr Misener, Professor Mantalaris, Professor Pistikopoulos and collaborators have developed a novel 3-D biomimetic bioreactor for growing red blood cells ex vivo. The bioreactor recapitulates architectural and functional properties of erythrocyte formation, reducing the need for expensive growth factors by an order of magnitude. Building on this, ongoing work involves developing a global superstructure optimization for improved bioreactor design. Another project is motivated by the treatment protocols in Acute Myeloid Leukaemia, which relies on cell cycle phase-specific chemotherapeutic drugs. A platform is developed combining experiments, modelling of the cell cycle, and modelling of cell populations using population balance models. This platform can be the basis of improving chemotherapy planning through such cell cycle phase-specific drugs, leading to optimizing drug dosages and timings in a systematic manner. Overall, these projects involve a combination of mechanistic mathematical modelling, in some cases at multiple levels, design and optimization.

Dr. Kontoravdi and co-workers are developing process models to enable the implementation of Quality by Design in bioprocessing. Model development centres around two main themes: the mechanisms involved in protein glycosylation and the release of host cell contaminants. Protein glycosylation is a type of non-template modification that affects the efficacy, stability and immunogenicity of therapeutic proteins. It is, in turn, affected by process conditions, cell metabolism and intracellular regulation events. The group is working towards understanding these interactions and eventually providing a platform for glycosylation optimisation and control with a view to producing a narrow and targeted set of structures. In parallel, Dr. Kontoravdi is collaborating with Prof. Shah and colleagues in Chemistry and Life Sciences on the design and fabrication of a synthetic enzymatic reactor that will perform protein glycosylation ex vivo in a fully controlled manner. In the second theme, the release of host cell contaminants is a poorly understood process that largely depends on process conditions and cell health. The group is currently focused on developing a mechanistic understanding of the contaminants content with respect to process conditions and linking this knowledge to the efficiency of the primary purification step, affinity chromatography. Overall this work involves mechanistic mathematical modelling of the relevant cellular biochemical steps and their effect at the process level, with associated tools of analysis and design.

Professor Bogle along with colleagues at the UCL Institute for Liver and Digestive Health have used process systems engineering approaches and tools to tackle medical problems which involve complex chemical transformations and spatial phenomena looking in particular at the liver system, the body’s chemical factory. This involves modelling distributed behaviour necessary to predict the behaviour of drugs for treating liver disease. The model developed has been used to predict the effects of suppression of de novo lipogenesis, stimulation b-oxidation and a combination of the two.

In non-alcoholic fatty liver disease (NAFLD), lipid build-up and the resulting damage is known to occur more severely in perivenous cells. Due to the complexity of studying individual regions of the sinusoid, the causes of this zone specificity and its implications on treatment are largely ignored. A computational model of liver glucose and lipid metabolisms has been developed which treats the sinusoid as the repeating unit of the liver rather than the single hepatocyte. By simulating insulin resistance (IR) and high intake diets leading to the development of steatosis in the model, the work identifies key differences between periporal and perivenous cells accounting for higher susceptibility to perivenous steatosis. Secondly, variation between individuals is seen in both susceptibility to steatosis and its development across the sinusoid. Sensitivity analysis was used to identify the processes which have the largest effect on both total hepatic triglyceride levels and on the sinusoidal location of steatosis. Results confirm phenomena seen in vivo. Overall, this work involves multiscale and multilevel modelling, and systems engineering tools for their analysis.

Work in Dr Krishnan’s group focuses on information processing in cells and tissues using a combination of mathematical modelling across a range of scales and levels, theoretical and systems analysis, and collaboration with experimentalists. Recent work has focused on information processing in multisite phosphorylation, connecting the
enzymatic mechanism to the molecular information processing behaviour. This in turn plays an important role in signalling networks, where such enzymatic mechanisms are implicated. Another project in the area of mRNA translation combines experiments (in the group of Ian Stansfield) and modelling to develop a systems analysis for connecting ribosomal recycle, feedback, nonsense mediated decay and mRNA stability. A complementary approach in this area has been to develop new Probabilistic Boolean Network tools to facilitate analysis of these stochastic transport models. At the network level, recent work has focused on the effects of spatial regulation and compartmentalization in biochemical networks, an aspect of increasing importance in both systems and synthetic biology. Another project examines the effect of dynamic environments on the progression of the cell cycle in budding yeast. Using a multiplicity of models, as well as different experimental data, a number of underlying features of cell cycle progression in dynamically varying environments has been demonstrated. A platform for connecting the effects of the environment, the cell cycle and growth has also been created. Finally, at the cell and tissue levels the effects of different modes of intrinsic and induced drug resistance mechanisms in tumours at the cellular and tissue levels has been studied. This work clearly demonstrates the need to account for both cellular and tissue levels simultaneously, in a systematic manner in this context. Overall, the projects described above involve a combination of mathematical models (temporal, spatial, stochastic) and tools from nonlinear dynamical systems analysis, systems and control engineering and networks for analysis.

Taken together, the above research snapshots clearly demonstrate a number of features. Firstly, biological systems are complex in many ways and present a range of challenges at different scales. Secondly, systems engineering approaches are essential to tackle these challenges, and further different kinds of systems engineering tools are needed in different contexts. Thirdly, a combination of modelling, experiments and the deployment of appropriate systems engineering tools can prove to be very effective. Fourthly, new systems engineering approaches need to be developed in certain cases. Finally, systems engineering provides vital input in the life sciences in areas ranging from basic biology, biomedical engineering, biotechnology and synthetic biology. All these areas in turn provide new impetus for systems engineering itself.
Application Domain
Energy Systems Engineering

The importance of Energy Systems Engineering as an application domain within CPSE has increased over the last few years. Concerns over the cost and integrity of supply, coupled with the apparent inability to control greenhouse-gas emissions resulting from the increased use of fossil fuels, has amplified the need to focus not only on a less carbon-intense supply but the efficiency of energy generation and use together with strategies for carbon mitigation.

CPSE is engaged in a number of these areas of research including Urban Energy Systems, Bioenergy Systems, Hydrogen Networks and Polygeneration, Energy Storage, Carbon Capture and Storage, and Network Systems.

Urban Energy Systems
Cities use up approximately three-quarters of the world’s energy and play a major role in issues such as economic security and climate change. Work continues in the area of Urban Energy Systems, building on the £4 million, 5-year collaborative project with BP that investigated the technologies and systems used in cities to distribute and consume energy. Understanding these systems in more detail can provide valuable insights into how to make the distribution and consumption of energy more cost effective and sustainable in cities in the future. State of the art Urban Energy Systems Model (URBEN) is a comprehensive optimisation tool that enables urban planners, property developers and equipment manufacturers to determine the optimum mix of technologies in order to meet policy goals and cost constraints for both retrofit and new urban build projects. Research continues on new approaches to designing our urban energy infrastructure so that it is more efficient and has less impact on the environment. (Shah, Kierstead)

Molecular Energy Systems
Energy is a key area in which Molecular Systems Engineering approaches have been developed and applied to key problems. The general approach is to develop molecular equations of state for phase behaviour and thermodynamic properties and integrate these into process system design and optimisation approaches, using for instance gPROMS, for combined fluids/materials and process design. A good recent example of this involves an integrated molecular and process design of separation of carbon dioxide from natural gas (methane) for well-head applications. Here we have used our group contribution SAFT-γ Mie approach to design new solvents for CO₂/methane separation using a unified process/solvent optimisation of the process. Similar approaches are being applied to high-pressure amine solvent design for separation with membrane contactors. The other main line of work involves addressing climate-change mitigation issues: integrated solvent and process design of carbon dioxide capture from power station flue gas at low pressures. With a detailed SAFT description of the thermodynamics of the reactive dissolution equilibria we can successfully model the process by focusing on the mass transport with just a single transferable modulation of the diffusivity of carbon dioxide in the solvent. (Jackson, Adjiman, Galindo, Pantelides)

Energy Storage
We are modelling integrated energy systems for off-grid mining operations to identify the trade-offs between reliability of energy provision, due to the use of variable renewable energy generation such as solar and wind, with the cost of large scale energy storage. The system model includes the variable and stochastic behaviour of renewable energy. Storage technologies include compressed air, molten salts and pump-hydraulic systems with energy efficiency and losses. The approach includes the use of case studies of large scale mining operations with both heat and power demands in Chile and Canada. (Fraga)

Local Energy Systems
This area involves the design of neighbourhood-level energy systems, incorporating local distribution and sharing of both heat and power amongst dwellings. Local energy generation includes combined heat and power units, such as fuel cells using grid supplied gas, solar thermal, solar photo-voltaic and wind turbines. Energy storage in the form of hot water tanks is included. A key consideration is the regulatory framework to support energy integrated at this neighbourhood scale and the impact of such regulations on the systems design. (Fraga)

Nuclear Reprocessing
Recently research has started on looking at the design of nuclear reprocessing using intensified operations. Traditional technologies for separation are mixer-settlers; we are looking at micro-channels for intensified operations to reduce the volume of solvents required and improve the separation performance. (Fraga)
Multiscale Modelling of Integrated Energy Systems

There is a strong CPSE engagement (Mac Dowell, Shah, Maitland) within the CleanFAB (Clean Fossil and Bioenergy) Group, an interdisciplinary team of researchers studying how fossil fuels and bioenergy, in conjunction with CCS, will be key to enabling our stable, cost-effective transition to a low-carbon energy system. From engineering to economics, we are determined to make this adaptation as successful as possible. The work focuses on the multi-scale modelling of clean fossil and bioenergy as part of the diverse energy system of the 21st century. An example of the work we are carrying out in this space is the MESMERISE-CCS project wherein we are integrating energy system, electricity market, CCS-power plant, CO₂ transport and CO₂ storage models. This work is driven by the view that the role that thermal power plants will play in the energy system going forward will be distinct to that which they played historically. In particular, the concept of baseload or indeed mid-merit power plants will be a thing of the past– in order to be successful, thermal power plants will need to operate in a much more flexible fashion than in the 20th century. The objective of this work is therefore to understand how flexible the CCS chain needs to be, to identify the flexibility-limiting links in the CCS chain and to gain insight into the value of re-engineering these systems to provide enhanced flexibility to the energy system, thus enabling the integration of increased quantities of renewable power, hastening our transition to a low-carbon energy system. (Mac Dowell)

Carbon Storage

The Qatar Carbonates and Carbon Storage Research Centre (QCCSRC) is a 10 year, $70m research programme funded by Qatar Petroleum, Shell and Qatar Science and Technology Park. It is the largest industry-funded research programme at Imperial and aims to provide the underpinning science and engineering to enable the optimised design and operation of large-scale carbon dioxide storage operations in carbonate reservoirs typically found in Qatar and other parts of the Middle East.

The activity is a close collaboration between the Departments of Chemical Engineering and Earth Science and Engineering and involves the close interplay of experimental and theoretical/numerical modelling research. Molecular Systems Engineering and Multiscale Modelling within CPSE are a key part of this activity and the programme has enabled a unique partnership of modelling and experimental work, the one driving the other in terms of new insights and improved predictive capability.

The experimental work involves characterisation of the rocks, the properties of reservoir fluids mixed with supercritical CO₂ and the multiphase flow of such fluids in the porous and fractured carbonate rocks. Imaging using X-ray micro-tomography and modified body-scanners plays a major role in this. The modelling work comprises prediction of the thermophysical properties (phase behaviour, interfacial properties, transport properties) of the fluids involved under high temperature-pressure reservoir conditions. Molecular Systems Engineering plays a major role here, and new developments of the SAFT approaches, are transforming our ability to predict accurately the way complex fluid mixtures behave under such extreme conditions. These models feed into simulations of multiphase fluid flow in the storage rocks on a wide range of length-scales, from the pore scale (pore network models and Lattice Boltzmann) through core and metre block scales up to the kilometre distances of CO₂ plume development at the reservoir scale. Once robust reservoir models are developed, the challenge will be to use systems engineering approaches to aid in the design, optimisation, monitoring and control of these complex operations. (Maitland, Jackson, Galindo)
Application Domain
Environmental Systems Engineering

The application of system engineering techniques to environmental problems is relatively nascent within CPSE, but is a rapidly emerging area. The dynamics of the interactions, in both length- and time-scales, between human-natural systems are complex and nuanced, often involving multiple stakeholder groups. Thus the tools and techniques developed within CPSE are ideally poised to make a sizable contribution to this emerging area, in the context of process and systems optimisation and also in the provision of decision support tools to the industrial and policy-making communities.

Plant-wide Optimization of Full-Scale Wastewater Treatment Plants

Improving operational and process control strategies has become key for the sewage industry to reduce their energy consumption without compromising effluent quality. These strategies may be particularly useful for energy-intensive processes such as activated sludge aeration, which can account for 45-75% of a plant’s energy expenditure. Overall, it is estimated that energy consumption of most wastewater treatment plants (WWTPs) may be reduced by 10-40% this way. Nevertheless, WWTPs are comprised of a large number of treatment and separation units, which involve a great variety of processes acting on different time scales and interacting with each other via recycling loops. Failure to account for these interactions, e.g., by optimizing in a unit-wise manner, may not lead to the largest possible improvements and could even be detrimental from a plant-wide standpoint.

The group of Dr Chachuat is working on the development and application of a model-based methodology in order to provide a better understanding of the impacts of changing effluent quality targets on plant-wide energy use and fugitive emissions. Two industrial case studies corresponding to existing activated sludge plants (including sludge treatment), owned and operated by Sydney Water (Australia), were investigated. Plant-wide dynamic models were assembled and calibrated using historical data for both plants, paying special attention to closing the solids balances in the main treatment/separation units. A scenario-based optimization approach was used in an objective to determine the best possible performance with respect to a variety of economic and environment sustainability metrics. In turn, these results could feed into decisions revolving around treatment-plant operation and asset management as well as inform the next major plant license review. An inherent advantage of this methodology is that it can be used for analysing other ‘what-if’ scenarios or for assessing the performance of other WWTPs.

Figure 1: Comparison of various strategies for an optimal interplay between plantwide power consumption and NO₃ emissions in the treated effluent

Figure 2
Multi-Scale Modeling of Microalgae Culture for Optimization and Control
Andreas Nikolaou, Benoît Chachuat
Microalgae have long been identified as a promising candidate for biofuel production. These microorganisms have fast growth rates and a rich protein content, in addition to being able to produce and accumulate lipids under certain stress conditions. They are considered by many to be a viable alternative to conventional oil crops due to a higher biomass productivity and independence towards arable land and fresh water. Moreover, the downstream processing of microalgae in biorefineries opens the perspective for producing a wide spectrum of valuable products in addition to biofuel, including cosmetics, pharmaceuticals and nutraceuticals, while treating nutrient-rich effluents from wastewater treatment works or CO₂ from power-plant flue gas, all in the same process. Despite these promises, mass production of microalgae for large-scale biofuel production is yet to be demonstrated, especially in regards of their high nutrient requirements, the trade-off between biomass growth and lipid productivity, and the lipid extraction challenges.

The group of Dr Chachuat is working on the development of mathematical models capable of capturing the processes governing light-limited growth in microalgae. Particularly important in outdoor culture systems, where the light irradiance vary greatly, are the mechanisms of photoinhibition and photoacclimation, which act on a wide range of time-scales (from seconds to days).

Our recent focus is on integrating microalgae growth models at the cell level with CFD and light attenuation models describing the mixing conditions and the vertical light distribution in raceway ponds and other cultivation systems. These models provide a way of assessing various scale-up effects and how certain key parameters may affect microalgae productivity. The ultimate goal is to provide reliable predictions in large-scale production systems, as a means for optimizing their design and operation. This work is a collaboration with the University of Padova (Prof. Bezzo, Prof. Morosinotto) and BIOCORE-INRIA (Dr. Bernard).

Water and Energy Systems in Sustainable City Development – Resilience.IO platform
The grand challenges facing human societies are closely interconnected with the sustainable provisioning of energy, water and material resources, for growing and developing populations, and the subsequent processing and management of waste and pollution. Current urban water and energy systems are expanding increasing attention paid to their economic and environmental impacts. However, there is a lack of a sufficiently systematic approach to address these impacts and evaluate optimal strategies, either in the context of research or real-world decision making.

The group of Professor Nilay Shah took advantage of their strength in urban energy and transportation systems to expand the study to water, sanitation, and hygiene sector (WASH). The current regional demographics, land-use, infrastructure and economic information is used as input for the initial state of the focused urban system incorporating energy, water and other related resources.

Detailed spatio-temporal demand data, obtained by simulating a synthetic population using agent-based models, is further used to plan capacity utilization and expansion by supply-side matching on a cost optimal basis, eventually aiming to explore the optimal design and operational strategies for residential, commercial, industrial, and other sectors. Moreover, long-term socio-economic scenarios are addressed in the urban system development through a real-time feedback loop.

The team developed a prototype based on the Greater Accra Metropolitan Area (GAMA) city-region in Ghana, as part of the Department for International Development (DfID) funded Future Cities Africa (FCA) project. The outputs depict an overall resource landscape of the studied urban area, but also provide the material and energy balance of supply and demand from both macro and micro perspectives, which is used to propose environmentally friendly and cost effective sustainable city-development strategies. This work is to become a core component of the Resilience.io platform as an open-source, data-driven, integrated systematic tool gathering social, environmental and economic data to inform urban planning, investment and policy-making for city-regions globally.

Figure 3 (right and left plots): Velocity field in raceway pond (left plot) and simulated microalgae production over several weeks (right plot)
Figure 4: Example of simulated wastewater flow in GAMA (top plot) and optimized investment strategies for water and wastewater technologies (bottom plot)

Model Predictive Control of Post-Combustion CO₂ Capture Process integrated with a power plant

The process of CO₂ capture and storage is a potential way to control the emissions of CO₂ from large-scale power plants. A favoured CCS (Carbon Capture and Storage) strategy is the post-combustion CO₂ capture process using MEA. However, in a gas-fired power station, the power plant has to respond to dispatching signals from the transmission operator in order to provide load balancing. Frequent changes in operating point create significant disturbances to the CO₂ capture plant. Therefore, the integration of the CO₂ capture process and gas-fired power plants will increase the need to design advanced model-based control systems to overcome the process interactions and maintain dynamic operability of power plant and CCS unit. The dynamic behaviour of the capture plant was implemented in gCCS [1], a tool developed within gPROMS for the modelling of the capture plant units. In order to show how the proposed control scheme responds to a real operation during a day, fluctuation of the flue gas flowrate was implemented in the model. A Model Predictive Control (MPC) strategy was implemented in Matlab in order to maintain the dynamic operability of the CO₂ capture plant in the presence of changes in the load [2]. In order to implement the MPC control strategy, the detail dynamic model of the capture unit was approximated by a state-space model of five inputs and five outputs. A key advantage of the MPC control scheme is that it uses an optimisation framework which makes use of explicit process models to predict the future behaviour of the plant. The results demonstrated that the MPC control strategy can compensate for disturbances. Moreover, the work also studied flexibility scenarios involving changes to the set point for the carbon capture rate thus allowing an economic trade-off between use of steam (and the consequent increase in use of natural gas) versus decreased capture rate which could incur penalties for CO₂ emissions. The work was funded by EPSRC through grant EP/J020788/1 GasFACTS: Gas – Future Advanced Capture Technology Options.

Understanding Methane and Carbon Dioxide Emissions from the Natural Gas Supply Chain

When you compare natural gas to other fossil fuels such as coal, its combustion generates approximately half as much carbon dioxide (CO₂) emissions. However, natural gas is also mainly composed of methane, which is itself a strong greenhouse gas, and is emitted at different stages along the natural-gas supply chain. While methane dissipates from the atmosphere more quickly than CO₂, it is considered to have a higher global warming potential and therefore a more potent short-term effect on climate change than carbon dioxide.

The big question is: do these methane emissions along the supply chain undermine natural gas’s lower carbon credentials? Over the last five years, a large number of studies have estimated how much methane is emitted through the whole natural-gas supply chain from exploring, extracting, producing, processing and transporting natural gas. These studies have used a variety of methods to understand the issue, but so far have differed significantly in their findings.

Professor Nigel Brandon and Dr Adam Hawkes and colleagues at the Sustainable Gas Institute (SGI) have undertaken a comprehensive review of all the available global data on both CO₂ and methane emissions from the natural-gas supply chain to fully understand the scale of the issue. This briefing note summarises the main findings and recommendations of the Institute’s first White Paper. By systematically assessing the literature in terms of transparency, relevance and accuracy, the paper assembles and analyses the current state of our knowledge on emissions globally.

Key Questions

• How much methane and CO₂ is emitted from the natural gas supply chain?
• What methods are being used to estimate these emissions?
• What factors affect emission ranges?
• Why do we see such a big range?
This review analysed over 250 studies and reports. These studies covered natural gas from both conventional wells and unconventional wells at every stage in the supply chain, as well as examining the liquefied natural gas (LNG) process.

KEY FINDINGS:

1. The range of estimated emissions across the supply chain is vast.
   - Combined methane and CO₂ emissions from the supply chain are between 14 and 302 gCO₂eq/kWh.
   - A small number of studies estimate exceptionally high emissions from specific supply chain stages or facilities. However, the average estimates lie towards the lower end (see Figure 5).
   - Methane emissions are estimated to be between 0.2% and 10% of total produced methane.

2. Key emissions sources are during well completions, liquids unloading, and the use of pneumatic devices and compressors.
   - Studies show that the use of Reduced Emission Completions (RECs) equipment can significantly reduce methane emissions by over 75%. This technique is now compulsory in the United States.
   - Emissions from both unconventional and conventional wells are comparable as long as methane is captured rather than flared during well completion.
   - Gas venting and leakage from compressors and pneumatic devices across the supply chain contribute significantly to emissions.
   - More research is needed to quantify the factors affecting the emissions from the liquids unloading process.

3. There is evidence of ‘super emitter’ facilities all along the supply chain.
   - A small number of high-emitting facilities strongly impact the emissions profile at every stage in the production process.
   - These may be a result of the use of ineffective process equipment and poor operational and maintenance strategies, and could be eliminated and reduced if the best available techniques were applied.

4. Some of the emissions estimates are considerable, but there is potential to reduce these emissions.
   - If modern equipment with appropriate operation and maintenance regimes were to be used, the total supply chain emissions should lie within the range of 19–212 gCO₂eq/kWh with a central estimate of 92 gCO₂eq/kWh. If the natural gas was used in a power plant, these supply chain emissions would contribute between 4%–35% of the total greenhouse gas emissions per kWh of electricity generation.
   - Methane emissions are expected to be 0.3%–2.4% of total produced methane, with a central estimate of 1.4%.
   - Further reductions could be made, particularly for emissions from transport, storage and distribution, and also at the point when gas is extracted.

5. A wide variety of techniques are used to monitor emissions which means supply chain emissions estimates vary greatly in the literature.
   - Many studies apply a top-down approach to measuring methane emissions which involves measuring or inferring the concentration of methane in the atmosphere within a region, and then attributing emissions to specific sources within that region. A more thorough approach would involve a bottom-up point measurement at specific places on the ground in combination with local leak detection.
   - Methodological assumptions vary significantly across the literature and have a major effect on the estimated emissions (e.g., total production volume of a well and the assumed methane content of the extracted natural gas).

6. There is a significant lack of data, particularly for regions other than the US.
   - More data are required globally for offshore extraction, coal-bed methane extraction, liquids unloading, well completions with RECs, transmission and distribution pipelines, and methane emission measurement from all LNG stages.

7. Further research is needed to determine the potential role of natural gas in a low-carbon energy mix.
   - Research exploring the technological, operational or regulatory mechanisms is required to achieve emission reductions.
   - Further studies are also necessary to quantify the potential reduction in supply-chain emissions and to examine factors affecting different supply-chain emissions in order to understand the mitigation potential at each stage and also to look at the impact of regional regulation (e.g., regulation for continuous monitoring of ‘super-emitting’ facilities).

References
Application Domain
Supply Chains of the Future

Supply chains of the future will have to deal with a host of new challenges facing us in the 21st century, including:

• Exploiting new energy and material sources
• Cleaner exploitation of existing sources (e.g. high-carbon fossil fuels)
• Resource efficiency to deal with increasing scarcity of non-fuel resources (e.g. water and minerals)
• Decarbonised supply chains
• Customisation of products and services (e.g. healthcare) closer to the point of use.

A key feature of supply-chain optimisation is the need to include multiple objective functions when considering the design or operation of a supply chain. These may reflect for example economics, sustainability and responsiveness metrics. An example of an industrial case study which employs multi-objective optimisation is discussed below.

Incorporating sustainability measures in supply chains
Sustainability plays a key role in the management of a successful and responsible business. When trying to improve the sustainability performance of a business, there are three major challenges that need to be addressed. First, assessment of sustainability requires consideration of not just economic, but also environmental and social impacts. Second, we need to find appropriate sustainability indicators and gather the necessary data in order to quantify sustainability performance. Finally, sustainability has to be seen in the context of the whole system, i.e., it has to include all activities along the supply chain. In this work, we consider all three aspects and propose a multi-objective optimisation framework for the optimisation of a sustainable supply chain.

Three sustainability indicators have been considered, namely the total cost (reflecting economics), GHG emissions (reflecting sustainability) and lead time (reflecting responsiveness). We apply this framework to an industrial test case using real-world data drawn from an industrial collaborator. The results show clear trade-offs between the three different objectives. However, we can also observe that typically a considerable decrease in GHG emissions or lead time can already be achieved with only a relatively small increase in cost. The proposed framework enables us to determine such trade-off relations and consequently make decisions that improve the sustainability performance of the supply chain.

Case study and results
A case study explored the allocation of production of multiple products to seven plants around the world, and their subsequent distribution to markets, using the supply chain structure as below:

A trade-off curve between the three objectives was developed by the use of classical multi-objective optimisation procedures. The overall trade-offs between the objectives can be seen below:

It can be seen that GHG emissions can be reduced considerably without a significant cost increase initially, but then they are very hard to reduce. Shorter lead times can only be achieved by compromising both emissions and cost.
“CPSE academics are expected to span several disciplines including systems modelling, optimisation and control and computing.”
Nilay Shah FREng

Professor of Process Systems Engineering, Director CPSE, Department of Chemical Engineering, Imperial College London

Qualifications
MEng in Chemical Engineering (Imperial College London)
PhD in Chemical Engineering (Imperial College London)

Awards and Distinctions
Fellow of the Royal Academy of Engineering
Fellow of the IChemE
RAEng MacRobert Award and Prize (2007)
RSC/SCI/IOM Bailey Medal (2005)
ICI/RAEng Fellowship (1997-2002)
Imperial College Faculty of Engineering Teaching Award (2009)
IChemE Hutchison Medal (2012)

Research Interests
Design and analysis of energy and process systems:
- Bioenergy/Biorenewable systems and technologies.
- Modelling and optimisation of low-carbon technologies and systems (e.g., CCS, hydrogen infrastructure etc).

Supply-chain design and optimisation:
- Development of new algorithms for large-scale supply-chain models.
- Application to sector-specific processes (e.g., pharmaceuticals, oil and gas, consumer goods)

Process synthesis and development for fine chemicals, pharmaceutical and biochemical processes:
- Combination of chemistry with modelling and engineering to improve process designs and to speed up process development.
- Performing rapid economic assessments for different manufacturing routes.
- Developing long-term capacity and investment plans.

Safety in design and operation, especially the application of formal mathematical techniques to assess and improve process safety

Other Activities
Co-founder of Process Systems Enterprise Ltd
EPSRC college member
EPSRC Manufacturing Strategy Advisory Team
BBSRC Industrial Biotechnology and Bioenergy Strategic Advisory Team
IChemE Transactions editorial board member Director, Imperial College Manufacturing Futures Lab

Reviewer for
AIChE Journal
Chemical Engineering Research and Design
Computers and Chemical Engineering
Chemical Engineering Science
A-Star Research Council (Singapore)
Science Foundation Ireland

Academic Collaborations
University College London, Department of Chemical Engineering
Newcastle and Strathclyde Universities, CPACT
National University of Singapore
Delft University of Technology
Rothamsted Research
IBERS – University of Aberystwyth
University of York
Aston University
Newcastle University
Cardiff University
Industrial Collaborations
Shell (Energy Efficient Refining)
Syngenta (Supply Chain Optimisation)
Sainsbury’s (Store of the Future)
Unilever (Sustainable Supply Chains Design)
Energy Technologies Institute (Bioenergy Value Chains)
Biosep (Biomass Fractionation)
Petronas (Novel Gas Separation Technologies)

Publications
Journal Articles (A * indicates open-access publication)


Conference Papers


3. Pantaleo AM, Ciliberti P, Camporeale S, Shah N, 2015, Thermo-economic assessment of small scale biomass CHP: steam turbines vs ORC in different energy demand segments, 7th International Conference on Applied Energy (ICAЕ), Publisher: ELSEVIER SCIENCE BV, Pages: 1609-1617, ISSN: 1876-6102


5. Elahi N, Shah N, Korre A, Durucan S., 2014, Multi-period least cost optimisation model of an integrated carbon dioxide capture transportation and storage infrastructure in the UK, 12th International Conference on Greenhouse Gas Control Technologies (GHGT), Publisher: ELSEVIER SCIENCE BV, Pages: 2655-2662, ISSN: 1876-6102


7. Mac Dowell N, Shah N, 2014, Optimisation of post-combustion CO2 capture for flexible operation, 12th International Conference on Greenhouse Gas Control Technologies (GHGT), Publisher: ELSEVIER SCIENCE BV, Pages: 1525-1535, ISSN: 1876-6102

Claire S. Adjiman FREng
Professor of Chemical Engineering, Department of Chemical Engineering, Imperial College London

Qualifications
MEng in Chemical Engineering, Imperial College London
PhD in Chemical Engineering, Princeton University

Awards and Distinctions
Fellow of the Royal Academy of Engineering
Fellow of the Institution of Chemical Engineers
Chartered Engineer
EPSRC Leadership Fellowship, 2012-2017
Philip Leverhulme Prize for Engineering, 2009
Research Excellence Award for Molecular Systems Engineering team, Imperial College, 2009
Rector’s Excellence Award, Imperial College, 2007
Royal Academy of Engineering ICI Fellowship, 1998-2003
Porter Ogden Jacobus Honorary Fellowship, Princeton University, 1997

Secondments

Research Interests
Systematic methodologies for integrated molecular and process design for reactive processes: development of modelling and optimisation tools and applications (e.g., solvent design for reactions or CO2 capture, risk management). Model-based assessment of design of energy-conversion systems including solid-oxide fuel cells. Development of property-prediction techniques integrating different scales of modelling (from quantum mechanics to advanced equations of state). Global analysis techniques, such as global optimisation and safety analysis

Other Activities
Associate Editor, Chemical Engineering Science
Associate Editor, Journal of Global Optimization
Editorial Board, Fluid Phase Equilibria
AIChE: Technical area co-chair/chair for CAST10a, 2006-2008
IChemE: Committee Member, Computer-Aided
Process Engineering Group
EPSRC: Member of Peer Review College
Co-chair, Foundations of Molecular Modeling and Simulations 2015 (FOMMS 2015), Oregon

Reviewer for

Academic Collaborations
Argonne National Laboratory, UCL, University of Manchester, University of Edinburgh, University of Cardiff, University of Paderborn, University of Pannonia, ETH Zürich, National Technical University of Athens, Centre for Research and Technology-Hellas, University of Notre-Dame.

Industrial Collaborations
BP, CaO Hellas, Dynamic Extraction, Julius Montz, Novartis, Pfizer, Process Design Center, Procter & Gamble, Process Systems Enterprise, Public Power Corporation, Scottish Power, Syngenta

Publications
Journal Articles
6. Papaioannou V, Calado F, Laffitte T, Dufal S, Sadeqzadeh M, Jackson G, Adjiman CS, Galindo A, 2015, Application of the SAFT-γ Mie group contribution equation of state to fluids of relevance to the oil and gas industry, Fluid Phase Equilibria, ISSN: 0378-3812
I David L. Bogle CEng FREng FIChemE

Professor of Chemical Engineering, Department of Chemical Engineering, University College London

Qualifications
PhD in Chemical Engineering (Imperial College London)
MSc in Chemical Engineering (Imperial College London)
DIC in Engineering (Imperial College London)
BEng with honours in Chemical Engineering (Imperial College London)

Awards and Distinctions
Fellow of the Royal Academy of Engineering (2005)
Fellow of Institution of Chemical Engineers (1997)
IChemE Council Medal (2005)

Research Interests
Numerical global optimisation techniques for process design.
Controllability analysis of nonlinear systems. Process modelling of pressure swing adsorption and desalination units. Systems Biology and Systems Medicine with particular focus on liver physiology and protein networks in cancer.

Other Activities
Pro-Vice-Provost, Head of the UCL Doctoral School
Member of College of Engineering for the Engineering & Physical Sciences Research Council (EPSRC)
Vice Chair of BBSRC Multidisciplinary Synthetic Biology Research Centres panel (2014)
Vice Chair of EPSRC Engineering Fellowships for Growth – Synthetic Biology panel (2014)
Committee member of Computer Aided Process Engineering Subject Group of Institution of Chemical Engineers
Member of European Federation of Chemical Engineers Working Party on Computer Aided Process Engineering (UK representative)
Member of International Federation of Automatic Control (IFAC) Technical Committee on Control of Environmental Systems
Member of Royal Academy International Committee
Chair Royal Academy of Engineering Distinguished Visiting Fellowship Scheme
Chair Royal Academy of Engineering Industry Academic Partnerships Programme Steering Group (from 2016)
Chair League of European Research Universities Doctoral Studies Community
UK representative on European Research Area Steering Group on Human Resources and Mobility Working Group on Doctoral Education
Advisory Board of University of Zurich Graduate Campus
Advisory Board AICES (Aachen Institute for Computational Engineering Science) RWTH Aachen

Reviewer for

Academic Collaborations
UCL Chemical Engineering, Centre for Mathematics and Physics in the Life Sciences and Experimental Biology (UCL), UCL Hepatology, UCL Cancer Institute, University of Palermo.

Industrial Collaborations
PricewaterhouseCoopers
Nigel Brandon OBE FREng
Director of the Sustainable Gas Institute (SGI), Department of Earth Science & Engineering, Imperial College London

Qualifications
PhD in Electrochemical Engineering (Imperial College London)
BSc (Eng) in Minerals Technology (Imperial College London)

Awards and Distinctions
2014 Francis Bacon Medal, American Society of Mechanical Engineers
2014 RISE (Recognising Inspirational Scientists and Engineers) Fellow
2014 Co-Director, Energy SuperStore
2014 Director Sustainable Gas Institute
2013 Member of Council, Royal Academy of Engineering
2012 Director Hydrogen and Fuel Cells Supergen Hub
2012 Director Energy Storage Research Network
2012 BRE Fellow
2012 Visiting Professor, Energy Research Institute, NTU Singapore
2011 Baker Medal, Institute of Civil Engineering
2011 OBE for services to UK-China science
2008 Fellow of the Royal Academy of Engineering
2008 Fellow of the City and Guilds of London Institute
2007 Royal Academy of Engineering Silver Medal
2006 Chartered Engineer
2006 Fellow of the Institute of Materials, Minerals and Mining
2006 Fellow of the Energy Institute
2006 Inaugural Energy Senior Research Fellow to the Research Councils Energy Programme

Publications
Journal Articles

Research Interests
Professor Brandon’s research is focused on electrochemical power sources for fuel cell and energy storage applications. He collaborates extensively with industry in this field, as well with other research centres and universities around the world, and he is Director of the RC Energy programme funded Hydrogen and Fuel Cells SUPERGEN Hub (www.h2fcsupergen.com). He was the founding Director of the Energy Futures Lab at Imperial College (www.imperial.ac.uk/energyfutureslab), and a founder of Ceres Power (www.cerespower.com), an AIM listed fuel cell company spun out from Imperial College. In 2014 he was appointed to the BG Chair in Sustainable Gas and as Director of the Sustainable Gas Institute at Imperial College.

Publications
Journal Articles


11. Ruiz-Trejo E, Zhou Y, Brandon NP, 2015, On the manufacture of silver-BaCe0.5Zr0.5O3-δ electrodes for hydrogen separation membranes, INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, Vol: 40, Pages: 4146-4153, ISSN: 0360-3199


26. Kishimoto M, Lomberg M, Ruiz-Trejo E, Brandon NP, 2014, Enhanced triple-phase boundary density in infiltrated electrodes for solid oxide fuel cells demonstrated by high-
resolution tomography, JOURNAL OF POWER SOURCES, Vol: 266, Pages: 291-295, ISSN: 0378-7753


Conference Papers


5. Maskell WC, Brett DJL, Brandon NP, 2014, Thick-film amperometric zirconia oxygen sensors: influence of cobalt oxide as a sintering aid, Publisher: IOP PUBLISHING LTD, ISSN: 0957-0233


Invited Lectures


3. Electrochemistry in energy applications: policy drivers, commercial opportunities and research challenges, Conference plenary lecture, ECS conference on electrochemical energy conversion and storage, Glasgow, 26th to 31st July 2015.

4. Visualisation and quantification of microstructural change in battery electrodes, Invited lecture, ECS conference on electrochemical energy conversion and storage, Glasgow, 26th to 31st July 2015.


8. Making Gas Greener, Invited lecture, Flame, Amsterdam, 14th April 2015.


13. The role and value of fuel cells and energy storage in low carbon energy systems, Zandmer Distinguished lecture, University of Calgary, Canada, 19th November 2014.
17. Solid Oxide Fuel Cells – from concept to commercialisation, Francis Bacon Medal award lecture, 12th ASME Fuel Cell Science, Engineering and Technology Conference, Boston, USA, June 30th to July 2nd 2014.

Benoît Chachuat

Reader in Process Systems Engineering, Department of Chemical Engineering, Imperial College London

Qualifications
MEng in Environmental Engineering (1998, with Distinction – ENGEES, Strasbourg, France)
MSc in Engineering Science (1998, with Distinction – Universite Louis Pasteur, Strasbourg, France)
PhD in Chemical Engineering (2001, with Distinction – INPL, Nancy, France)

Awards and Distinctions (Selection)
Certificate of Excellence in Reviewing, Computers & Chemical Engineering, 2013
CAST Outstanding Young Researcher Award, AIChE, 2014
CAST Directors Award, AIChE, 2015

Research Interests
1. Environmental systems engineering: design and operation of wastewater treatment and recovery plants; multiscale modeling, design and operation of microalgae culture systems.
2. Integrated membrane processes: OSN membrane cascades for separation of organic mixtures; modeling and optimization of membrane contactors; water network synthesis with membrane regenerators.
3. Analysis of uncertainty propagation in dynamic systems optimization-based control and real-time optimization of dynamic systems.
4. Complete search methods and tools for global optimization and constraint satisfaction.

Other Activities (Selection)
Program Coordinator (Elect.), Area 10D (Applied Mathematics and Numerical Analysis), AIChE Computing & Systems Technology (CAST) division, 2015-2016
Member of International Programming Committee, 9th IFAC Symposium on Advanced Control of Chemical Processes (ADCHEM), June 2015
UK Representative of IFAC Technical Committee on Chemical
Process Control, since March 2015
Visiting Scientist, Department of Industrial Engineering, University of Padova, Italy (June 2014)
Invited Professor, Automatic Control Laboratory, EPFL (August-September 2015)

Plenary and Keynote Lectures
9th IFAC Internation Symposium on Advanced Control of Chemical Processes (ADCHEM), Plenary address, June 2015
AIChE Annual Meeting, CAST Division Plenary, November 2014

Editorial and Peer-Review Activities
Associate Editor, Journal of Process Control (Elsevier)
Associate Editor, Journal of Optimization Theory & Applications (Springer)
Guest Editor, Optimal Control Applications & Methods (Wiley), special issue on Global and Robust Optimization of Dynamic systems

Academic Collaborations
EPFL, Switzerland, Automatic Control Lab (Prof. Bonvin)
INRIA Sophia Antipolis, France, BIOCORE Group (Dr. Bernard)
INRA, France, LBE Narbonne (Dr. Steyer)
MIT, Dpt Chemical Engineering (Prof. Barton)
RWTH Aschen, Dpt Mechanical Engineering (Prof. Mitsos)
STU Bratislava, Slovakia, Dpt Chemical Engineering (Prof. Fikar)
University of Padova, Dpt Industrial Engineering (Prof. Bezzo), Dpt Biology (Prof. Morosinotto)

Industrial Collaborations
Petronas, Praxair, Sydney Water, Syngenta

Publications

Journal Articles

Peer Reviewed International Conference Papers
Marc Deisenroth

Lecturer in Statistical Machine Learning, Department of Computing, Imperial College London

Qualifications
PhD in Computer Science (Karlsruhe Institute of Technology)

Awards and Distinctions
Best Cognitive Robotics Paper Award at ICRA 2014

Research Interests
Machine Learning, Robotics, Optimization

Other Activities
Area Chair at NIPS 2015

Reviewer for
JMLR, ICRA, RLDM, Cambridge University Press, AISTATS

Academic Collaborations
MIT, TU Darmstadt, AIMS Senegal, Uppsala University

Book Chapters
Roberto Calandra, Nakul Gopalakrishnan, Marie Seyfarth, Jan Peters, Marc P. Deisenroth. Bayesian Gait Optimization for Bipedal Locomotion, volume 8426 (Lecture Notes in Computer Science), pp.274–290, 2014

Publications

Journal Articles

Conference Contributions

Invited Lectures and Seminars 2015 (Talks/Seminars)
University of Edinburgh
ETH Zurich
University of Washington
Sloan Summit at London Business School (Keynote)
International Conference on Machine Learning (Contributed Talk)
Workshop on Autonomous Citizens (Keynote)
AI Society, Queen Mary University London
Robotics Society, Imperial College London
NIPS Workshop on Bayesian Optimization (Contributed Talk)
Tesco
2015 (Tutorials)
Machine Learning Summer School (Chalmers University)
Gaussian Process Winter School (University of Sheffield)

2014 (Talks/Seminars)
Microsoft Research
University of Sheffield
TU Darmstadt
University of Hertfordshire
University College London
Georgia Institute of Technology
International Conference on Artificial Intelligence and Statistics (Contributed Talk)
International Conference on Robotics and Automation (Contributed Talk)
Chalmers University
University of Oxford
British Petroleum
Workshop on Policy Learning at International Conference on Humanoid Robotics (Invited Talk)

Peter DiMaggio
Senior Lecturer, Department of Chemical Engineering, Imperial College London

Qualifications
BSc in Chemical Engineering
PhD in Chemical Engineering

Awards and Distinctions
Ruth L. Kirschstein National Research Service Award: NIH
Postdoctoral Research Fellowship, Princeton U., 2010-2012
Porter Ogden Jacobus Honorary Fellowship, Princeton U., 2008-09
Kristine M. Layn Award for Outstanding Achievement in Research, Princeton U., 2007

Research Interests
Holistic integration of proteomics and genomics data to understand the epigenetic basis of disease regulation Combinatorial optimisation and multivariate statistical tools for the interpretation and integration of large-scale omics datasets.

Reviewer for

Academic Collaborations
MRC Clinical Sciences Centre (London), Hammersmith Hospital (London), Institut Pasteur, The Francis Crick Institute, The University of Edinburgh, Howard Hughes Medical Institute, University of Rhode Island.

Industrial Collaborations
GSK
AstraZeneca

Publications
Journal Articles

Invited Lectures and Seminars
1. ELRIG Drug Discovery Meeting, September 2015, Telford UK.
2. Wellcome Trust Epigenomics of Common Diseases, November 2015, Wellcome Trust Genome Campus, Cambridge, UK.
Vivek Dua

Senior Lecturer and Departmental Tutor, Department of Chemical Engineering, UCL

Qualifications
PhD in Chemical Engineering, Imperial College London
MTech in Chemical Engineering, Indian Institute of Technology, Kanpur
BE (Honours) in Chemical Engineering, Panjab University, Chandigarh

Research Interests
Model Reduction, Parameter Estimation, Mixed-Integer Optimisation, Refinery-wide optimization, Solvent Extraction based Water Desalination, Synthetic Biology, Cystic Fibrosis

Other Activities
Member Synthetic Biology Network
Co-editor of Process Systems Engineering book series

Reviewer for

Publications

Journal Articles

Conference Contributions

Eric S Fraga

Professor of Process Systems Engineering, Department of Chemical Engineering, University College London

Qualifications
BSc in Applied Mathematics (University of Alberta)
MSc in Computer Science (University of Alberta)
PhD in Computer Science (University of Waterloo)

Research Interests
Professor Fraga’s interests lie at the interfaces between engineering, mathematics and computer science. He is specifically interested in the design of novel computer algorithms and mathematical
techniques and their application to problems in process engineering. In the past, his research has concentrated on the development of methods for automated process design, or process synthesis, with the development of tools for the design of profitable, safe, environmentally benign chemical plants. These tools, including most prominently the Jacaranda system, use a variety of optimization methods and specially targeted visualization and interaction procedures to provide a system which is both powerful and easy to use.

Other activities
EPSRC: Member of Peer Review College
Member of the International Editorial Board for the Journal of Industrial Biotechnology and Biorefineries
The Information Technology and Control journal
The Journal of Optimization
Revista Scientia Alimentaria
Member of Programme Committee for META’2016

Reviewer for
A number of journals and funding agencies, covering the interfaces between computer science, mathematics and engineering.

Academic Collaborations
Universitat d’Alacant, Spain; University of Edinburgh, UK; University of Essex, UK; University of Leeds, UK.

Publications
Journal Articles

Conference Contributions
Amparo Galindo
Professor of Physical Chemistry, Department of Chemical Engineering, Imperial College London

Qualifications
PhD in Physical Chemistry, University of Sheffield
BSc Chemistry, Universidad Complutense de Madrid (Spain)

Awards and Distinctions
Imperial College Research Excellence Award as part of the Molecular Systems Engineering Team for high academic achievement and significant future potential (2009)
Imperial College Award for Excellence in Research Supervision for exemplary activity in inspiring and supporting research students (2007)
Imperial College Award for Excellence in Teaching for outstanding contribution to undergraduate teaching (2007)
ExxonMobil Teaching Fellow (2005-2009), ExxonMobil – Royal Academy of Engineering, 2005

Research Interests
My research interests are two-fold: the development of statistical mechanical approaches for complex systems, and their application to processes relevant to industry. The tools of statistical mechanics and computer simulations offer a privileged molecular perspective of increasingly complex systems. My interest in this field is to develop fundamental approaches to contribute to the understanding of experimental systems, with a special focus on chemical processes. The goal is to be able to predict bulk properties of complex systems. We are currently concentrating on the advancement of group contribution methodologies targeting specifically solubility prediction of organic molecules (usually active pharmaceutical ingredients) and their use for the development of coarse grained force fields for use in molecular dynamics simulations. Increasingly the use of quantum mechanics and statistical mechanics to predict reaction rate constants and guide solvent design is a major interest. The impact and exposure of this work is maximised through collaborative efforts in which the aim is to promote the transfer of the theoretical developments into tools for the design and synthesis of chemical processes and products.

Other activities
Member of the Royal Society of Chemistry (RSC)
Member of the peer review college of the Engineering and Physical Sciences Research Council (EPSRC)
Member of the International Scientific Advisory Committee of the European Symposium on Applied Thermodynamics (ESAT)

Editorial Activity
Journal of Chemical Engineering Data Editorial Advisory Board
Molecular Physics Editorial Advisory Board

Industrial Collaborations
P&G, Petronas, Pfizer, PSE Ltd., Qatar Petroleum, Shell, Syngenta.

Publications
Journal Articles


Conference contributions


Federico Galvanin

Lecturer, Department of Chemical Engineering, University College London

Qualifications

BSc in Chemical Engineering, University of Padova
PhD in Chemical Engineering, University of Padova

Awards and Distinctions


Research Interests

Dr Galvanin’s research interests lie at the interface between mathematical modelling and experimentation. The research activity is particularly focused on the use of advanced computational tools for the development of predictive models for the characterisation of complex systems in both chemistry and physiology. He has a specific expertise in the following areas:

- Design of Experiments (DoE) and statistical planning
- Model-based Design of Experiments (MBDoE) for model identification
- Kinetic modelling, chemical reactor modelling
- Pharmacokinetics/pharmacodynamics modeling
• Modeling of physiological systems
• Parameter Estimation

The current research activity is primarily focused on the optimal design of experiments for i) the identification of kinetic models in flow reactors; ii) the development of pharmacokinetic models for the detailed study of physiological systems (diabetes and rare coagulation diseases).

Teaching Interests
Teaching activities are in the areas of process design and simulation of chemical processes. Below are the modules he is currently teaching:
• CENGM01P/CENGG01P Process Systems Modelling and Design
• CENG207P Process Design Principles

He is the Deputy Departmental Admissions Tutor at UCL Chemical Engineering.

Reviewer for

Academic Collaborations
University of Padova on the project: “Optimal design of experiments for the identification of physiological models of Von Willebrand Disease” Cardiff Catalysis Institute, Liverpool University, UCL Chemical Engineering (Catalysis Hub) on the project: “Merging information from batch and continuous flow experiments for the identification of kinetic models of benzyl alcohol oxidation”

Industrial Collaborations
Collaboration with Syngenta (Bracknell, UK) on the MSc project: “Bringing plant potential to life through optimisation of traveling traders’ exchanges”.

Publications
Journal Articles

Gonzalo Guillén Gosálbez
Reader in Process Systems Engineering, Department of Chemical Engineering, Imperial College London

Qualifications
MEng in Chemical Engineering (Top Student Award, Universidad de Murcia, Murcia, Spain)
PhD in Process Systems Engineering (Top Student Award, UPC, Barcelona, Spain)

Awards and Distinctions
Outstanding Young Investigator Award “Juan López de Peñalver” (Spanish Royal Academy of Engineering), Oct-2012
Erasmus Staff Mobility for Training (ETH Zürich), June-2012

doi:10.1016/j.foodeng.2013.07.027
Fulbright Postdoctoral Fellowship (Carnegie Mellon University), Oct-2006
Top Doctoral Student Award (UPC), Dec-2005
FPU Pre-doctoral Scholarship (Spanish Ministry of Education and Science-UPC), Jan-2002-Jan-2006
Top Student Award in Chemical Engineering (Spanish Ministry of Education-UMU), Jun-2001

Research Interests
Dr. Guillén-Gosálbez’s research interests lie at the interface of engineering, environmental sciences and computer aided systems design. Areas of particular interest include: Sustainable engineering, Multi-objective optimisation of sustainable processes, Life cycle assessment, Eco-efficiency assessment and optimisation, Stochastic programming and multi-criteria decision-making under uncertainty.

Reviewer for
Member of the Editorial Board of The Scientific World Journal.

Referee for a number of journals

Referee for international funding bodies
Spanish Ministry of Science and Innovation (Spain); CONICET (Argentina); Fonds National de la Recherche (Luxembourg); National Agency for the Evaluation of Universities and Research Institutes (ANVUR) (Italy); Qatar National Research Fund (Qatar).

Academic Collaborations (leading to joint publications)
ETH Zürich (Switzerland): Prof. Stefanie Hellweg, Life Cycle Assessment.
Polytechnic University of Catalonia (Barcelona, Spain): Prof. Christian Blum, Hybrid Meta-heuristics.
The University of Manchester (UK): Prof. Adisa Azapagic, Sustainable Industrial Systems.
Universidad de Alicante (Alicante, Spain): Prof. José Caballero, Simulation-Optimisation for Process Synthesis.
Universidad de Santander (Santander, Spain): Prof. Ángel Ibrahim, Design of Energy Systems.
Universidad Michoacana de San Nicolás de Hidalgo (Mexico): Prof. Ponce-Ortega, Sustainable Supply Chains.
Universidad Nacional de Tucumán (San Miguel de Tucumán, Argentina): Prof. Fernando Daniel Mele, Biofuels Supply Chains.
Universitat de Lleida (Spain): Prof. Albert Sorribas, Systems Biology.

Industrial Collaborations
Messer Ibérica de Gases; REPSOL; ExxonMobil Research and Engineering Company.

Publications
Book Chapters

Journal Articles (“*“ stands for corresponding author)


Conference Contributions


Invited Lectures and Seminars

1. Benchmark analysis of a top British University in Chemical Engineering, Universitat Rovira i Virgili (Tarragona, Spain), January 2015.

2. Multi-objective optimisation coupled with life cycle assessment for the development of sustainable processes, Luxembourg Institute of Science and Technology (LIST) (Luxembourg City, Luxembourg), January 2015.
3. Systematic tools based on mathematical programming for the life cycle optimisation of sustainable processes, BASF (Ludwigshafen, Germany), June 2015. Systematic optimisation tools applied to sustainable engineering, Joint Research Centre in Ispra (Ispra, Italy), May 2015.
4. Teaching Design Project at The University of Manchester (Reading, UK), December 2014.
5. Systematic multi-criteria decision-making tools for the design and planning of more sustainable processes, Northwestern University (Evanston, US), May 2014.

Adam Hawkes

Senior Lecturer in Energy Systems, Department of Chemical Engineering, Imperial College London

Qualifications
PhD in Energy Systems Modelling
B.Eng (Hons)

Awards and Distinctions
Baker Medal, Institution of Civil Engineers, 2011

Research Interests
Adam’s areas of research interest fall into five categories:
1. Economy-wide energy systems modelling
2. Technologies and pathways for low-carbon heat
3. Design and operation of microgrids and more integrated/coordinated energy systems
4. Fuel cells, polygeneration, and other cutting-edge energy conversion technologies
5. Residential energy supply and demand, with a focus on microgeneration

In the field of energy systems modelling, Adam’s research seeks to bridge the gap between siloed energy technology assessment and the role of those technologies in integrated energy systems. Multi-scale modelling is applied to reflect the critical design and operational parameters of energy technologies and infrastructures into the energy system as a whole, providing engineers and policy makers with insight into the value of particular technology characteristics, and aiding prioritisation of technology R&D.

Other Activities
Member, European Council for an Energy Efficient Economy (ECEEE), 2013–2015

Member, Energy Institute
Chartered Engineer, Engineering Council UK

Reviewer for

Academic Collaborations
Collaborator, IEA ECBCS Annex 54 on Residential Microgeneration
Collaborator, IEA Annex 42 on Residential Cogeneration
Researcher, UKERC Microgeneration Theme

Industrial Collaborations
Ceres Power Ltd, Techno Economic Modelling of Solid Oxide Fuel Cells
EDF, Techno Economic Modelling of Micro-CHP Systems

Publications
Reports

Journal Articles

Conference Contributions
George Jackson

Professor of Chemical Physics, Department of Chemical Engineering, Imperial College London

Qualifications
DPhil in Physical Chemistry, Exeter College, University of Oxford
BSc Chemistry, Chelsea College, University of London

Awards and Distinctions
Guggenheim Medal for Excellence in Thermodynamics, Institution of Chemical Engineers (IChemE, 2015)
Fellow of the Mexican Academy of Molecular Engineering (2001)
Fellow of the Royal Society of Chemistry (FRSC), Chartered Chemist (CChem, 1995)

Research Interests
A molecular description of matter is the key to understanding and predicting the properties of dense fluids and materials. The latest developments in statistical-mechanical theories and computer simulation (Monte Carlo and molecular dynamics) are used by my group to provide a reliable predictive platform for complex fluids and ordered materials at the molecular level. The focus is on the phase equilibria of systems which are of industrial relevance, e.g., mixtures containing hydrogen fluoride (production of refrigerants), aqueous solutions of surfactants (enhanced oil recovery), and hydrogen-bonded liquid crystals (optical devices).

One of our main achievements has been the development of a highly accurate equation of state for the thermodynamic properties of complex fluid mixtures: the statistical associating fluid theory for potentials of variable range SAFT-VR. We are currently embarking on extensions of the formalism to polymers, electrolytes, and inhomogeneous systems. A recent advance is the formation of the Molecular Systems Engineering (MSE) Group in which we are incorporating advanced thermodynamics modelling in process design and optimisation.

In the area of liquid-crystal modelling, the aim is a fundamental understanding of the effect of association, polar interactions and molecular flexibility on the stability of liquid-crystalline phases (nematic, biaxial, smectic, etc.). We are currently simulating molecules which incorporate molecular flexibility and dipolar interactions as well as chiral centres.

Other Activities
1. 1991-1996, Member of the Executive Committee of the Statistical Mechanics and Thermodynamics Group (SMTG) of the Faraday Division of the Royal Society of Chemistry
2. 1992-1998, Founder member of the Centre for Molecular Materials, Sheffield University
3. 1993-1996, Member of the Executive Committee of the Collaborative Computational Project 5 (CCP5)
4. 1994-1998, Editor of Molecular Physics
5. 1995-date, Fellow of the Royal Society of Chemistry, Chartered Chemist (FRSC, CChem)
6. 1997-2000, Member of Chemistry Programme (Structure and Bonding College) of the EPSRC
7. 1998-2013, Member of Executive Committee and Special Issue Editor of Molecular Physics
8. 1998-2002, Member of Editorial Board of Molecular Simulation
9. 2000-date, Member of Editorial Board of Fluid Phase Equilibria
10. 2000-2007, Member of Peer Review College of the EPSRC
11. 2001-date, Fellow of the Mexican Academy of Molecular Engineering
12. 2003-date, Member of the Centre for Process Systems Engineering
14. 2006-2011, Council Member of the Faraday Division of the Royal Society of Chemistry
15. 2006-2011, Member of the Faraday Standing Committee on Conferences
16. 2006-2013, Member of Management Committee of the Liquids and Complex Fluids Group of the Institute of Physics
17. 2007-2008, Member of Appointments Committee of the Department of Physics, University of Bergen, Norway
18. 2007-date, External Examiner, Physical Chemistry, Univ. of West Indies (Barbados, Jamaica, Trinidad and Tobago)
19. 2007-2013, UK Representative to European Federation of Chemical Engineering (EFCE), Thermodynamics/Transport
20. 2008-2011, Honorary Secretary and Treasurer of Faraday Council of the Royal Society of Chemistry

Reviewer for

Industrial Collaborations
BASF, BCURA, Power Ltd, Borealis AS, Britest Ltd., BP, ICI Research/Akzonobel, Ineos Fluor/Mexichem, P&G, Pfizer, Novartis, Qatar Petroleum, Shell International, Schiumberger Syngenta, Total, Unilever Research.
Publications

Journal Articles
1. GV Lau, PA Hunt, EA Müller, G Jackson, UJ Ford, 2015, Water droplet excess free energy determined by cluster mitosis using guided molecular dynamics, Journal of Chemical Physics 143, 244709
2. B Rotenberg, G Jackson, D Frenkel, 2015, Jean-Pierre Hansen – a stimulating history of simulating fluids, Molecular Physics 113, 2363-2375
4. L Wu, A Malíjevs'ký, G Jackson, EA Müller, C Avendaño, G Jackson, 2015, The A in SAFT: developing the contribution of association to the Helmholtz free energy within a Wertheim TPT1 treatment of generic Mie fluids, Molecular Physics 113, 948-964
5. S Dufal, T Lafitte, AJ Haslam, A Galindo, GNI Clark, C Vega, G Jackson, 2015, A hierarchical method to integrated solvent and process design of physical CO2 adsorption using the SAFT-y Mie approach, AIChE Journal 61, 3249-3269
6. GV Lau, UJ Ford, PA Hunt, EA Müller, G Jackson, 2015, Surface thermodynamics of planar, cylindrical, and spherical vapour-liquid interfaces of water, Journal of Chemical Physics 142, 114701
7. J Burger, V Papaioannou, S Gopinath, A Galindo, CS Adjiman, 2015, A single-site coarse-grained model of water applicable over a wide temperature range, Molecular Physics 113, 1228-1249
11. G Jackson, GV Lau, EA Müller, PA Hunt, UJ Ford, 2015, Water droplet excess free energy determined by cluster mitosis using guided molecular dynamics, American Institute of Physics (AIP)
16. EA Müller, G Jackson, 2014, Force field parameters from the SAFT-y equation of state for use in coarsegrained molecular simulations, Annual Review of Chemical and Biomolecular Engineering 5, 405-427

Keynote/plenary talks given at international conferences
1. 2014 “Computing the Pressure and Interfacial Tension of Inhomogeneous Nanoscopic Systems Including Drops and Confined Anisotropic Phases: The Devil Is in the Detail,” Annual AIChE Meeting, Atlanta, USA.
3. 2015 “SAFT-γ force fields for molecular simulations of the thermodynamic, structural and transport properties of complex fluids and mixtures,” SAFT 25th Anniversary Conference, Houston, USA.
4. 2015 “Guggenheim Medal Award: The legacy of Edward Guggenheim to Statistical Thermodynamics,” Thermodynamics 2015 Conference, Copenhagen, Denmark
James Keirstead
Lecturer in Urban Energy Systems, Department of Civil and Environmental Engineering, Imperial College London

Qualifications
BSc in Civil Engineering (First Class Honours, Queen’s University, Canada),
MSc Environmental Change and Management (Distinction, University of Oxford)
DPhil (University of Oxford).

Awards and Distinctions
Chartered Engineer, Member of the Energy Institute
Commonwealth Scholar, 2003-2006
British Council Chevening Scholar, 2001-2002
Guinness Book of World Records, 2000, Longest Distance Travelled by Solar Powered Vehicle

Secondments
October 2010, University of Tokyo, Institute for Industrial Science.

Research Interests
1. Urban energy systems including systems integration, technologies, and policies
2. Optimisation methods, agent-based simulation, uncertainty/sensitivity analysis
3. Industrial ecology, particularly urban metabolism

Other Activities

Reviewer Activities

Academic Collaborations
University of Toronto, Prof. Chris Kennedy
University of Minnesota, Prof. Anu Ramaswami
Arizona State University, Dr. Mikhail Chester
University of Surrey, Prof. Roland Clift
University of Bath, Dr Nick McCullen

Industrial Collaborations
Arup, AECOM, Hildebrand Ltd

Alexandros Kiparissides
Lecturer in the Department of Biochemical Engineering, University College London

Qualifications
Diploma in Chemical Engineering (Aristotle University of Thessaloniki, Greece)
PhD in Bioprocess Systems Engineering (Imperial College London, UK)

Research Interests
Recombinant protein production in mammalian cell cultures, algae biotechnology and bioprocessing. Development of an integrated methodology combining Multi-scale & Metabolic Modelling, Metabolic Engineering and wet-lab experiments in order to: (i) Better understand cell physiology and metabolism under industrial bioprocessing conditions; (ii) Identify key parameters affecting culture efficiency at the metabolic, bioprocess and reactor design level; (iii) Enable the model based design and optimisation of industrial scale bioreactors.

Other Activities
Member of the SIG: Biochemical Engineering – IChemE
MSc Admissions Tutor – Department of Biochemical Engineering, UCL
Reviewer for
Biochemical Engineering Journal
BMC Bioinformatics
Chemical Engineering Research and Design Computers & Chemical Engineering
Algal Research, Technology
Biomass & Bioenergy

Academic Collaborations
Imperial College London (UK), University College Dublin (IRL), University of Surrey (UK), Tufts University (USA), Ecole Polytechnique Fédérale de Lausanne - EPFL (CH), Austrian Centre of Industrial Biotechnology (AUT), Cyprus University of Technology (CY), Centre for Research and Technology Hellas (GR).

Industrial Collaborations
Lonza Biologics
Medimmune

Publications
Journal Articles

Conference Presentations and Posters

Cleo Kontoravdi
Senior Lecturer, Department of Chemical Engineering, Imperial College London

Qualifications
PhD in Chemical Engineering, Imperial College London
MEng in Chemical Engineering, Imperial College London

Research Interests
Mathematical modelling, experiment design and optimisation for biological processes
Protein-producing animal cell cultures
Protein glycosylation

Industrial Collaborations
Lonza Biologics
MedImmune
GSK
Symphogen

Reviewer for
Biotechnology Progress
Biotechnology and Bioengineering
Analytical Biochemistry
Biochemical Engineering Journal
PLoS ONE
Cytotechnology
Biotechnology and Applied Biochemistry
Bioprocess and Biosystems Engineering
Chemical Engineering Science
Computer Applications in Biotechnology
Biochemical Engineering Journal

Publications
Journal Articles
CHO cell culture, Biotechnology and Bioengineering, 112: 2172- 2184


Invited talks
2nd BioProNet Symposium, Manchester, U.K., October 2015
Cell Line Development & Engineering, Vienna, Austria, February 2014.

J Krishnan
Senior Lecturer, Department of Chemical Engineering, Imperial College London. Affiliated with: Institute for Systems and Synthetic Biology, Centre for Bioinformatics

Qualifications
B.Tech Indian Institute of Technology, Madras
Ph.D Princeton University (Chemical Engg)
Associate Research Scientist, Electrical Engg, Johns Hopkins University

Research Interests
Information processing in cells and tissues with applications in systems and synthetic biology combining (i) mathematical modelling (ii) theoretical work (iii) systems analysis including tool development (iv) experimental collaboration. Mathematical modelling involves temporal, spatial and stochastic descriptions as appropriate, and some of the mathematical modelling is explicitly multi-level (e.g., cells and tissues). This is complemented by theoretical and systems work involving tools from dynamical systems, systems engineering, control engineering, and network analysis. Modelling and systems analysis spans a whole range of levels and scales from the enzymatic (multi-site phosphorylation), to the gene regulatory (mRNA translation), to the network (information processing in network modules, regulation of the cell cycle in dynamic environments, spatial control of biochemical cascades and pathways), to the cell and tissue levels (effect of intrinsic and induced drug resistance mechanisms at the cell and tissue scales, engineering of patterns at the tissue level). We are also interested in non-biological analogues of such work in engineered and related physico-chemical systems.

Reviewer for Systems and Synthetic Biology

**Biomedical Engineering**
Annals of Biomedical Engineering, Fundamental and Clinical Pharmacology.

**Dynamical Systems/Control/Systems Engg**
IEEE Transactions on Automatic Control, Automatica, Computers and Chemical Engineering, Chemical Engineering Research and Design.

**Academic Collaborations**
Collaborations with experimental groups in systems and synthetic biology (mRNA translation, cell signalling and decision making, spatial engineering at cell and tissue levels).

**Publications**

**Journal Articles**


**Book Chapters**


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Niall Mac Dowell

**Lecturer in Energy and Environmental Technology and Policy, Centre for Environmental Policy, Imperial College London**

**Qualifications**

PhD in Chemical Engineering, Imperial College London (2010)
B.E. in Chemical Engineering, University College Dublin, (2005)

**Awards and Distinctions**

Nicklin Medal, Institution of Chemical Engineers, 2015
Chartered Chemical Engineer, CEng, Institution of Chemical Engineers, 2013
The Qatar Petroleum Award for PhD Research Excellence in Clean Fossil Fuels, Qatar Petroleum, 2010

**Research Interests**

Clean Fossil Fuels
Carbon Capture and Storage (CCS)
Low carbon electricity generation
Biomass Enhanced Carbon Capture and Storage (BECCS) CO2 Capture and utilisation (CCu)
Ionic liquids
Dynamic Process Modelling, Simulation and Optimisation
Mathematical Modelling

**Other Activities**

Visiting Academic in the Department of Mechanical Engineering, University of Sheffield
Secretary of the Executive Board of the IChemE Energy Centre
Appointed to the Technical Working Group of the Zero Emissions Platform (ZEP)
Appointed to the Technical Working Group of the Carbon Capture and Storage Association Member, Royal Society of Chemistry, 2015
MAiChE, American Institution of Chemical Engineers, 2008
MIChemE, Institution of Chemical Engineers, 2004

**Reviewer for**

Energy and Environmental Science
Molecular Systems Design and Engineering
Publications

Journal Articles


Conference Contributions


4. Mac Dowell N, Shah N, 2014, Optimisation of post-combustion CO₂ capture for flexible operation, 12th International Conference on Greenhouse Gas Control Technologies (GHGT), Publisher: ELSEVIER SCIENCE BV, Pages: 1525-1535, ISSN: 1876-6102

Invited Lectures and Seminars
1. CO₂ capture and storage without the Geography, Alternative Carbon Capture and Storage (CCS) Pathways Workshop, June 2014, St Catherine’s College, Oxford

2. On the use of advanced association theories in process engineering, SAFT Meeting 2014, April 2014, Tróia, Portugal

3. Optimisation of post-combustion CO₂ capture for flexible operation, keynote lecture at UKCCSRC Biannual meeting, April 2014, Queens’ College Cambridge, UK

4. UK power generation: carbon source or sink?, UKCCSRC workshop on Direct Air/Negative Emissions, March 2014, Imperial College London

Geoffrey C. Maitland FREng

Professor of Energy Engineering, Department of Chemical Engineering, Imperial College London

Qualifications
MA in Chemistry (Oxford University)
DPhil in Physical Chemistry (Oxford University)

Awards and Distinctions
Fellow of the Royal Academy of Engineering
Fellow of IChemE
President of IChemE 2014-15
Salters’ Scholar 1969-72
ICI Fellowship 1972-74
Hutchison Medal of the IChemE, 1999
ICheE Envoy Award 2010
RSC/SCI Rideal Award 2012

Research Interests
Clean production and use of fossil fuels
Carbon capture and storage
Recovery of non-conventional hydrocarbons
Real-time control and management of oil and gas reservoirs
Thermophysical properties of fluids
Rheology of complex fluids and soft materials
Rock-fluid interactions
Renewable solar production of hydrogen from water using green algae and cyanobacteria

Other Activities
President, Institution of Chemical Engineers 2014-15
Deputy President, Institution of Chemical Engineers 2013-14
EPSRC: Member of Peer Review College
Editor, Chemical Engineering Research and Development Soft Matter Journal: Founder Member of Editorial Board
Member of IChemE Council and UK Board
Member of Royal Society of Chemistry Publications Board Member of Royal Society of Chemistry Faraday
Council with responsibility for liaison with IChemE Associate Member University of Wales Institute of Non-Newtonian Fluid Mechanics
Chair, EPSRC Steering Group, Portfolio Grant on Complex Fluids and Complex Flows, Swansea University
Chair, UK Offshore Oil and Gas Regulatory Review Panel

Reviewer for
ACS Petroleum Research Fund
Chemical Engineering Research and Development
Chemical Engineering Science
Journal of Chemical and Engineering Data
Journal of Materials Chemistry
Journal of Non-Newtonian Fluid Mechanics
Journal of Rheology Langmuir
Molecular Physics
Nature
Physical Chemistry Chemical Physics
Soft Matter

Publications
Journal Articles
5. Hou S-X, Maitland GC, Trusler JPM, 2015, Phase equilibria of (CO2 + butylbenzene) and (CO2 + butylcyclohexane) at temperatures between (323.15 and 423.15) K and at pressures up to 21 MPa, FLUID PHASE EQUILIBRIA, Vol: 387, Pages: 111-116, ISSN: 0378-3812
8. Peng C, Crawshaw JP, Maitland GC, Trusler JPM, 2015, Kinetics of calcite dissolution in CO2-saturated water at temperatures between (323 and 373) K and pressures up to 13.8 MPa, CHEMICAL GEOLOGY, Vol: 403, Pages: 74-85, ISSN: 0009-2541


20. Maitland G, 2014, Putting CO$_2$ in its place. TCE The Chemical Engineer, Pages: 34-37, ISSN: 0302-0797

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Athanasios (Sakis) Mantalaris

Professor in BioSystems Engineering, Department of Chemical Engineering, Imperial College London

Qualifications
PhD in Chemical Engineering, University of Rochester
MSc in Chemical Engineering, University of Rochester

Awards and Distinctions
Fellow of the American Institute of Biological and Medical Engineers 2013
European Research Council Advanced Investigator Award 2012
Fellow, American Institute of Medical & Biological Engineering, 2011
1st Prize Award, Hellenic Association of Orthopaedics Surgery & Traumatology, 2009
Rector's Award for Research Excellence, Imperial College, 2006
Live Demo Award, ISCAS, 2006
Jounitor Moulton Award, IChemE, 2004

Research Interests
Modelling of Biological Systems, Mammalian Cell Bioprocessing, Stem Cell Bioprocessing and Tissue Engineering.

Other Activities
Member of the Executive Board of the European Society for Biochemical Engineering Sciences (ESBES)
Member of the Advisory Board for Prometheus Catholic University of Leuven

Reviewer for
Tissue Engineering Biomatertials, Stem Cells & Development
Biochemical Engineering Journal
Biotechnology & Bioengineering

Academic Collaborations
University of Thessaloniki ETH
Temple University
NTU
Industrial Collaborations
Novalung

Publications
Journal Articles


Conference Contributions

Ruth Misener
Lecturer & Royal Academy of Engineering Research Fellow, Department of Computing, Imperial College London

Qualifications
BSc in Chemical Engineering (Massachusetts Institute of Technology) PhD in Chemical Engineering (Princeton University)

Awards and Distinctions

Research Interests
Research Domain: Optimisation Methods & Computation. Foundations: Global optimisation of mixed-integer nonlinear programs (MINLP); Numerical optimisation algorithms; Computational optimisation frameworks; Implementations and software for global optimisation. Applications: Optimal chemotherapy scheduling for leukaemia; Bioprocess optimisation under uncertainty; Cell cycle modelling; Superstructure optimisation of chemical and petrochemical plants for energy efficiency; Process network design and operations.

Other Activities
Software development/maintenance of MINLP global optimization solvers ANTIGONE and GloMIQO.

Reviewer for

Academic Collaborations
MIT, Texas A&M, University of Liége

Industrial Collaborations
GAMS Development Corp

Publications
Book Chapters
Journal Articles


Conference Contributions


Invited Lectures and Seminars


4. Misener R. Global Optimisation; Centre for Process Systems Engineering Advanced Optimisation Course, Imperial College London, England; Invited by Prof C Adjiman; 04/2015.


Erich A. Müller

Professor of Thermodynamics, Department of Chemical Engineering, Imperial College London

Qualifications
Ph.D. in Chemical Engineering, Cornell University (USA)
M.Sc. in Chemical Engineering (honor mention), Universidad Simón Bolívar, (Venezuela)

Research Interests
- Molecular simulation of complex fluids (liquid crystals, asphaltenes, polymers, etc.) adsorption and interfacial phenomena (activated carbons, nanotubes, colloids)
- Phase equilibria and thermophysical properties (VLE, supercritical fluids, etc.) bridging size scales from atomistic simulations to equation of state modelling (SAFT)
- Focus on application to engineering, environmental problems and high performance computing for engineering

Other Activities
- Fellow, Royal Society of Chemistry, 2011
- Member, International Adsorption Society
- Senior Member, AIChE

Links with Other Academic Bodies
- Visiting Professor, Universidad de Concepcion
- Visiting Researcher, Cornell University
- Visiting Researcher, North Carolina State University
- Visiting Researcher, Danmarks Tekniske Højskole
- Visiting Researcher, Universidad de Sevilla
- Visiting Professor, Universidad Pablo de Olavide

Publications

Journal Articles


Costas C. Pantelides FREng
Professor of Chemical Engineering, Department of Chemical Engineering, Imperial College London

Qualifications
BSc (Eng.) in Chemical Engineering (Imperial College London)
MSc in Chemical Engineering (MIT)
PhD, DIC in Symbolic & numerical solution methods (Imperial College London)

Awards and Distinctions
2015 The Sargent Medal, The Institution of Chemical Engineers
2015 The President’s Medal for Excellence in Innovation and Entrepreneurship, Imperial College London
2010 Fellow of the Royal Academy of Engineering
2009 Fellow of the Institution of Chemical Engineers
2007 MacRobert Award of the Royal Academy of Engineering, awarded for the innovation of gPROMS
1998 Beilby Medal from the SCI, RSC and IoM for contributions to process systems engineering

Research Interests
Process modelling methodologies & tools
Systems-based Pharmaceuticals
Ab initio prediction of crystal structures

Other Activities
Managing Director, Process Systems Enterprise Ltd.

Publications
Journal Articles
2. Vasileiadis M, Pantelides CC, Adjiman CS, 2015, Prediction of the crystal structures of atenolol, a polymorphic pharmaceutical molecule, CHEMICAL ENGINEERING SCIENCE, Vol: 121, Pages: 60-76, ISSN: 0009-2509
Conference Contributions

Lazaros G. Papageorgiou
Professor in Chemical Engineering, Department of Chemical Engineering, University College London

Qualifications
Dipl. Eng. in Chemical Engineering (NTUA, Greece)
PhD in Chemical Engineering (Imperial College London)

Research Interests
Computer-aided process engineering, production planning and scheduling, supply-chain optimisation, mixed-integer optimisation

Other Activities
Member of IChemE CAPE Subject Group Committee
Member of EPSRC Peer Review College
International Programme Committee member – ESCAPE21, ESCAPE22
Editorial board member of Current Opinion in Chemical Engineering
Editorial board member of ISRN Chemical Engineering

Reviewer for

Academic Collaborations
Imperial College London, King’s College London, University College London, Technical University of Crete, Aristotle University of Thessaloniki, National Technical University of Athens, University of Wisconsin, Instituto Superior Tecnico.

Industrial Collaborations
Bayer, Syngenta, Unilever.

Publications
Journal Articles

Academic Collaborations
Imperial College London, King’s College London, University College London, Technical University of Crete, Aristotle University of Thessaloniki, National Technical University of Athens, University of Wisconsin, Instituto Superior Tecnico.

Panos Parpas
Senior Lecturer, Department of Computing, Imperial College London

Qualifications
PhD in Computer Science, Imperial College London (2006)
MSc in Computer Science, Imperial College London (2002)

Awards and Distinctions
MIT CIY Fellowship

Research Interests
Development and analysis of algorithms for large scale optimisation problems

Other Activities
Athena-Swan representative for the Department of Computing

Reviewer for

Academic Collaborations
MIT Engineering Systems Division
Department of Statistical Science Duke University
Department of Mathematics Edinburgh
School of Pharmacy Nottingham

Industrial Collaborations
IBM

Publications
Journal Articles
Berc Rustem

Professor of Computational Methods in Operations Research, Department of Computing, Imperial College London

Qualifications
B.S. MSc, PhD, FIMA, CMath

Awards and Distinctions
President of Society of Computational Economics, 2002-04
Special issue of Computational Economics in honour of Berc Rustem (V. 27, Nos 2-3, 2006)
Special issue of Computational Management Science in honour of Berc Rustem (V. 11, No. 3, 2014)

Research Interests
Optimisation Algorithms, Decision and Design Under Uncertainty, Worst-Case Design, Stochastic Optimisation

Other Activities

Academic Collaborations
University of Warwick; University of Florida

Industrial Collaborations
Commerzbank; BAE Systems

Editor
Automatica (2003-2015)
Computational Management Science (2002-2012)

Editorial Advisory Board
Journal of Economic Dynamics & Control

Associate Editor
Royal Society Proceedings (Series A; 2008-14)
Computational Economics
Journal of Global Optimization
Optimization Letters
Computational Science & Engineering

Book Series Editor
Advances in Computational Management Science
Advances in Computational Economics

Organiser & Programme Committee Co-chair

Activities
Associate Director - Research - Centre for Process Systems Engineering, Imperial College

Eva Sørensen

Professor of Chemical Engineering, Department of Chemical Engineering, University College London
Deputy Head of Department (Education)

Qualifications
MSc in Chemical Engineering (NTNU, Norway)
PhD in Chemical Engineering (NTNU, Norway)
MA in Education (University College London)
Chartered Engineer (CEng)
Chartered Scientist (CSci)

Awards and Distinctions
Fellow of the Institution of Chemical Engineers (IChemE)
Fellow of the Higher Education Academy (HEA)
IChemE Sustainability Teaching Award (2015)
ExxonMobil Award for Excellence in Teaching
Royal Academy of Engineering (2013)

Publications
Journal Articles
Royal Academy of Engineering Secondment Award (2005)
Faculty Teaching Award for Outstanding Achievements in Teaching Faculty of Engineering,
University College London, UK (2001)
Postdoctoral Research Scholarship, Norwegian Research Foundation (1995-1996)
Research Scholarship, Norwegian Research Foundation (1993-1994)
University Scholarship, NTNU, Norway (1990-1993)

Secondments
BP Refining Technology (2005)

Research Interests
Systematic methodologies for mathematical modelling of fluid separation processes, in particular, distillation, membrane separation, chromatography and hybrids thereof
Optimal design and operation of fluid separation processes
Micro-scale separation processes
Optimal separation process selection
Optimal process design, operation and control

Education

Other Activities
Editor-in-Chief of Chemical Engineering Research & Design
Member of the European Federation of Chemical Engineers (EFCE) Executive Board
Member of EFCE's Working Party on Fluid Separations
Member of IChemE’s Education & Accreditation Board
Member of Engineering Council’s Engineering Accreditation Board
Member of IChemE’s Education Special Interest Group Committee
Member of IChemE’s Fluid Separations Special Interest Group Committee
Member of American Institute of Chemical Engineers (AIChE) Executive Board
Member of European Society for Engineering Education (SEFI) Executive Board
Editorial Board Member of Chemical Engineering & Technology
Chair of Organising Committee for Distillation & Absorption Conference, 2006

Reviewer for
Deutsche Forschungsgemeinschaft (DFG)
Dutch Technology Foundation (STW)
CONICYT Chile
AIChE Journal
Biomass and Bioenergy
Chemical Engineering & Processing
Chemical Engineering & Technology
Chemical Engineering Science
Computers and Chemical Engineering
Journal of Membrane Science
Journal of the Science of Food and Agriculture
Journal of European Engineering Education

Academic Collaborations
University College London, Department of Biochemical Engineering
Imperial College London, Department of Chemical Engineering
Dortmund University, Germany

Industrial Collaborations
BioMarin, Eli Lilly

Publications

Journal Articles
Michail Stamatakis

Lecturer in Chemical Engineering, Department of Chemical Engineering, University College London

Qualifications
MEng in Chemical Engineering (NTUA, Greece)
PhD in Chemical and Biomolecular Engineering (Rice University, USA)

Awards and Distinctions
2015 - Shortlisted for IChemE Global Awards – Research Project of the Year
2013 - Top Reviewer, Computers & Chemical Engineering
2007 - Outstanding Teaching, Department of Chemical and Biomolecular Engineering, Rice University
2007 - Kobayashi Fellowship, Department of Chemical and Biomolecular Engineering, Rice University

Research Interests
First-principles based chemical process modelling tools
Computational catalyst engineering

Reviewer for

Academic Collaborations
Thomas Young Centre, UK Catalysis Hub, University College London, Oxford University, University of Pittsburgh, University of Wisconsin at Madison, Tufts University, Integrated Mesoscale Architectures for Sustainable Catalysis – Energy, Frontier Research Centre, Harvard University.

Publications
Journal Articles

Conference Contributions

Invited Lectures and Seminars


Nina F. Thornhill FREng

Professor of Process Automation, Department of Chemical Engineering, Imperial College London, Holder of ABB/Royal Academy of Engineering Research Chair in Process Automation

Qualifications
BA in Physics (Oxford University)
MSc in Control Systems (Imperial College)
PhD (UCL)

Awards and Distinctions
Fellow of the Royal Academy of Engineering
Fellow of the IChemE
Fellow of the IET

Secondments
Marie Curie Fellowship secondment to ABB Corporate Research, Poland, 2012 and 2013
Royal Academy of Engineering Global Research Award with ABB Corporate Research, Norway, April-September 2005
Royal Academy of Engineering Foresight Award with University of Alberta, Canada, January-September 2001

Research interests
Industrial data analysis using time series analysis and signal processing; Plant-wide performance assessment; Applications in oil and gas, chemicals, bioprocesses and electricity supply.

Other Activities
IChemE: Chair of Process Management & Control Subject Group
Associate Editor of Control Engineering Practice 2006-2013

Reviewer for
Automatica
Biotechnology and Bioengineering
Chemical Engineering Research and Design
Computers & Chemical Engineering
Control Engineering Practice
IEEE Transactions on Control System Technology
Industrial and Engineering Chemistry Research
Journal of Process Control

Academic Collaborations
Helmut Schmidt University, Hamburg, Institut für Automatisierungstechnik
Imperial College London, Department of Electrical and Electronic Engineering
Imperial College London, Department of Mechanical Engineering
Norwegian University of Science and Technology – NTNU Trondheim
University of Alberta, Department of Chemical and Materials Engineering
University College London, Department of Biochemical Engineering

Industrial Collaborations
ABB Corporate Research
ABB Strategic R&D for Oil, Gas and Petrochemicals
ESD Training Simulation
BASF
BP Exploration and Production
Fingrid Oyj
National Grid
Statnett SF

Publications
Journal Articles


Conference Presentations


Wolfram Wiesemann

Associate Professor of Management Science and Operations; Fellow of the KPMG Centre for Advanced Business Analytics, Imperial College London

Qualifications
MSc in Management and Computing at Darmstadt University of Technology (2006)
PhD in Operations Research at Imperial College London (2010)

Research Interests
Dr Wolfram Wiesemann’s research focuses on the development of tractable computational methods for the solution of stochastic and robust optimisation problems, as well as, applications in operations management, finance and health care.

Reviewer for
Annals of Operations Research, Applied Mathematical Modelling,
Asia-Pacific Journal of Operational Research, Automatica,
Computational Management Science, The Computer Journal,

Academic Collaborations
Carnegie Mellon University
Columbia University
National University of Singapore
Princeton University

Publications
Journal Articles

Invited Lectures and Seminars
1. Tesco Analytics, Welwyn Garden City (UK), November 2015.
2. Faculty of Economics and Business, KU Leuven (Belgium), October 2015.
3. International Workshop on Vehicle Routing under Uncertainty, TU Dortmund (Germany), September 2015.
5. 21st International MENDEL Conference, Brno (Czech Republic), June 2015.
6. School of Mathematics, University of Edinburgh (UK), March 2015.
7. School of Mathematics, Computer Science & Engineering, City University London (UK), February 2015.
8. London Optimization Workshop, King’s College London (UK), June 2014.
9. Operations Group, Judge Business School, University of Cambridge (UK), April 2014
Imperial College London

**Department of Chemical Engineering**
Professor Nilay Shah, FREng, Professor of Process Systems Engineering, Director CPSE
Professor Claire S. Adjiman, FREng, Professor of Chemical Engineering
Dr Benoît Chachuat, Reader in Process Systems Engineering
Dr Peter DiMaggio, Senior Lecturer
Professor Amparo Galindo, Professor of Physical Chemistry
Dr Gonzalo Guillén-Gosálbez, Reader in Process Systems Engineering
Dr Adam Hawkes, Senior Lecturer in Energy Systems
Professor George Jackson, Professor of Chemical Physics
Dr Cleo Kontoravdi, Senior Lecturer
Dr J Krishnan, Senior Lecturer
Professor Geoffrey C. Maitland, FREng, Professor of Energy Engineering
Professor Athanasios (Sakis) Mantalaris, Professor of BioSystems Engineering
Professor Erich Müller, Professor of Thermodynamics
Professor Costas C. Pantelides, FREng, Professor of Chemical Engineering
Professor Nina F. Thornhill, FREng, Professor of Process Automation

**Business School**
Dr Wolfram Wiesemann, Assistant Professor

**Centre for Environmental Policy**
Dr Niall MacDowell, Lecturer in Energy and Environmental Technology and Policy

**Department of Civil and Environmental Engineering**
Dr James Keirstead, Lecturer

**Department of Computing**
Dr Marc Deisenroth, Lecturer in Statistical Machine Learning
Dr Ruth Misener, Lecturer in Computing
Dr Panos Parpas, Senior Lecturer

**Department of Earth Science & Engineering**
Professor Nigel Brandon, OBE FREng, Director of the Sustainable Gas Institute (SGI)

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Emeritus and Honorary Academics
Professor Roger Benson
Dr Graham Elkes
Professor John Perkins
Professor Efstratios (Stratos) Pistikopoulos
Professor Berc Rustem, Professor of Computing
Professor Paul Rutter
Professor Roger W. H. Sargent

University College London

**Department of Chemical Engineering**
Department of Chemical Engineering
Professor I. David Bogle, FREng, Professor of Chemical Engineering and Head of UCL Graduate School
Dr Vivek Dua, Senior Lecturer
Professor Eric S. Fraga, Professor of Process Systems Engineering
Dr Federico Galvanin, Lecturer
Professor Lazaros Papageorgiou, Professor of Chemical Engineering
Professor Eva Sørensen, Deputy Head for Education and Professor of Chemical Engineering
Dr Michail Stamatakis, Lecturer

**Department of Biochemical Engineering**
Dr Alexandros Kiparissides, Lecturer
Academic Staff

Professor Nilay Shah (CPSE Director)  n.shah@imperial.ac.uk
Professor Claire S Adjiman  c.adjiman@imperial.ac.uk
Professor I David L Bogle  d.bogle@ucl.ac.uk
Professor Nigel Brandon  n.brandon@imperial.ac.uk
Dr Benoît Chachuat  b.chachuat@imperial.ac.uk
Dr Marc Deisenroth  m.deisenroth@imperial.ac.uk
Dr Peter DiMaggio  p.dimaggio@imperial.ac.uk
Dr Vivek Dua  v.dua@ucl.ac.uk
Professor Eric S Fragal  e.fraga@ucl.ac.uk
Professor Amparo Galindo  a.galindo@imperial.ac.uk
Dr Federico Galvanin  f.galvanin@ucl.ac.uk
Dr Gonzalo Guillén-Gosálbez  g.guillen05@imperial.ac.uk
Dr Adam Hawkes  a.hawkes@imperial.ac.uk
Professor George Jackson  g.jackson@imperial.ac.uk
Dr James Keirstead  j.keirstead@imperial.ac.uk
Dr Alexandros Kiparissides  alex.kiparissides@ucl.ac.uk
Dr Cleo Kontoravdi  cleo.kontoravdi@ucl.ac.uk
Dr J Krishnan  j.krishnan@imperial.ac.uk
Dr Niall Mac Dowell  n.mac-dowell@imperial.ac.uk
Professor Geoffrey C Maitland  g.maitland@imperial.ac.uk
Professor Athanasios Mantalaris  a.mantalaris@imperial.ac.uk
Dr Ruth Misener  r.misener@imperial.ac.uk
Professor Erich Müller  e.muller@imperial.ac.uk
Professor Costas C Pantelides  c.pantelides@imperial.ac.uk
Professor Lazaros Papageorgiou  l.papageorgiou@ucl.ac.uk
Dr Panos Parpas  p.parpas@imperial.ac.uk
Prof Berc Rustem  b.rustem@imperial.ac.uk
Professor Eva Sørensen  e.sorensen@ucl.ac.uk
Dr Michel Stamatakis  m.stamatakis@ucl.ac.uk
Professor Nina F Thornhill  n.thornhill@imperial.ac.uk
Dr Wolfram Wiesemann  wv@imperial.ac.uk
Dr Do Yeon Kim  d.kim@imperial.ac.uk
Dr Oleksiy Klymenko  o.klymenko@imperial.ac.uk
Dr Sergei Kucherenko  s.kucherenko@imperial.ac.uk
Dr Kamal Kurian  k.kurian@imperial.ac.uk
Dr Romain Lambert  romain.lambert@imperial.ac.uk
Dr Lianfang Cai  l.cai@imperial.ac.uk
Dr Songsong Liu  s.liu@ucl.ac.uk
Dr Ryan Luong  vu.luong@imperial.ac.uk
Dr Evgenia Mehtleri  e.mehtleri@imperial.ac.uk
Dr Marta Moreno Benito  martas.moreno@imperial.ac.uk
Dr Jordan Muscatello  jordan.muscatello@imperial.ac.uk
Dr HongXing Niu  n.niu@imperial.ac.uk
Dr Antonio Marco Pantaleo  a.pantaleo@imperial.ac.uk
Dr Remigijus Paulavicius  remigijus.paulavicius@imperial.ac.uk
Dr Bharat Kumar Varma Penmuthsa  b.penmuthsa@imperial.ac.uk
Dr Pedro Rivotti  p.rivotti@imperial.ac.uk
Dr Nouri Samatelli  n.samatelli@imperial.ac.uk
Dr Sheila Samatelli  s.samatelli@imperial.ac.uk
Dr SaurabhMahesh Kumar Shah  saurabh.shah@imperial.ac.uk
Dr Mahdi Sharifzadeh  mahdi.sharifzadeh@imperial.ac.uk
Dr Javier Silvénte  j.silvente@ucl.ac.uk
Dr Edward Smith  edward.smith@ucl.ac.uk
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Dr H. Sugden  h.sugden@imperial.ac.uk
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Head of Computing Services
Mr Graham Stuart  g.stuart@imperial.ac.uk
“Continuing advances in computing power and artificial intelligence will extend the reach, capability and usability of process systems engineering to help industry and society deal with the challenges that confront us all in the next century.”
CPSE Research Project List

Ali Salim Al Qahtani
*Technical, Economic and Environmental Impact of Future Fuel Formulations*
Supervisor: Prof Nilay Shah
Start date: October 2010
Finish date: October 2016

Adam Alexandros
*Integrated Heating and Power Systems for Dwellings*
Supervisor: Prof Eric Fraga
Start date: October 2011
Finish date: May 2016

Folashade Akinmolayan
*Real-Time Operational Risk Management through Advanced Multi-Scale Modelling*
Supervisors: Prof Eva Sørensen and Prof Nina Thornhill
Start date: August 2011
Finish date: July 2016

Yasmeen Aldawsari
*Systems Analysis of Transport Decarbonisation Options*
Supervisor: Prof Nilay Shah
Start date: September 2013
Finish date: September 2017

Amos B. Aleji
*Experimental and Modelling of Viscosity and Density of Mixtures of Crude oil + CO₂*
Supervisors: Prof Geoffrey Maitland and Prof Martin Trusler
Start date: February 2011
Finish date: August 2016

Sakhr Alhuthali
*Understanding the Interplay Between Upstream and Downstream Bioprocessing by a Sequence of Mathematical Models*
Supervisor: Dr Cleo Kontoravdi
Start date: October 2015
Finish date: May 2019

Mark C. Allenby
*Development of a Bio-Inspired in Silico-in Vitro Platform: Towards Personalised Healthcare through Optimisation of a Bone Marrow Mimicry Bioreactor*
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: October 2013
Finish date: April 2017

Nihal Almuraikhi
*Stem Cell Bioprocessing*
Supervisor: Prof Athanasios Mantalaris
Start date: October 2010
Finish date: August 2016

Diego Alonso Martinez
*Profiling the Methylome Targets of Histone Lysine Methyltransferases*
Supervisor: Dr Peter DiMaggio
Start date: September 2013
Finish date: September 2017

Tamador Alsobaie
*Stem Cell Bioprocessing*
Supervisor: Prof Athanasios Mantalaris
Start date: May 2012
Finish date: January 2016

Daniel E. Aluma
*Model-Based Optimisation of the Operation of Integrated Natural Gas Production & Processing Networks*
Supervisors: Prof Nilay Shah and Prof Costas Pantelides
Start date: November 2012
Finish date: November 2016

Oluwamayowa Amusat
*Design of Renewables-Based Integrated Energy Systems for Stand-Alone Continuous Processes*
Supervisor: Prof Eric Fraga
Start date: November 2013
Finish date: November 2016
Benaiah Uchechukwu Anabaraonye
Experimental and Modelling Studies of Reservoir Minerals
Dissolution Following CO₂ Injection
Supervisor: Prof Geoffrey Maitland
Start date: October 2013
Finish date: October 2016

William Ashworth
Systems Biology of the Liver
Supervisors: Prof David Bogle and Dr Nathan Davies (UCL Division of Medicine)
Start date: October 2013
Finish date: May 2017

Vitali Avagyan
Essays on Risks and Profitability of the UK Electricity Industry
Supervisors: Prof Berc Rustem, Dr Panos Parpas and Prof Richard Green
Start date: October 2012
Finish date: September 2016

Vijay Avinash
Integration of Decentralised Energy Resources with the Electricity Balancing System
Supervisor: Dr Adam Hawkes
Start date: April 2014
Finish date: April 2017

Styliani Avraamidou
Distributed Multi-Parametric Model Protective Control Applied on Biological and Biomedical Processes
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: October 2014
Finish date: April 2018

Radu Baltean-Lugojan
Structure Exploitation in Large Scale Non-Convex Optimization
Supervisor: Dr Ruth Misener
Start date: April 2015
Finish date: April 2018

Davide Bascone
Modelling and Optimisation of the Nuclear Fuel Cycle
Supervisor: Prof Eric Fraga
Start date: March 2015
Finish date: March 2019

Asif Bhatti
Synthesis and Design of Biological Systems Under Uncertainty
Supervisor: Dr Vivek Dua
Start date: October 2010
Finish date: September 2016

Hao Bian
Studies of Production, Inhibition and Exchange Processes for Gas Hydrates
Supervisor: Prof Geoffrey Maitland
Start date: July 2013
Finish date: June 2016

Moiz Bohra
Optimising Qatar’s Transition to Renewable Energy through Model-Based Analysis
Supervisor: Professor Nilay Shah
Start date: April 2016
End date: December 2019

Aaron Borg
Characterising the Function of Chromatin-Modifying Protein Complexes
Supervisor: Dr Peter DiMaggio
Start date: August 2012
Finish date: July 2016

Jonathan Bosch
Supervisor: Dr Adam Hawkes
Start date: October 2014
Finish date: June 2017

Susana Isabel Brito dos Santos
In Vitro Erythropoiesis in a 3D Bone Marrow Biomimicry: Reproducing Physiologic Biochemical and Microenvironmental Factors Involved in Red Blood Cell Formation
Supervisors: Prof Athanasios Mantalaris and Dr Nicki Panoskaltsis
Start date: March 2014
Finish date: March 2018

Pantelis Broukos
Urban Energy Systems
Supervisors: Prof Nilay Shah and Dr James Keirstead
Start date: September 2012
Finish date: December 2015

Sara Budinis
ENERGY-SMARTOPS
Supervisor: Prof Nina Thornhill
Start date: September 2011
Finish date: December 2015

Gizem Buldum
Bacterial Cellulose Production
Supervisor: Prof Athanasios Mantalaris
Start date: October 2011
Finish date: October 2016

Gonzalo Bustos-Turu
Integrated Modelling of Future Urban Energy Systems
Supervisor: Prof Nilay Shah
Start date: March 2014
Finish date: March 2017
Renato Cabral
A Quantification of the Value Provided by Flexible Oxy-Combustion CCS to the UK Energy System
Supervisor: Dr Niall Mac Dowell
Start date: October 2015
Finish date: September 2018

Claudio Calabrese
Viscosity and Density of Reservoir Fluids under CO₂ Addition
Supervisors: Prof Geoffrey Maitland and Prof Martin Trusler
Start date: November 2013
Finish date: October 2016

Andres Calderon Vargera
Optimisation of Biomass-Based Supply Chains
Supervisor: Prof Lazaros Papageorgiou
Start date: May 2013
Finish date: April 2017

Raúl Calvo Serrano
Process Optimisation and Sustainability Analysis
Supervisor: Dr Gonzalo Guillén Gosálbez
Start date: April 2016
Finish date: March 2019

Juan Sebastian Campos Salazar
Multilevel Optimization for Large Scale Semidefinite Programming
Supervisor: Dr Panos Parpas
Start date: October 2013
Finish date: October 2017

Vassilis M. Charitopoulos
Uncertainty-Aware Planning and Scheduling in the Process Industries
Supervisors: Dr Vivek Dua and Prof Lazaros Papageorgiou
Start date: September 2015
Finish date: September 2019

Florence Yu Tsing Chow
The Effect of Impurities on the Interfacial Tension between CO₂ and Reservoir Fluids
Supervisor: Prof Geoffrey Maitland
Start date: September 2012
Finish date: September 2015

Cheng-Ta Chu
Global Electricity Sector Decarbonisation Modelling
Supervisor: Dr Adam Hawkes
Start date: October 2015
Finish date: October 2019

Edward James Close
The Derivation of Bioprocess Understanding from Mechanistic Models of Chromatography
Supervisors: Prof Eva Sørensen and Dr Dan Bracewell (UCL)
Start date: September 2010
Finish date: October 2014

Constanza Cumicheo Melgarejo
The Combination of Bioenergy, Natural Gas and CCS for Negative Emissions
Supervisors: Dr Niall Mac Dowell and Prof Nilay Shah
Start date: November 2015
Finish date: June 2019

Ibrahim Daher
The Effect of Salt Precipitation on Permeability and Porosity in Fractured Carbonates System
Supervisors: Dr John Crawshaw and Prof Geoffrey Maitland
Start date: January 2013
Finish date: January 2017

Matthew Thomas Darby
First-Principles Simulations of Molecular Phenomena on Bimetallic Hydrogenation Catalysts
Supervisor: Dr Michail Stamatakis
Start date: October 2013
Finish date: May 2016

Pedro de Oliveira Filho
Development, Implementation and Application of a Language for Modelling Uncertainty in Design and Process Optimisation
Supervisor: Prof Eric Fraga
Start date: October 2015
Finish date: September 2019

Aikaterini Diamanti
Design of Optimal Reaction Conditions: Temperature and Solvent Effects
Supervisors: Prof Claire Adjiman and Prof Amparo Galindo
Start date: October 2012
Finish date: October 2016

David Dorantes Romero
Capture and Analysis of Process Connectivity and Topology
Supervisor: Prof Nina Thornhill
Start date: October 2012
Finish date: September 2018

Daniel Kunisch Eriksen
Molecular Modelling and Thermodynamics of Oil Systems in the Presence of Brine and CO₂
Supervisors: Prof Amparo Galindo and Prof George Jackson
Start date: October 2012
Finish date: August 2016

Karl Fairhurst
Molecular Simulation of Associating Fluids, Using a Combination of Molecular Dynamics (MD) and Monte Carlo (MC) Simulations, with Coarse-Grained Models
Supervisors: Prof Erich Müller and Prof George Jackson
Start date: October 2015
Finish date: September 2019
Sara Febra  
Molecular Systems Engineering Methods for Solubility Prediction of Active Pharmaceutical Ingredients  
Supervisor: Prof Amparo Galindo  
Start date: March 2014  
Finish date: March 2017

Christina-Anna Gatsiou  
Crystal Structure Prediction  
Supervisors: Prof Claire Adjiman and Prof Costas Pantelides  
Start date: March 2012  
Finish date: March 2016

Anastasia Georgiou  
Generation of Mineralised Cellular Constructs Using Mouse Embryonic Stem Cells Encapsulated in Alginate Hydrogels and Cultured within a Custom-Made Rotating Wall Vessel Perfusion Bioreactor  
Supervisor: Prof Athanasios Mantalaris  
Start date: October 2009  
Finish date: January 2016

Solomos Georgiou  
Decarbonisation of Food Supply Chains: A Holistic Approach  
Supervisors: Prof Nilay Shah and Dr Christos Markides  
Start date: October 2015  
Finish date: September 2019

Cher Hui Goey  
Cascading Effects in Bioprocessing: The impact of Cell Culture Environment on Mammalian Cell Behaviour and Host Cell Protein Species  
Supervisor: Dr Cleo Kontoravdi  
Start date: February 2013  
Finish date: February 2017

Smitha Gopinath  
Developing a Methodology for Integrated Molecular and Process Design  
Supervisors: Prof George Jackson, Prof Claire Adjiman and Prof Amparo Galindo  
Start date: September 2013  
Finish date: March 2017

Edward Graham  
The Integrated Molecular and Process Modelling of Carbon Dioxide Capture in Amine Solvents  
Supervisors: Prof Claire Adjiman, Prof George Jackson and Prof Amparo Galindo  
Start date: December 2014  
Finish date: December 2017

Boram Gu  
Modelling of RO Membrane Process Performance and Transport Phenomena for Performance Analysis and Optimisation  
Supervisors: Prof Claire Adjiman and Prof Yun Xu  
Start date: April 2014  
Finish date: October 2016

Yingjian Guo  
Modelling the Role of Gas T&D Infrastructure in Future Low Carbon Energy Systems  
Supervisor: Dr Adam Hawkes  
Start date: October 2015  
Finish date: April 2019

Clara Heuberger  
Energy System Optimisation and Technology Valuation, in Particular of Flexible CCS  
Supervisors: Dr Niall Mac Dowell, Prof Nilay Shah and Dr Iain Staffell  
Start date: January 2015  
Finish date: June 2018

Ching-Pang Ho  
Optimization Algorithms for Multiscale Models  
Supervisors: Dr Panos Parpas and Dr Wolfram Wiesemann  
Start date: October 2012  
Finish date: September 2016

Rayane Hoballah  
Solubility of Gases in Water or Brines at Reservoir Conditions  
Supervisors: Prof Martin Trusler and Prof Geoffrey Maitland  
Start date: December 2012  
Finish date: February 2017

Vahan Hovhannisyan  
Multi-Level Convex Optimisation in Machine Learning  
Supervisors: Dr Panos Parpas and Dr Stefanos Zafeiriou  
Start date: September 2013  
Finish date: September 2017

Sei Howe  
Singly Perturbed Optimal Control Systems  
Supervisor: Dr Panos Parpas  
Start date: October 2012  
Finish date: March 2017

Panatpong Hutacharoen  
Prediction of Octanol-Water Partition Coefficients of Active Pharmaceutical Ingredients by the SAFT-γ Mie Group- Contribution Equation of State  
Supervisors: Prof Claire Adjiman, Prof Amparo Galindo and Prof George Jackson  
Start date: May 2013  
Finish date: October 2016

Frederike Jaeger  
Flow of Fluids through Porous Media with Application to Membranes: from the Molecular to the Continuum Scale  
Supervisors: Prof Erich Müller and Prof Omar Matar  
Start date: October 2014  
Finish date: September 2017
Francisca Jalil Vega  
**Novel Approaches to Modelling Whole System Heat Decarbonisation**  
Supervisor: Dr Adam Hawkes  
Start date: December 2013  
Finish date: April 2017

Elnaz Jamili  
**Model-Based Optimal Control of Non-Viral Gene Delivery**  
Supervisors: Dr Vivek Dua and Dr Michail Stamatakis  
Start date: November 2012  
Finish date: October 2016

Erin Johnson  
**UK Green Gas: Exploring Sustainable Gas Potential as a Relevant Low Carbon Energy Stream**  
Supervisor: Professor Nilay Shah  
Start date: October 2015  
Finish date: October 2018

Suela Jonuzaj  
**Optimisation Approaches to Mixture Design**  
Supervisor: Prof Claire Adjiman  
Start date: August 2013  
Finish date: July 2017

Ashkan Kavei  
**Development and Application of Stack Segmented Fuel Cell Systems**  
Supervisors: Prof Nigel Brandon, Dr Gregory J Offer, Dr Billy Wu and Dr Vladimir Yufit  
Start date: September 2015  
Finish date: September 2019

Nikolaos Kazazakis  
**Development of Deterministic Global Optimization Methods**  
Supervisor: Prof Claire Adjiman  
Start date: September 2012  
Finish date: August 2016

Esma Koca  
**Product Release Strategies in Single and Multiple Markets**  
Supervisors: Dr Wolfram Wiesemann and Prof Tommaso Valletti  
Start date: October 2013  
Finish date: September 2017

Mariya Koleva  
**Optimisation of Wastewater Systems**  
Supervisor: Prof Lazaros Papageorgiou  
Start date: March 2013  
Finish date: December 2016

Clea Kolster  
**Multi-Scale Modelling and Analysis of the Dynamic CO2 Injection and Storage**  
Supervisors: Dr Niall MacDowell and Dr Sam Krevor  
Start date: October 2014  
Finish date: October 2017

Qingyuan Kong  
**An Optimisation-Based Framework for the Conceptual Design of Reaction-Separation Processes**  
Supervisor: Prof Nilay Shah  
Start date: October 2014  
Finish date: June 2018

Georgia Kouyialis  
**Exploiting Symmetry in Mixed Integer Non-Linear Optimisation**  
Supervisor: Dr Ruth Misener  
Start date: October 2014  
Finish date: September 2017

Gabriel Lau  
**Droplets: From Molecular Nanoclusters to the Atmospheric Aerosols**  
Supervisor: Prof George Jackson  
Start date: March 2013  
Finish date: September 2016

Georgia Lazarou  
**Modelling the Effect of pH on the Thermodynamics of Electrolyte Solutions Using the Statistical Associating Fluid Theory**  
Supervisors: Prof Claire Adjiman, Prof Amparo Galindo, Prof George Jackson and Prof Erich Müller  
Start date: October 2013  
Finish date: September 2017

Duncan Leeson  
**Energy Cascading in Complex Downstream Operations**  
Supervisors: Prof Nilay Shah, Dr Paul Fennell and Dr Niall MacDowell  
Start date: October 2014  
Finish date: April 2018

David Leng  
**Fault Propagation, Detection and Analysis in Process Systems**  
Supervisor: Prof Nina Thornhill  
Start date: September 2013  
Finish date: June 2018

Yunjie Liao  
**Development and Validation of a Model of Energy Differential Production Across the Liver Sinusoid**  
Supervisors: Prof David Bogle and Dr Nathan Davies (UCL Division of Medicine)  
Start date: October 2015  
Finish date: September 2019

Phantisa Limleamthong  
**Systematic Computer Aided Process Engineering Tools for the Optimal Design and Planning of Sustainable Chemical Processes**  
Supervisor: Dr Gonzalo Guillén-Gosálbez  
Start date: April 2016  
Finish date: March 2019
Tom Lindeboom  
Molecular Origins of the Thermodynamic Properties, Phase Separation Behaviour and Structure of Biomolecules in Aqueous Solutions  
Supervisors: Prof George Jackson and Prof Amparo Galindo  
Start date: October 2015  
Finish date: September 2019

Maximilian Lularevic  
A Combined Multi-Scale Modelling and Experimental Investigation of the Effects of Lactate Metabolism on Mammalian Cell Bioprocessing  
Supervisors: Dr Alexandros Kiparissides and Dr Cleo Kontoravdi  
Start date: September 2015  
Finish date: September 2019

Robert MacFarlane  
The Production of 3-Dimensional Mineralised Cellular Implants for Bone Tissue Engineering Applications  
Supervisor: Prof Athanasios Mantalaris  
Start date: October 2013  
Finish date: September 2017

Nikiforos Maragkos  
Novel Composite Materials Design for Economic Infrastructure Equipment  
Supervisors: Prof Efstratios Pistikopoulos and Prof Alexander Bismarck  
Start date: October 2009  
Finish date: PENDING (Interruption of Studies)

Amit M. Manthanwar  
Multiscale Design, Robust Optimisation and Robust Model Predictive Control of Fuel Cell Energy Systems  
Supervisor: Prof Efstratios Pistikopoulos  
Start date: February 2012  
Finish date: May 2016

Kristian Mc Caul  
A Multiscale and Multiphysics Modelling Framework for Processes Involved in Production of Fuels from Lignocelluloses  
Supervisors: Prof Nilay Shah, Dr Cleo Kontoravdi and Prof Yun Xu  
Start date: September 2013  
Finish date: March 2017

Calum J McIntosh  
Controlling the Quality of Novel Glycoprotein Therapeutics  
Supervisor: Dr Cleo Kontoravdi  
Start date: November 2015  
Finish date: November 2019

Govind Menon  
Elucidating Temporal and Spatial Aspects of Cellular Information Processing  
Supervisor: Dr J Krishnan  
Start date: October 2014  
Finish date: April 2018

Miten Mistry  
Integrating Mixed Integer Nonlinear Programming and Satisfiability Modulo Theories for Next-Generation Optimisation Algorithms  
Supervisor: Dr Ruth Misener  
Start date: October 2015  
Finish date: September 2019

Nur Amirah Izzati Mohd Noor  
Industrial Smart Grid  
Supervisor: Prof Nina Thornhill  
Start date: September 2013  
Finish date: September 2017

Eðvald Moller  
Model Development and Evaluation  
Supervisors: Prof Nilay Shah and Prof Lazaros Papageorgiou  
Start date: November 2010  
Finish date: January 2018

Ioana Nascu  
Advances in Explicit/Multi-Parametric Model Predictive Control with applications in Anaesthesia  
Supervisor: Prof Efstratios Pistikopoulos  
Start date: January 2012  
Finish date: April 2016

Dimitrios Nerantzis  
Deterministic Global Optimisation Techniques  
Supervisor: Prof Claire Adjiman  
Start date: September 2012  
Finish date: September 2016

Andreas Nikolaou  
Multi-Scale Modelling of Light-limited Growth in Microalgae Production Systems  
Supervisor: Dr Benoît Chachuat  
Start date: November 2011  
Finish date: November 2015

Richard Oberdieck  
Theoretical and Algorithmic Developments in Multi-Parametric Optimization and Control  
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos  
Start date: September 2013  
Finish date: August 2016

Funmilyayo Olabode  
Parameter Estimation Using Neural Networks  
Supervisor: Dr Vivek Dua  
Start date: January 2014  
Finish date: January 2019
Anna Panteli  
Biorenewable Value Chain Optimization with Multi-Layered Value Chains and Advanced Analytics  
Supervisor: Prof Nilay Shah  
Start date: July 2014  
Finish date: July 2017

Maria Papathanasiou  
Multi-Parametric Model Based Control for Nonlinear, Periodic Systems: An Application to Biopharmaceutical Processes  
Supervisors: Prof Efstratios Pistikopoulos and Prof Athanasios Mantalaris  
Start date: November 2012  
Finish date: November 2016

Nehal Patel  
Comparison of Chromatographic and Two-Phase Separations for Novel Biopharmaceuticals  
Supervisor: Prof Eva Sørensen  
Start date: September 2012  
Finish date: September 2016

Carlos Perez-Galvan  
Global Optimisation of Dynamic Process Systems  
Supervisor: Prof David Bogle  
Start date: January 2013  
Finish date: December 2016

Nikola Peric  
Towards the Next Generation of Algorithms and Software for Global Optimization of Energy and Environmental Systems  
Supervisor: Dr Benoît Chachuat  
Start date: October 2013  
Finish date: September 2016

Stefan Pfenninger  
Multi-Scale Energy Systems Modelling  
Supervisor: Dr James Keirstead  
Start date: October 2012  
Finish date: September 2015

Catalina Pino  
Electrodes by Design - Improved Electrodes for Redox Flow Batteries  
Supervisor: Prof Nigel Brandon  
Start date: October 2015  
Finish date: September 2019

Channarong Puchongkawarin  
Optimisation-Based Methodology for the Design and Operation of Sustainable Wastewater Treatment Facilities  
Supervisors: Dr Benoît Chachuat and Prof David Stuckey  
Start date: November 2011  
Finish date: February 2016

Ana Luz Quiroga Campano  
Mathematical Modelling and Experimental Validation for the Optimization and Control of Mammalian Cell Culture Systems  
Supervisor: Prof Athanasios Mantalaris  
Start date: October 2012  
Finish date: October 2016

Sadia Rahman  
Computer Simulation of Coarse-Grained Models of Ionic Surfactants  
Supervisors: Prof Erich Müller, Prof Amparo Galindo and Prof George Jackson  
Start date: September 2012  
Finish date: August 2016

Jai Rajyaguru  
Rigorous Numerical Analysis with Polynomial Models: Applications to Implicit and Differential-Algebraic Equations  
Supervisor: Dr Benoît Chachuat  
Start date: October 2011  
Finish date: February 2016

Shakeel Ramjanee  
Integrated Production Modelling Systems for the Upstream Oil & Gas Industry and Field Performance  
Supervisors: Prof Nilay Shah, Dr Benoît Chachuat and Prof Ann Muggeridge  
Start date: October 2015  
Finish date: October 2018

Kristzian Ronaszegi  
Water Splitting for Hydrogen Production for Use in Dwellings  
Supervisor: Prof Eric Fraga  
Start date: May 2011  
Finish date: September 2016

Daniel Ross  
Multi-Scale Simulation of the Transport of Hydrocarbons in Porous Engine Deposits  
Supervisor: Prof Erich Müller  
Start date: October 2012  
Finish date: September 2016

Victor Sanchez Tarre  
A Combined Multi-Scale Modelling and Experimental Approach to Optimize Algal Culture Efficiency at the Metabolic, Process and Reactor Design Level  
Supervisors: Dr Alexandros Kiparissides and Dr Gary Lye  
Start date: September 2015  
Finish date: September 2019

Symeon Savvopoulos  
Mathematical Modelling of Chronic Lymphocytic Leukaemia  
Supervisor: Prof Athanasios Mantalaris  
Start date: March 2014  
Finish date: March 2018
Oliver Schmidt
Supervisor: Dr Adam Hawkes
Start date: October 2015
Finish date: October 2018

Marzia Sesini
Gas Storage and its Strategic Coordination within the EU Market: A Qualitative and Quantitative Approach
Supervisor: Dr Adam Hawkes
Start date: October 2015
Finish date: October 2019

Olivia Sloan
Combined CO$_2$ Storage and Enhanced Oil Recovery in the North Sea. Rock Heterogeneity and Flow in Geologic Systems with Low Flow Potential – applications to Subsurface CO$_2$ Injection
Supervisors: Dr Sam Krevor, Dr Niall McDowell and Dr Jerome Neufeld (University of Cambridge)
Start date: October 2015
Finish date: October 2019

Bowen Song
Solid Oxide Fuel Cell
Supervisor: Prof Nigel Brandon
Start date: October 2015
Finish date: October 2018

Si Nga Sou
Understanding the Impact of Bioprocess Conditions on Monoclonal Antibody Glycosylation in Mammalian Cell Cultures through Experimental and Computational Analyses
Supervisors: Dr Cleo Kontoravdi and Dr Karen M Polizzi
Start date: October 2011
Finish date: February 2016

Graham Stevenson
Engineering Ceramic Scaffold Electrodes for Solid Oxide Fuel Cells and Solid Oxide Electrolyzer Cells
Supervisor: Prof Nigel Brandon
Start date: September 2015
Finish date: September 2019

Flávio Strutzzel
Economically Optimal Integrated Process and MPC Control Design
Supervisor: Prof David Bogle
Start date: October 2014
Finish date: September 2018

Carlos Ricardo Suarez Heredia
Development of a Combined Mathematical and Experimental Platform for the Design and Optimisation of Metabolically Balanced Nutrient Supplementation Strategies in Semi-Continuous Mammalian Cell Cultures
Supervisor: Dr Alexandros Kyparissidis
Start date: April 2016
Finish date: March 2020

Muxin Sun
Design of Tractable MPC and NCO-Tracking Controllers using Parametric Programming
Supervisors: Prof Efstratios Pistikopoulos and Dr Benoit Chachuat
Start date: September 2013
Finish date: September 2016

Thapanar Suwanmajo
Modelling and Systems Engineering Approaches for Elucidating Dynamics and Information Processing of Multi-Site Phosphorylation Systems
Supervisor: Dr Jawahar Krishnan
Start date: April 2011
Finish date: July 2016

Asma Tahlawi
Development of a Three-Dimensional Biomimicry for the Culture of Normal and Abnormal Haematopoietic Cells
Supervisor: Prof Athanasios Mantalaris
Start date: September 2013
Finish date: November 2017

Naveed Tariq
Model Based Analysis of Low Carbon Energy Pathways based on Natural Gas
Supervisor: Prof Nilay Shah and Prof Paul Fennell
Start date: October 2012
Finish date: October 2016

Quang Tran
Sampling Algorithms for Stochastic Programming Using Importance Sampling and Markov Chain Monte Carlo
Supervisors: Prof Berc Rustem and Dr Panos Parpas
Start date: October 2011
Finish date: June 2016

Cristian Triana
Heat Integration for Bioethanol Process from Lingocellulosic Biomass
Supervisors: Prof Eric Fraga and Prof Eva Sørensen
Start date: October 2011
Finish date: June 2016

Argyro Tsipa
Connecting Transcriptional Regulation to Microbial Growth Kinetics in Cultures of Pseudomonas Putida
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: September 2011
Finish date: February 2016
Chonlatep Usaku
An Integrated Experimental and Modelling Approach for the Study of Apoptosis in GS-NS0 Cell Cultures
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: October 2010
Finish date: March 2016

Mario Villanueva
Set-Theoretic Methods for Analysis, Estimation and Control of Nonlinear Systems
Supervisor: Dr Benoît Chachuat
Start date: October 2011
Finish date: September 2015

Yukun Wang
Set Theoretic Approaches in Estimation and Optimization of Large-Scale Process Systems
Supervisor: Dr Benoît Chachuat
Start date: October 2015
Finish date: March 2019

Carmen Wouters
Optimal Design and Regulation of Residential Distributed Energy Systems
Supervisors: Prof Eric Fraga and Dr Adrian James
Start date: February 2013
Finish date: February 2017

Dionysios Xenos
ENERGY-SMARTOPS
Supervisor: Prof Nina Thornhill
Start date: September 2011
Finish date: December 2015

Iván Ying Xuan
Electricity Demand-Side Response from Heavy Industrial Loads
Supervisor: Prof Nina Thornhill
Start date: October 2015
Finish date: October 2018

Joseph Yao
Biomass Combustion with In-Situ CO₂ Capture Via the Calcium Loop
Supervisor: Prof Geoffrey Maitland
Start date: October 2012
Finish date: September 2015

Mauricio Javier Zamorano Mosnaim
Human Dental Pulp Stem Cells: Characterisation and In Vitro 3D Bone Ontogenesis
Supervisor: Prof Athanasios Mantalaris
Start date: January 2012
Finish date: February 2016
**PhD Graduates 2014–2015**

On completion of their studies, our graduates quickly find employment in many sectors including: industry, academia, consulting, finance and software.

**Dr Ozlem Akgul**  
Optimisation of Bioenergy Supply Chains  
Supervisors: Professor Lazaros Papageorgiou and Professor Nilay Shah  
Employer: Baringa

**Dr Alireza Behjousiar**  
*In Situ* FRET Biosensors for the *In Vivo* Measurement of Important Metabolites during Cell Culture  
Supervisors: Dr Cleo Kontoravdi and Dr Karen Polizzi  
Employer: Gap year

**Dr Aiman Alam Nazki**  
Elucidating the Spatial Organization and Control of Information Processing in Cell Signalling Networks: From Network and Enzymatic Building Blocks to Concrete Systems  
Supervisor: Dr Jawahar Krishnan  
Employer: Awarded EPSRC Prize Fellowship, Imperial College London

**Dr Shane Cadogan**  
Diffusion of CO₂ in Fluids Relevant to Carbon Capture, Utilisation and Storage  
Supervisors: Professor Geoffrey Maitland and Professor Martin Trusler  
Employer: Erlangen Graduate School in Advanced Optical Technologies (SAOT) Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Germany

**Dr Saif Al Ghafri**  
Phase Behaviour and Physical Properties of Reservoir Fluids Under Addition of Carbon Dioxide  
Supervisors: Professor Martin Trusler and Professor Geoffrey Maitland  
Employer: Research Fellow, University of Western Australia

**Dr Ahmed Alhajaj**  
Multiscale Design and Analysis of CO₂ Capture, Transport and Storage Networks  
Supervisors: Professor Nilay Shah, Professor Nigel Brandon and Professor Velisa Vesovic  
Employer: Masdar Institute

**Dr Inês Da Mata Cecilio**  
Study of Simulated Moving Bed Reactor (SMBR) for Para-Xylene Production  
Supervisor: Professor Nina Thornhill  
Employer: Research Scientist at Schlumberger

**Dr Emily Chapman**  
Micro-Model Pore-Scale Flow Studies of Fluid Displacement in Carbonate Rock with Application to CO₂ Storage  
Supervisor: Dr Edo Boek  
Employer: Associate at Expand Research - A Company of the Boston Consulting Group

**Dr Donald O’Donoghue**  
Mathematical Modelling of Ion Transport in Healthy and Cystic Fibrosis Human Airway Epithelia  
Supervisor: Dr Vivek Dua  
Employer: Quantitative Analyst at Irish Life Investment Managers

**Dr Pongsathorn Dechatiwongse**  
A Study of the Growth and Hydrogen Production of Cyanothece sp. ATCC 51142  
Supervisors: Professor Klaus Hellgardt and Professor Geoffrey Maitland  
Employer: Walailak University, Nakhon Si Thammarat, Thailand

**Dr Christos Argyropoulos**  
A Combined Immersed Boundary/Phase-Field Method for Simulating Two-Phase Pipe flows  
Supervisor: Dr Edo Boek  
Employer: Postdoctoral Research Associate at Texas A&M University and Mary Kay O’Connor Process Safety Center at Qatar

**Dr Joakim Beck**  
Efficient Targeted Optimisation for the Design of Pressure Swing Adsorption Systems for CO₂ Capture in Power Plants  
Supervisor: Professor Eric Fraga  
Employer: Department of Statistical Science, UCL
Dr Nasim Elahi  
*Multiscale Modelling of Carbon Capture and Storage*
Supervisor: Professor Nilay Shah  
Employer: Research Associate, Supply Chain Optimisation, Machine learning, Data Science, Imperial College

Dr Hendrik Frentrup  
*Molecular Simulation of Diffusive Mass Transport in Porous Materials*
Supervisor: Professor Erich Müller  
Employer: R&D Engineer, Dyson

Dr Maria Fuentes Gari  
*A Mathematical Model of Cell Cycle Heterogeneity for Personalizing Leukemia Chemotherapy*
Supervisor: Professor Athanasios Mantalaris  
Employer: Process System Enterprise Limited (PSE), London, United Kingdom

Dr Zara Ganase  
*An Experimental Study on the Effects of Solvents on the Rate and Selectivity of Organic Reactions*
Supervisors: Professor Clare Adjiman, Professor Amparo Galindo and Professor Alan Armstrong (Imperial Chemistry)  
Employer: Intel, Ireland

Dr David Garcia Munzer  
*Cell Cycle Heterogeneity Study by an Integrated Modelling and Experimental Approach*
Supervisors: Professor Athanasios Mantalaris and Professor Efstratios Pistikopoulos  
Employer: Postdoctoral Associate, Novartis, Switzerland

Dr Michael Hadjiyiannis  
*Decision Under Uncertainty: Problems in Control Theory, Robust Optimization and Game Theory*
Supervisor: Dr Daniel Kuhn  
Employer: A company in Cyprus

Dr Grani Hanasusanto  
*Decision Making Under Uncertainty: Robust and Data-Driven Approaches*
Supervisors: Dr Daniel Kuhn and Dr Wolfram Wieseman  
Employer: Faculty member at UT Austin

Dr Abdihakim Hassan  
*Modelling Solvent Mixtures and their Effects on Reactions*
Supervisors: Professor Claire Adjiman and Professor Amparo Galindo  
Employer: Shell

Dr Philip Jedrzejewski  
*A Platform for the Optimisation of Metabolic Pathways for Glycosylation to Achieve a Narrow and Targeted Glycoform Distribution*
Supervisor: Dr Cleo Kontoravdi  
Employer: Gap year

Dr Alexandra Krieger  
*Modelling, Optimisation and Explicit Model Predictive Control of Anaesthesia Drug Delivery Systems*
Supervisor: Professor Efstratios Pistikopoulos  
Employer: Research Assistant, RWTH Aachen, Germany

Dr Sarantos Kyriakopoulos  
*Amino Acid Metabolism in Chinese Hamster Ovary Cell Culture*
Supervisor: Dr Cleo Kontoravdi  
Employer: BioMarin, Ireland

Dr Romain Lambert  
*Approximation Methodologies for Explicit Model Predictive Control of Complex Systems*
Supervisor: Professor Efstratios Pistikopoulos  
Employer: Research Associate, Imperial College London

Dr Olga Lobanova  
*Development of Coarse-Grained Force Fields from a Molecular Based Equation of State for Thermodynamic and Structural Properties of Complex Fluids*
Supervisors: Professor George Jackson and Professor Erich Müller  
Employer: Syngenta

Dr Duy Luong  
*Optimisation for Image Processing*
Supervisors: Professor Berc Rustem, Dr Panos Parpas and Professor Daniel Rueckert  
Employer: Imperial College London

Dr Mithila Manage  
*An Investigation into the Feasibility of Integrating Intermediate-Temperature Solid Oxide Electrolysers with Power Plants*
Supervisor: Professor Eva Sørensen  
Employer: NNL

Dr Jan Marzinek  
*Molecular Dynamics Modelling of Skin and Hair Proteins*
Supervisors: Professor Athanasios Mantalaris and Professor Efstratios Pistikopoulos  
Employer: Postdoctoral Research Fellow, A *STAR/National University of Singapore, Singapore

Dr Ali Mehdizadeh  
*Food Industry Supply Chain Planning with Product Quality Indicators*
Supervisor: Professor Nilay Shah  
Employer: Strategy and Operation, Supply Chain (Consultancy), Birds Eye Iglo Limited

Dr Silvia Padula  
*Capacity Planning for Water Supply Networks*
Supervisor: Professor Lazaros Papageorgiou  
Employer: University of Manchester
Dr Antonio Marco Pantaleo  
*Perspectives on the Role of Bioenergy for Distributed Heat and Power Generation*  
Supervisor: Professor Nilay Shah  
Employer: Imperial College London

Dr Nicole Papaioannou  
*Environmental Impact Assessment and Optimization of Urban Energy Systems*  
Supervisor: Professor Nilay Shah  
Employer: Principal Consultant - Gas & Power at Wood Mackenzie

Dr Olga Parkes  
*Defining a Comprehensive Methodology for Sustainability Assessment of Mega-Event Projects*  
Supervisors: Professor David Bogle and Professor Paola Lettieri  
Employer: UK Dept of Energy and Climate Change

Dr Eleni Pefani  
*Modelling and Optimisation Based Drug Delivery Systems for the Treatment of Acute Myeloid Leukemia (AML)*  
Supervisors: Professor Efstratios Pistikopoulos and Dr Nicki Panoskaltsis  
Employer: GlaxoSmithKline, Stevenage, United Kingdom

Dr Cheng Peng  
*Chemical Interactions Between CO2 Acidified Aqueous Fluids and Carbonate Minerals*  
Supervisors: Professor Geoffrey Maitland, Professor Martin Trusler and Dr John Crawshaw  
Employer: Shell Global Solutions International B.V., Rijswijk, Netherlands

Dr Vladimir Roitch  
*Optimisation Applied to Cloud Computing*  
Supervisors: Dr Daniel Kuhn and Dr Wolfram Wiesemann  
Employer: Lecturer at City University

Dr Pedro Rivotti  
*Multi-Parametric Programming and Explicit Model Predictive Control of Hybrid Systems*  
Supervisor: Professor Efstratios Pistikopoulos  
Employer: Research Associate, Imperial College London

Dr Cyrus Siganporia  
*Production Planning for Biopharmaceuticals*  
Supervisor: Professor Lazaros Papageorgiou  
Employer: Research Associate, University College London

Dr Erini Siougkrou  
*Systematic Methods for Solvent Design: Towards Better Reactive Processes*  
Supervisors: Professor Claire Adjiman and Professor Amparo Galindo  
Employer: Marie Curie Research Fellow at National Technical University of Athens

Dr Saurabh Mahesh Kumar Shah  
*Multi-Scale Pore Imaging of Multiphase Flow in Porous Media*  
Supervisor: Dr Edo Boek  
Employer: QCCSRC Experimental Officer, Imperial College London

Dr Roochi Solanki  
*Modelling of a Two-Phase Thermofluidic Oscillator for Low-Grade Heat Utilisation*  
Supervisors: Dr Christos Markides and Professor Amparo Galindo  
Employer: Carbon Credentials

Dr Ioanna Stefani  
*Unravelling the Progression of Endoplasmic Reticulum Stress in Familial Alzheimer’s Disease*  
Supervisors: Dr Cleo Kontoravdi and Dr Karen Polizzi  
Employer: ICON (Medical Consulting)

Dr Ailing Teo  
*Exploring New Bioprocess Considerations for Cardiomyogenesis of Embryonic Stem Cells*  
Supervisors: Professor Athanasios Mantalaris and Professor Lim Mayasari  
Employer: Associate Patent Examiner at Intellectual Property Office of Singapore

Dr Lingjian Yang  
*Optimisation Approaches for Data Mining in Biological Systems*  
Supervisor: Professor Lazaros Papageorgiou  
Employer: PDRA at University of Manchester

Dr Lara Yaroson  
*Force Field Parameters from the SAFT Equation of State for the Molecular Simulation of Fused Molecules*  
Supervisors: Professor George Jackson, Professor Erich Müller and Professor Amparo Galindo  
Employer: Syngenta

Dr Stamatina Zavitsanou  
*Modeling and Multi Parametric Control Drug Delivery Systems for Diabetes Type 1*  
Supervisor: Professor Efstratios Pistikopoulos  
Employer: Postdoctoral Research Scholar at SEAS, Harvard University