Centre for
Process
Systems
Engineering

cpse

Centre for Process Systems Engineering

Annual Report 2012 – 2013

Imperial College London | UCL

Contents
2012–2013 CPSE Annual Report

Welcome to the 2012–13 CPSE Annual Report

Professor Nilay Shah

CPSE Director

"CPSE has enjoyed great success during the past couple of years. This is due to the hard work of our academics, students, researchers and the loyal support of our industrial partners."

Introduction
2012/13 CPSE Annual Report

The Centre for Process Systems Engineering draws upon the world-leading science and engineering based skills of Imperial College London and University College London

World renowned academics use sophisticated modelling techniques and experimental studies where appropriate to study complex systems ranging from molecular structure and biological systems through to complex chemical/energy plants, urban environments and supply chains. The Centre has 27 academic staff, 124 PhD students and 52 research fellows and associates and a portfolio of grants worth more than £30 million.

CPSE History

CPSE was inaugurated in 1989 by Professor Roger W.H. Sargent, the founding Director of the Centre from 1989 to his retirement in 1992. Since then, CPSE has continued the legacy of Professor Sargent and remains a Centre of Excellence. Our academics come from multi-disciplinary backgrounds, including: chemical engineering, mathematics, physics and chemistry and are international leaders in their fields. We consistently attract major grants as well as high calibre PhD students and Research Associates from around the world.

The Centre's cutting-edge research has been recognized by many awards, including the Royal Academy of Engineering MacRobert Award in 2007 (the UK's highest award for innovation in engineering). This prestigious award was presented to the Centre's spin-out company Process Systems Enterprise Limited (PSE). The award was in recognition of PSE's highly innovative modelling software gPROMS which to date remains "the leading modelling product within the chemical industry." gPROMS is a mathematical modelling systems developed to help make chemical plants safer and more efficient. It continues to be successful. Previous winners of this esteemed award include IBM, Rolls Royce and BP.

Research programme

The research carried out in CPSE can be found in this report under the headings of Competence Areas that require similar research tools and approaches for their solution and the main industrial sectors or Domains where the research is applied.

CPSE Industrial Consortium Membership

CPSE's Industrial Consortium has been running for nearly 25 years. The membership provides opportunities for member companies 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. We have 9 multinational companies and recently AkzoNobel has become our newest member. AkzoNobel is a Global Fortune 500 company and has operations in more than 80 countries. AkzoNobel is also the largest global paints and coatings company and a major producer of specialty chemicals. We are delighted to have our latest member and welcome AkzoNobel in our consortium.

Detailed information on our Industrial Consortium can be found later in the report. Companies and organisations wishing to join the CPSE Consortium should contact me, Professor Nilay Shah at: **n.shah@imperial.ac.uk**.

Research Income

The Centre has research income portfolio of £30m. We have continued to attract major funding from industrial companies and organisations, such as: UK Research Councils, the European Union, and overseas governments. At a time when many Universities, Departments and Centres have seen their income decline due to the funding constraints, we have continued to secure funding for our research. We believe this is indicative of the quality of research conducted in the Centre.

Highlights
2012/13 CPSE Annual Report

It gives me pleasure to share with you our activities in CPSE. Due to the lack of space, I will only give a brief summary of some of our activities and accomplishments

New Academics

I am pleased to introduce 4 new CPSE academics:

Dr Peter DiMaggio, Lecturer, Department of Chemical Engineering Imperial College London. Dr DiMaggio, obtained his PhD in Chemical Engineering, in 2010 from Princeton University. Prior to joining Imperial College, he was NIH/NRSA Postdoctoral Fellow, Department of Molecular Biology, Princeton University. Dr DiMaggio is interested in the development and application of innovative experimental and computational platforms for characterizing chromatin-associated proteins and how their interactions and post-translational modifications cooperatively regulate nuclear processes, such as gene expression.

Dr James Keirstead, Lecturer, Department of Civil and Environmental Engineering, Imperial College London. Dr Keirstead obtained his DPhil in 2006 from University of Oxford where he also obtained his MSc in Environmental Change and Management (2003). Previously, he was a Research Fellow and Team Leader of the BP Urban Energy Systems project and lead editor of the resulting book Urban Energy Systems: An Integrated Approach (Earthscan, 2013). His research focuses primarily on urban energy systems.

Dr Panos Parpas, Lecturer, Department of Computing, Imperial College London. Prior to joining Imperial, Dr Parpas was a postdoctoral fellow at the MIT Energy Initiative (2009-2011). Before that he was a quantitative associate at Credit-Suisse (2007-2009). He completed his PhD in computational optimization in 2006 at Imperial College, where he also received his MSc in Advanced Computing in 2002. Dr Parpas' research interests are in the development and analysis of algorithms for large scale optimisation problems. He is also interested in exploiting the structure of large scale models arising in applications.

Dr Michail Stamatakis, Lecturer in Chemical Engineering, University College London. Dr Stamatakis received his diploma from the National Technical University of Athens, Greece in 2004, and his PhD from Rice University, Houston, Texas in 2009. He subsequently joined the University of Delaware as a Post-doctoral researcher, performing research on multiscale modelling of catalytic phenomena on transition metal surfaces. Dr Stamataki research interests are; Computational catalysis, chemical reaction engineering, multiscale modelling, microkinetic modelling, kinetic Monte Carlo.

Departing Academic

Dr Daniel Kuhn has sadly left Imperial College in 2013. He is now working as Associate Professor at the College of Management of Technology at EPFL where he holds the Chair of Risk Analytics and Optimization (RAO). Dr Kuhn has been with CPSE for many years and will be greatly missed.

Academic Promotions

- **Professor Nilay Shah**, Director of CPSE has been promoted to other roles: he is the Director of Research in the Department of Chemical Engineering in addition to being Director of the Manufacturing Futures Lab at Imperial.
- **Professor Nina Thornhill** has become the Director of Undergraduates Studies in Department of Chemical Engineering.
- **Professor Erich Müller** remains as the Director of Resource in Department of Chemical Engineering.
- **Lazaros Papageorgiou** has been promoted to Professor.
- **Professor Claire Adjiman**, **Professor Amparo Galindo** and **Professor Erich Müller** gave their Inaugural Lectures in summer 2013. It was a privilege for the Centre to share these huge milestones in their academic careers.

Highlights
2012–2013 CPSE Annual Report

Honours and Awards

Professor Geoffrey Maitland is currently the Deputy President of the Institution of Chemical Engineers (IChemE). Due to his prominent work, he has also been elected President from May 2014. IChemE is the global professional membership organisation for people with relevant experience or an interest in chemical engineering and has over 38,000 members across 120 countries.

Professor Geoffrey Maitland was awarded the 2013 Imperial President and Rector's Award for Excellence in Pastoral Care. This award is given by Imperial to outstanding individuals who have shown exemplary behaviour and actions in relation to pastoral care for students. In addition to this, Professor Maitland received 'Best Personal Tutor' Award by Chemical Engineering Undergraduates.

Professor Stratos Pistikopoulos was elected Fellow of the Royal Academy of Engineering in 2013, for his pioneering research on the development of theory, algorithms and computational tools in multi-parametric programming, explicit model based predictive control and process optimization under uncertainty.

Professor Stratos Pistikopoulos was the recipient of the 2012 Computing in Chemical Engineering Award given by the Computing and Systems Technology (CAST) Division of the American Institute of Chemical Engineers (AIChE). There are only 3 previous UK winners of the Award, one of them being Professor Roger W.H. Sargent in 1990. Professor Pistikopoulos is the fourth European to receive the CAST prize in its 33-year history.

Professor Nilay Shah and **Professor Lazaros Papageorgiou** were awarded the 2013 IChemE Hutchison Medal.

High Profile Events

Professor David Bogle co-organised the ESCAPE-22 Conference which was held in University College London in June 2012. The conference explored how computer aided process engineering (CAPE) plays a key design and operations role in the process industries.

Each year, the Centre celebrates its founding Academic Father **Professor Roger Sargent** through the Annual Professor Roger W.H. Sargent Lecture. This is a major event in the Centre's calendar created as a tribute to Professor Roger Sargent's legacy in the field of Process Systems Engineering. The distinguished speakers who delivered the lectures are:

2012 **Professor Sebastian Engell**, Technische Universität Dortmund "Optimization under lack of knowledge – the key to operational excellence"

2013 **Professor Francis J. Doyle III**, University of California, Santa Barbara "Engineering the Artificial Pancreas"

New Ventures

Professor Nilay Shah (MFL Director) and his team launched the new Manufacturing Futures Lab on 4th June 2013. The MFL (**www.imperial.ac.uk/manufacturingfutureslab**) brings together experts from Imperial to focus on improving the UK's manufacturing technologies and processes. The Lab involves researchers from the fields of chemistry, physics, materials engineering, composites, membrane technologies, control engineering, bioengineering, process systems engineering, synthetic biology, microelectronics design and management, who collectively are supported by over £100m of externally sponsored research.

ERC Advanced Investigator Grant

Professor Sakis Mantalaris has been awarded a €2.5m five year Advanced Grant by the European Research Council (ERC). Established under the EU's Seventh Research Framework Programme (FP7), the grants target distinguished researchers based in Europe. Of the five Advanced Grants awarded to Chemical Engineers in the UK since the scheme began in 2007, two have been based at CPSE (Professor Pistikopoulos and Professor Mantalaris). BioBlood is one of just 284 successful peer-reviewed bids from over 2,400 applications, in what is the final year of the €7.5b FP7 Programme.

New Book

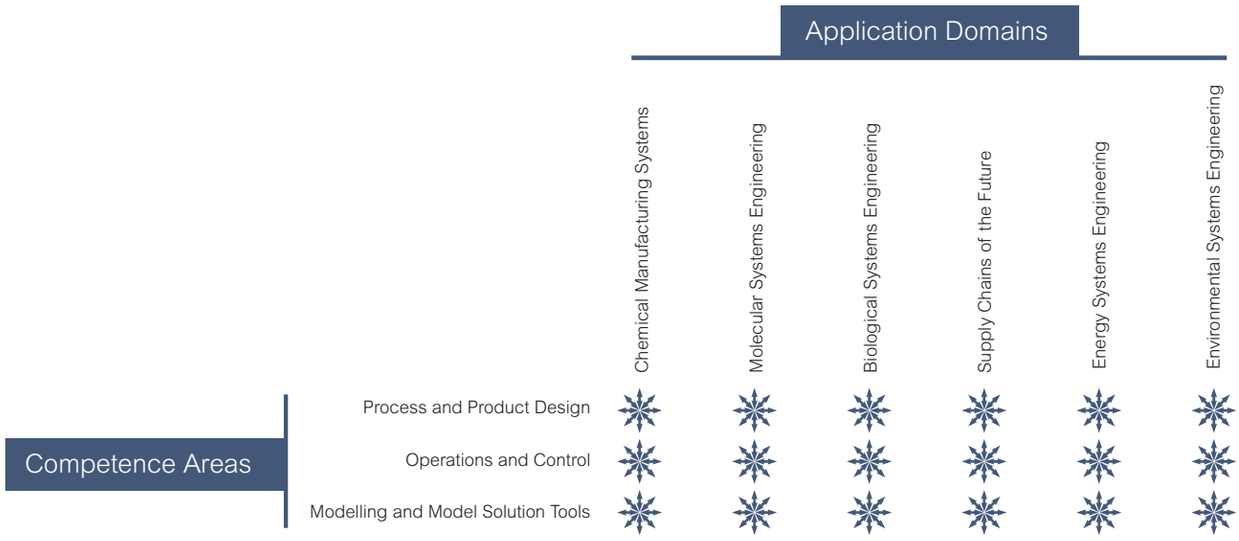
Dr James Keirstead and **Professor Nilay Shah** published a book titled 'Urban Energy Systems: An Integrated Approach.' The book brings together the major lessons learnt from a £4.5 million, 5-year collaborative project with BP that investigated the technologies and systems used in cities to distribute and consume energy.

Media Coverage

CPSE Director, **Professor Nilay Shah** and **Professor Geoffrey Maitland** were interviewed in several newspapers/ TV. Their expertise were sought after on various topics including recently when Professor Shah was interviewed following the launch of a report into global decarbonisation.

We hope that you will enjoy reading our 2012–2013 Annual Report as much as we have enjoyed putting it together. You can find out more about CPSE through our website: **http://www3.imperial.ac.uk/centreforprocesssystemsengineering**

Professor Nilay Shah
Director, Centre for Process Systems Engineering



Industrial Consortium
Graham Elkes

"Through the Industrial Consortium, CPSE can provide a tailor made service to individual Company members while fostering a broader cross-business sector understanding of process systems engineering developments."

CPSE Industrial Consortium
2012–2013 CPSE Annual Report

The Centre started the Industrial Consortium when it was inaugurated in 1989 to address challenges facing industry

Since then, it has continued to provide opportunities for member companies 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 are multinational companies from various industrial sectors including: gas, oil, pharmaceuticals and chemicals.

The Centre has tailored a unique relationship with member companies to prioritise and help solve issues associated with Process Systems Engineering.

Benefits for Members

Members have privileged access to CPSE academics, research staff and students. They also gain opportunities to network with other companies and organisations involved in Process Systems Engineering.

Each member company has a nominated CPSE academic as a point of contact or 'Friend'. The Friend is the first point of contact within CPSE and is responsible for tailoring the relationship to meet individual company needs. They will also facilitate informal interactions with the companies so member companies have an opportunity to build a close relationship with CPSE.

Members are invited to an annual meeting in December which includes:

- the Roger Sargent lecture by a distinguished international expert on a Process Systems topic;
- presentations by CPSE staff on key research areas;
- formal presentations and posters by CPSE research students.

The CPSE website also has a separate members only section. Member companies can maximize the benefits they gain through the following interactions:

Students
Meet and build relationships with CPSE MSc and Research students who might become future employees. Member companies can also link with MSc projects in the Process Systems and Engineering course through proposing areas for projects.

These projects could include add-ons to existing sponsored research in CPSE or scouting projects on areas of potential interest.

Academic staff
Build a close relationship with Imperial and University College CPSE staff through research projects of mutual interest. Gain access to strategic science and technology insight from the CPSE team. Enjoy assisted access to other Imperial College and University College research and development activities. Secondments can also be arranged where appropriate.

Future R&D
Develop company specific or collaborative, leveraged research projects through discussion with CPSE staff and Consortium members. Exploit technology transfer opportunities. Provide strategic input into the CPSE research portfolio in order to gain early competitive advantage.

Information
Access to pre-publication papers and reports, presentation materials, monthly CPSE seminars, project listings and the CPSE annual report either through the members-only website or as hard copy.

Current Member Companies

The Industrial Consortium presently has 9 members from different industries who are all major companies in their industry.

Company	Academic Friend
ABB Corporate Research	Professor Nina F Thornhill
AkzoNobel	Professor George Jackson
BP	Professor Nilay Shah
Petrobras	Professor David Bogle
Praxair	Dr Benoît Chachuat
PSE	Professor Costas Pantelides
Proctor and Gamble	Professor Erich Müller
Shell Research and Technology	Professor Geoffrey C Maitland
Syngenta	Professor Claire Adjiman

Companies and organisations wishing to join the CPSE Consortium should contact the CPSE Director, Professor Nilay Shah at **n.shah@imperial.ac.uk**

CPSE Research Programme
Professor Claire Adjiman

"The outstanding CPSE facilities and support team give CPSE researchers and collaborators the opportunity to take their ideas from concept to application."

Competence Area
Product and Process Design

The development of systematic model-based methodologies for the rational design of processes and products continues to be an important area of activity within CPSE

Product and Process Design

This area encompasses a growing range of scales, from nanoscale models for materials selection, to mesoscale models for the design of processes for specific tasks, as well as, overall process models for integrated plant design. The approaches we develop are generic and we aim to enable engineers to meet the constraints and objectives imposed by today's business environment, in particular, in the field of sustainable development. We consider not only economic aspects, but also environmental, safety and health factors and this is exemplified both in theoretical work and in technology development projects. Part of the work is focused on early process development. Other projects are applicable to later development stages, and focus on detailed design for separation, reaction, reactive separation, or operability issues such as controllability or maintenance. Modelling spans a range of scales and includes the design of devices where material issues play an important role such as solid oxide fuel cells, the level of process units, and entire process systems. This wide-ranging activity engages researchers along four main themes, and interacts very strongly with the Molecular Systems Engineering activity.

Materials design for process synthesis
The design of products and processing materials, such as solvents and catalysts, is tackled in a holistic manner, from the development of new property prediction techniques and modelling techniques to the use of these techniques in the design of environmentally benign yet functional systems. Problem formulation and the interplay between the mathematical form of the model and the optimisation techniques are key issues addressed in this area. The design problems we address have an increasing number of degrees of freedom: in addition to "standard" variables such as temperature and pressure, molecular structure, microstructure or formulation variables are considered explicitly in the problem formulation. Novel designs suggested by the modelling methodology are verified through targeted experiments in collaboration with experimentalists. The results of the experimental exercise are then fed back to the model, resulting in an iterative modelling-experimentation strategy.

Design of novel manufacturing processes
Models and techniques are developed for the design of state-of-the-art processes with a particular focus on fine chemicals and polymers. Separation and/or reaction systems with increasingly complex interactions are considered, which require the combination of detailed models and state-of-the-art numerical techniques.

Integrated process synthesis
The interactions of design and operability are used to create processes with better overall performance. Diverse tools such as life-cycle analysis, computational fluid dynamics and process modelling are combined to enable the consideration of multiple decision criteria.

Technology transfer
This activity is focused on facilitating the transfer of our more mature technologies to industrial partners.

New and noteworthy achievements in the past year:

Advanced process modelling of chromatography for industrial bioseparations
Edward Close & Eva Sørensen

Therapeutic proteins are well established as a clinically and commercially important class of therapeutics, and have played a key role in major advances in the treatment of various disorders and diseases over the last quarter century such as cancer and autoimmune diseases. Developing and operating biopharmaceutical processes is, however, extremely challenging and is traditionally almost completely reliant on an extensive experimental effort conducted at great effort, time and cost. In collaboration with Pfizer and the Department of Biochemical Engineering at UCL, we have been developing systematic approaches to bioprocess design by integrating high fidelity predictive models of chromatographic bioseparations and stochastic simulation methodologies with traditional experimentally based industrial bioprocess development platforms. The objective has been to accelerate the development of industrial purification processes and to increase process robustness, whilst deriving fundamental knowledge and process understanding.

We have developed detailed models of key purification steps in the production of multiple commercial therapeutic proteins with annual revenues totalling over $1 billion. These models have been used in various applications across the development timeline. During early phase development, models have provided a link between high throughput ultra-scale down experimentation and laboratory scale scouting column experiments, identifying robust operating parameter ranges for challenging separations and directing optimal performance, whilst decreasing total development times. For candidate molecules nearing commercialisation, models have been used to generate probabilistic design spaces in order to resolve process performance issues and reduce risk by quantifying the impact of this process variability on the design space. The successful application of process systems engineering approaches to industrial bioseparations in this work provides a basis for the next generation purification process development.

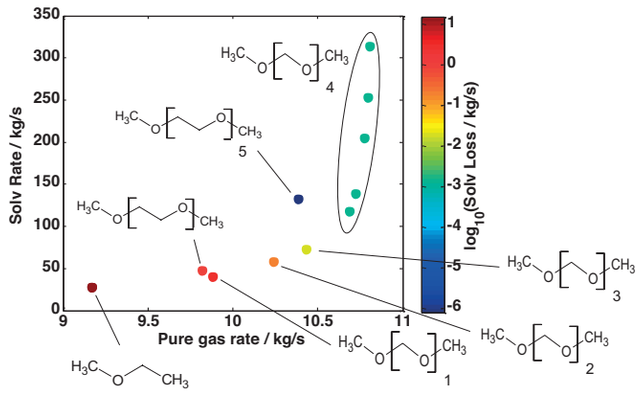


Figure (above). Solutions of the multi-objective optimisation used to determine suitable starting points for integrated process and solvent design. Solutions on the Pareto front are shown, based on three objective functions: solvent flowrate (vertical axis), methane production rate (horizontal axis) and solvent loss (colour scales).

Integrated process and solvent design for carbon capture

Jakob Burger (University of Kaiserslautern), Smitha Gopinath, Vasileios Papaioannou, Amparo Galindo, George Jackson, Claire Adjiman

We have been developing novel methodologies for the integrated design of processes and solvents by combining advances in the prediction of physical properties (see Molecular Systems Engineering) with computer-aided molecular design approaches. A specific challenge in this context is to handle the numerical complexities that arise from the simultaneous variation of the solvent and the process conditions, which can lead to large changes in the fluid phase behaviour within the process units. To address this issue, we have developed a hierarchical approach, in which an idealised process is first investigated using multi-objective optimisation. The best solutions (solvent molecular structure and process operating variables) that arise from this step are then used as starting points for a more reliable optimisation, in which a detailed process model is considered.

This hierarchical approach has been applied to the separation of carbon dioxide from methane via physical absorption. Natural gas streams often contain a large proportion of carbon dioxide which must be removed from the stream to increase its value. They are produced at a high pressure (typically a few MPa), which makes physical absorption a viable option. Using a simple absorption/desorption process consisting of one absorber and one flash unit, the SAFT-γ Mie equation of state was used in a predictive manner to model the impact of using different solvents on process performance (methane purity, recovery, net present value of the process). The class of solvent considered consisted of n-alkanes and linear ethers (methyl ethers, symmetric ethers, oxyethylene ethers and oxymethylene ethers). The hierarchical design approach allowed the identified of tetra(oxymethylene) dimethyl ether as the best solvent for this process, with a net present value 60% larger than that for the best n-alkane solvent.

Competence Area
Operations and Control

Process Operations uses mathematical models that capture the underlying science and adopts an optimization approach to give improved operation in terms of product quality, energy usage, environmental impact and sustainability

Operations and Control

Process Operations 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 with an emphasis on application to the process industries. Applied research covers a broad spectrum including within oil & gas, reaction and absorption, granulation and polymers. 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 broad range of activities in the past year includes:

Model-based optimization and control for process-intensification in chemical and biopharmaceutical systems
Process Intensification (PI) is the response to world-wide changes in the chemical/biopharmaceutical industry for specific end-use product properties and stricter energy and environmental constraints. In this framework, the OPTICO Project aims to overcome the limitations on implementing PI by establishing a new methodological design approach for sustainable, intensified chemical/biopharmaceutical plant design.

Within this scope, four specific processes (chromatography, polymerization, crystallization, oxidation) are examined in detail; the main focus thereby lies on the formulation of mathematical models of the processes as well as the identification of the bottlenecks of the process which limit its efficiency. Additionally, advanced control strategies are developed in order to enable a robust operation of the process which in return will enable the fulfilment of legal regulations while maintaining high process efficiency.

In collaboration with ETH Zurich and the ChromaCon AG, the CPSE mainly focuses on the optimization and control of a specific chromatographic system, the Multicolumn Solvent Gradient Purification (MCSGP) process. Due to its periodic and highly non-linear behaviour as well as the limited information available during operation, all model-based control strategies for this system have been unsuccessful so far. Using a multi-parametric programming approach we are aiming to develop not only a theoretical but also a practical approach to tackle this challenging class of problems. Theoretical work include devising new tools and algorithms for state estimation, and the solution of the multiparametric optimization problem. Applications include the use of system identification and model reduction techniques to recast the original model into a simpler form which then can be solved using the multi-parametric framework.

Theoretical advances in multi-parametric mixed-integer programming
The OPTICO project focuses on the theoretical aspects of multiparametric programming. Although the field of multiparametric programming involving only continuous variables has been explored in depth, such an analysis is missing for the hybrid case, where integer and continuous variables coexist in the problem formulation. The development of novel solution strategies for multiparametric Mixed-Integer Quadratic Programming (mp-MIQP) problems is therefore at the core of the work.

These strategies are also been considered within control formulations, especially in combination with dynamic programming. This combination has proven to be very efficient for the continuous case, and hopefully will have a similar effect for the hybrid case, opening up solutions for more complex (and therefore realistic) problems.

Novel state estimation techniques and their application in multi-parametric model predictive control
The implementation of explicit/multi-parametric MPC, and in general, MPC, is based on the assumption that the state values are readily available from the system measurements and that we have a clear measurable output with not much noise influence. Since information on the states is not always available due to difficulty to measure all the necessary states or expensive data acquisition equipment, advanced state estimation techniques are usually required. Dealing with system constraints entails the simultaneous use of moving horizon estimation (MHE) which can be implemented in a multi-parametric fashion. As a consequence the design and

implementation of mp-MPC together with state estimators is highly recommended.

Development of multi-parametric controllers for periodic, nonlinear systems

Industrial processes are commonly characterized by highly nonlinear models that follow a periodic operation profile. The demand for high product purity and low energy consumption render the development of advanced controllers, essential, as the process should always operate under optimal conditions that will assure fulfilment of the imposed constraints. It is therefore of vital importance to establish a holistic framework that will allow the development of multi-parametric controllers for nonlinear, periodic systems. Ultimately we are aiming to install the controllers on a bench-top experimental setup and test them against the original process.

Bioprocessing facility fit analysis

Due to limited information at pilot scale, facility fit assessments in industry are typically based on mass balance equations and former experience. The project provides systematic simulation tools and advanced decision support methods to predict the full range of possible outcomes of large scale facilities. It allows assessment of the trade-off between unexpected loss and the cost of oversized equipment. It solves facility fit issues arising during transfer of small pilot scale processes into large manufacturing scale facilities. Facility fit issues refer to any failure of requirement (e.g. unexpected mass loss, extra processing time) caused by mismatch of process equipment.

The outcome is a data mining decisional tool using decision tree classification method combined with Monte Carlo simulation for rapid prediction of facility fit issues and debottlenecking existing facilities. The industrially relevant case study demonstrated that this tool can be applied not only to predict the degree of facility fit of existing facilities by exploring the impact of process fluctuations on product mass loss but also to identify debottlenecking solutions worth pursuing with the series of if-then rules of the critical combinations of factors leading to different mass loss levels. The highlights are:

- A data mining decisional tool was created for prediction of facility fit issues
- Monte Carlo simulation was used to mimic biomanufacturing process fluctuations
- The decision tree discovered a set of rules to predict the root causes of mass loss
- Three different debottlenecking solutions were compared for a legacy facility

Furthermore, the innovation of my work has drawn great interest of MedImmune US and by great potential the tool will be applied to their manufacturing facilities in future demonstration projects. 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 such as GE Healthcare, GlaxoSmithKline, Pfizer and MedImmune.

A superstructure optimisation approach for clean water treatment

The water industry in England and Wales is one of the most heavily regulated industries, and water utilities are faced with increasingly stringent targets for the quality of the water received at customers' taps. The project is addressing the need for optimum functionality of water treatment plants to remain competitive by being able to make predictions on how the plants can be improved.

Due to the complex nature of the overall water treatment process and the interactions between unit operations, work in the literature has so far been focussing solely on the performance optimisation of individual water treatment units. This approach will inevitably lead to sub-optimal overall performance as the operation of one unit operation has an impact on the next, and their operations can therefore not be considered in isolation. A process-wide approach will therefore be of significant benefit to the water industry by increasing the overall process efficiency and thus decreasing plant costs. This is being done by taking into account the interactions between individual processing units to consider the plan as a whole. A design and operating procedure that considers an optimal series of several unit operations, including units which may run in parallel, whilst reducing the number of steps required for a given product quality, will improve the overall plant efficiency.

The use of superstructures, which contain all possible alternatives of a potential treatment network, has proved an effective tool for the synthesis of chemical engineering process flowsheets and for overall plant optimisation. This work addresses the current gap in water research by developing an approach based on superstructures for the synthesis of clean water treatment works through the application of mixed integer optimisation techniques. A systematic framework is presented for the representation of superstructures and derivation of optimisation models in process synthesis. The state task network (STN) and state equipment network (SEN) are proposed as the two fundamental representations of superstructures used to describe the overall plant operation including multiple sources of raw water and water treatment processes. Publications resulting from this work demonstrate that the approach can provide a valuable guidance in clean water treatment process design and operation.

Process Automation Research Programme:
Worldwide, there is a huge base 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 physical first principles.

Process plants also have mechanical and electrical equipment. We look 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

CO2 capture from gas-fired power plants (GAS-FACTS)
The Gas-FACTS project is funded by the EPSRC-Engineering and Physical Sciences Research Council. It started 01 April 2012 and involves a consortium of UK universities. Gas-FACTS will provide important underpinning research in for gas turbine modifications and post combustion capture technologies for gas power plants. These technologies are candidates for deployment between 2020 and 2030, and will be in operation until 2050 or beyond.

The challenge with CO2 capture in gas power plants is that gas-fired generators provide balancing services to the transmission grid in the presence of intermittent loads and variable generation from renewables. Such variable operation poses great challenges for the control and operation of carbon capture on gas power plants. The Process Automation group and the Thermophysics group at Imperial are working in the Gas-FACTS consortium on flexible capture systems for natural gas power plants through:

- Real time control of natural gas capture systems for power plants
- Experimental testing of liquid solvents including novel amine mixtures.
- Modelling and analysis for improved transient performance.

The aim is integration of the gas turbine and post-combustion capture to achieve excellent performance over a wide range of operating conditions, to allow rapid changes in output, to give an appropriate balance between fixed and variable costs, and to give good performance at a range of operating points. To date, a dynamic simulation Is complete and being used to explore operation and control in a range of scenarios.

Operations and Control – Highlighted project

Optimal operation of compressors in networks
It is well known that compressors consume large amounts of energy in different industrial sectors. In particular, compressors are one of the major energy consumers in many intensive chemical processes such as air separation. The focus of the project is to study optimization of the overall system, i.e the system in which multiple compressors operate in networks integrated with chemical process units.

The optimization of compressors leads to two different types of problem: (a) Real Time Optimization (RTO) related to optimal distribution of the load of compressors with a fixed configuration and (b) optimal scheduling and maintenance of compressors considering information for long time periods. The RTO scheme analyses raw data from the process to update models of the compressors to be used in the optimization to estimate the set points of the flows of the compressors which result in a more efficient operation compared to other conventional methods. The estimation of the best set points is called optimal distribution of load and it is also known as load sharing and multi-compressor capacity optimization. By contrast, optimal scheduling, which is given the forecast of the demand and other parameters, computes the optimal configuration of the compressors. Figure 1 shows the framework of these two interacting optimisation problems.

Study of the literature revealed a lack of a systematic way to optimally share the load of compressors considering varying operational conditions, such as atmospheric temperature and pressure, and demand. A common assumption is that individual compressors have the same characteristics and the same efficiencies, however many authors and practitioners reported that this is difficult or impossible. These characteristics and efficiencies change over time due to fouling and non-uniform maintenance plans. However, the conventional practice is to distribute the load evenly among the compressors or other similar strategies based on the assumption of constant performance and characteristics over time.

The RTO algorithm in Figure 1 solves the problem of the optimal load sharing. After data collection and conditioning, an NLP optimization problem employs data-driven models to estimate the optimal load sharing in the form of set points of the manipulated variables (opening of the actuators inlet guide vanes) and the controlled variables (mass flow rate). The set points are given to the control system whose role is to apply and keep these points until the next run of RTO.

The scheduling is formulated with as MINLP or MILP and decisions which involve discrete events (for example switching on or switching off a compressor). These decisions are used in the RTO. When the online compressors are not able to meet the requirements of the requested demand (due to disturbances coming from the customers), the scheduling problem updates the models and estimates a new schedule of the compressors which can satisfy the demand. The interactions between RTO and scheduling is part of the ongoing research.

Xenos et al. (2014a) presented the optimization of a compressor station with multi-stage centrifugal air compressors operating in parallel. Figures 2b and 2c show the electricity consumption of each compressor in the optimization case and the comparison of the total electricity consumption between the case of optimization and the case of equal distribution strategy. The study of the optimal distribution of load was examined for ten different cases with different demands. The results showed that the optimal distribution of load reduces the total electricity consumption compared to the case with equal split strategy.

The state-of-the-art of the scheduling of compressor networks examines the optimal operation and maintenance of compressors without considering the gradual degradation of a compressor over time. Xenos et al. (2014b) studied the scheduling and maintenance of compressor networks taking into account the deterioration of the performance of a compressor over time. An illustrative example considering the overall air separation plant (i.e. air compressors, separation units, storage tanks) compared the condition based maintenance optimization and a preventive maintenance optimization strategy. The condition-based maintenance optimization achieved 11% reduction in the overall cost, especially in the start-up, shut-down and maintenance costs compared to the benchmark preventive maintenance strategy (Fig 3).

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, in collaboration with the EPSRC Research Project EP/G059071/1 “Design Toolbox for Energy Efficiency in the Process Industry”.

References

Xenos D.P., Cicciotti M., Bouaswaig A.E.F., Thornhill N.F., Martinez-Botas R., 2014a, Modeling and optimization of industrial centrifugal compressor stations employing data-driven methods, Proceedings of ASME Turbo Expo 2014: Turbine Technical Conference and Exposition GT2014, June 16-20, 2014, Dussedorf, Germany. Xenos D.P., Kopanos G.M., Cicciotti M., Pistikopoulos E.N.,

Thornhill N.F., 2014b, Operational optimization of compressors in parallel considering condition-based maintenance, Proceedings of the 24th European Symposium on Computer Aided Process Engineering - ESCAPE 24, June 15-18, 2014, Budapest, Hungary.

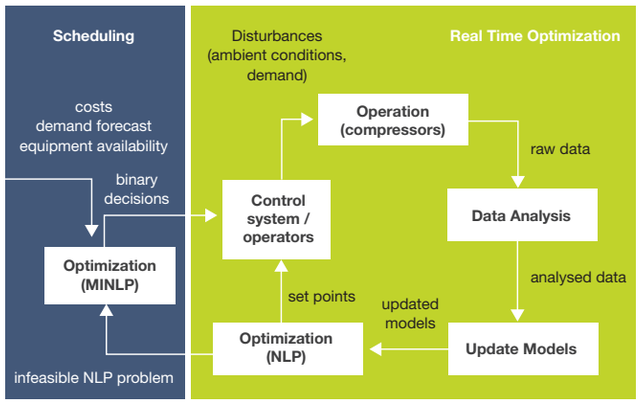


Figure (above). Framework for optimizing compressor stations.

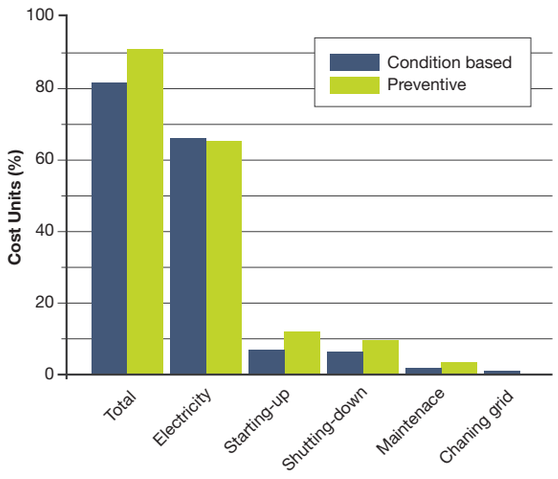
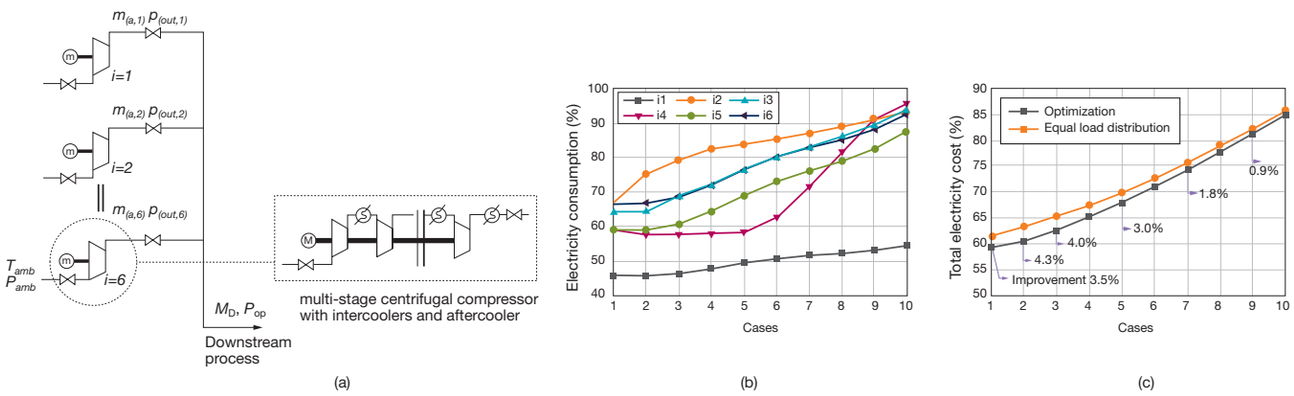


Figure (above). Comparison of costs between condition-based and preventive maintenance optimization.

Figure 2 (below). Compressors operating in parallel (a), electricity consumption of each compressor for each case studied (b) and total electricity cost for each case studied (c)



Competence Area
Modelling and Model Solution Tools

Modelling and tools for solving the models are the engines of Process Systems Engineering

Modelling and Model Solution Tools

As the economies around the world are becoming more inter-connected, the amount of the scientific and engineering data generated is skyrocketing and society demands a cleaner physical environment and better healthcare, we are ending up with having to build and solve very complex models. The complexity continues to grow in size on one hand and in terms of non-linearity, non-convexity, combinatorial nature and uncertain parameters on the other.
We are not only being expected to be able to solve these models fast (speed) but also have to ensure that the solution obtained is reliable (reliability); speed and reliability often conflict each other.
The highlighted developments reported below aim to address these issues.

OPTICO Project: Model-Based Optimization & Control for Process-Intensification in Chemical and Biopharmaceutical Systems **Ioana Nascu, Richard Oberdieck, Maria Papathanasiou, Stratos Pistikopoulos, Sakis Mantalaris; FP7 EU Commission**

Within this scope, four specific processes (Chromatography, Polymerization, Crystallization, Oxidation) are examined in detail; the main focus thereby lies on the formulation of mathematical models of the processes as well as the identification of the bottlenecks of the process which limit its efficiency. Additionally, advanced control strategies are developed in order to enable a robust operation of the process which in return will enable the fulfilment of legal regulations while maintaining high process efficiency.

In collaboration with ETH Zurich and the ChromaCon AG, the CPSE mainly focuses on the optimization and control of a specific chromatographic system, the Multicolumn Solvent Gradient Purification (MCSGP) process. Due to its periodic and highly non-linear behaviour, as well as, the limited information available during operation, all model-based control strategies for this system have been unsuccessful so far. Using a multi-parametric programming approach we are aiming to develop not only a theoretical but also a practical approach to tackle this challenging class of problems. On the theoretical side Ioana Nascu is devising new tools and algorithms for state estimation, while Richard Oberdieck focuses on the solution of the multiparametric optimization problem. On the practical side, Maria Papathanasiou uses system identification and model reduction techniques to recast the original model into a simpler form which then can be solved using the multi-parametric framework.

Modelling, Optimisation and Explicit Model Predictive Control of Anaesthesia Drug Delivery Systems **Alexandra Krieger, Stratos Pistikopoulos; European Research Council, MOBILE, ERC Advanced Grant, No: 226462**

Closed-loop model predictive control strategies for anaesthesia are aiming to improve patient's safety and to fine-tune drug delivery, routinely performed by the anaesthetist.

Towards this aim, the projects' objectives were (i) the development of a mathematical model for drug distribution and drug effect of volatile anaesthesia and (ii) model predictive control strategies for depth of anaesthesia control based on the derived model.
An individualised physiologically based model for drug distribution and uptake described by the pharmacokinetics was derived.
The pharmacokinetic model was adjusted to the weight, height, gender and age of the patient. The pharmacodynamic model, describing the drug effect, links the hypnotic depth measured by the Bispectral index (BIS), to the arterial concentration by an artificial effect site compartment and the Hill-equation. The individualised pharmacokinetic and pharmacodynamic variables and parameters were analysed with respect to their influence on the measurable outputs, the end-tidal concentration and the BIS. The validation of the model, performed with clinical data for isoflurane and desflurane based anaesthesia, showed a good prediction of the drug uptake, while the pharmacodynamic parameters were individually estimated for each patient.

In a consecutive step, the control strategy was derived. The control design combines a linear multi-parametric model predictive controller and a state estimator. The non-measurable tissue and blood concentrations were estimated based on the end-tidal concentration of the volatile anaesthetic. The designed controller adapts to the individual patient's dynamics based on measured data. An alternative approach uses the on-line parameter estimation of the patient's sensitivity solving a least squares parameter estimation problem to adapt the controller to the patient.

Multiscale Modelling of Molecules Interacting with Biosubstrate Systems **Jan Marzinek, Sakis Mantalaris, Stratos Pistikopoulos;** **MULTIMOD ITN, EC's Seventh Framework Programme, FP7/2007-2013 – Grant Agreement No 238013**

The binding free energy is one of the most important and desired thermodynamic properties in simulations of biological systems. The propensity of small molecules binding to macromolecules of human bio-substrates regulates their sub-cellular disposition. This subject is fundamental in transdermal permeation and hair absorption of cosmetic actives. Biomechanical and biophysical properties of hair and skin are related to keratin as their major constituent. A key challenge lies in predicting molecular and thermodynamic basis as the result of small molecules interacting with alpha helical keratin at the molecular level. In addition, elastic properties of human skin which are directly related to the interactions of keratin intermediate filaments remain a challenging subject.

Molecular dynamics (MD) simulations provide a possibility of observing biological processes within atomistic resolution providing more detailed insight into experimental results. However, MD simulations are limited in terms of the achievable time scales. Hence, in this work MD simulations were employed in order to provide better understanding of the experimental results conducted in parallel and to overcome the main limiting factor of MD – the simulation time. For this purpose, thermodynamic and detailed structural basis have been delivered for small molecules interacting with keratin explaining and validating experimental data. On the top of this, the fast free energy prediction tool has been built within all-atom force field by a use of steered molecular dynamics alone. Within the coarse grain approach, the force field was developed for the application of elastic properties of human skin enabling orders of magnitude faster than all-atom force fields simulations. The application of the force field, with water included within tabulated potentials enabled assessing the influence of the natural moisturizing factor composed of small molecules on the elastic properties of the outermost human skin layer. In this work, MD results reached excellent agreement with the experimental data.

Population balance modelling in cell culture systems **David García Münzer, Sakis Mantalaris, Stratos Pistikopoulos;** **MULTIMOD Training Network, European Commission, FP7/2007-2013**

The objective of the proposed research is the development of a framework, experimental and mathematical, that facilitates the study of mammalian cell cultures as a sum of subpopulations with individual growth/metabolic and productivity characteristics.

Closing the loop from in silico to in vivo: modelling and optimisation of bacterial cell culture systems **Argyro Tsipa, Sakis Mantalaris, Stratos Pistikopoulos;** **MULTIMOD Training Network, European Commission, FP7/2007-2013**

An important aspect in industrial bioprocesses is the capture of the biomass growth and substrate degradation via growth kinetic models. However, the most widely used models are empirical and unstructured. The solution for better models describing the cell growth, productivity and metabolism could be a combination of upstream and downstream events. In particular, when a substrate is induced in a cell culture, specific genes are expressed leading to enzymes production. These enzymes are the catalysts of the substrate degradation and biomass growth. Therefore, it is worthy studying the effect of gene expression in growth kinetic models. This concept is studied in the bacterium Pseudomonas Putida mt-2, which is a metabolically versatile soil bacterium able to degrade aromatic pollutants such as m-xylene and toluene. Pseudomonas Putida mt-2 harbours the TOL plasmid (pWW0). TOL plasmid is a paradigm of specific and global gene regulation and helps in the degradation of the same environmental pollutants as well. This idea was first developed in 2011 by Koutinas et al. using m-xylene as substrate, which triggers the TOL plasmid metabolic pathway, resulting to a hybrid growth kinetic model. In our project we extend this idea by using toluene as substrate which we observed that it triggers both the TOL plasmid and chromosomal pathways. Therefore by adding more genetic information and obtaining a clearer genetic map of the biosystem, the resulting hybrid kinetic model can become more accurate, efficient with increased predicting capability. As a result, a new approach starts to be applied in growth kinetic modelling. However the ultimate goal of this project is the development of a hybrid kinetic model in double substrate, which is usually the case in waste disposal, combining the microscale and macroscale level in cell cultures which will be a new proposal in research and we work towards this direction. This new proposal could lead to the optimisation of bioprocesses by reducing the cost and the labour time of the process and increasing the productivity and efficacy.

A Novel Fabrication Method for 3D Waveform Composite Architectures **Nikiforos Maragos, Alexander Bismarck, Stratos Pistikopoulos, Helmut Boehm**

We report a novel fabrication method for 3D waveform composite products. This arises from effects of material anisotropy of a novel composite architecture. A possible material translation looks into a fibre reinforced polymer material system. Design-for-Manufacturing criteria are further introduced to identify a meaningful processing route.

Experimental work aims to verify the concept with various precursor materials, namely pre-impregnated products or raw fibre, polymer constituents. In the latter case an intermediate 2D textile preform product is proposed for melt impregnation and resin infusion process routes. The design variables can thus be rigorously identified and a problem formulated.

A thermo-mechanical analysis via a numerical scheme leads to calculation of the design objectives. Design parameters necessary involve temperature-dependent Elasticity constants at the constituent or composite system level for every discrete fibre-matrix combination considered. Physical experiments are necessary to determine the design parameters to solve the problem.

The problem may be further formulated for discrete and continuous design variables for the textile preform architecture that meaningful design constraints can be built from. An optimization problem is proposed via a surrogate model fitting to a DOE setup.

Design of Tractable MPC and NCO-Tracking Controllers using Parametric Programming **Muxin Sun, Stratos Pistikopoulos, Benoit Chachuat**

The optimization of dynamic processes has received great attention in recent years for the need of reducing economic cost, improving system performance as well as satisfying corresponding constraints. Due to the uncertainty stemming from model mismatch and process disturbances, robust optimization or measurement-based optimization method needs to be applied. Traditional method such as model predictive control and dynamic real-time optimization will result in a lot of computation effort due to the repetitive solving optimization problem online. In contrast, multi-parametric programming allows determining the optimal solution of an optimization problem as a function of parameters, instead of repeatedly solving online optimization problem. Thus online control problem can be computed efficiently by substituting the explicit solution mapping for the optimization problem. The measured-based method of NCO-tracking enforces optimality by directly tracking the necessary conditions of optimality in the presence of uncertainty, transforming a dynamic optimization problem into a feedback control problem. However, the multi-parametric approach has not yet been incorporated into the NCO-tracking method. The current research is to further develop and unify the theories and algorithms of mp-MPC and NCO-tracking and exploit techniques for nonlinear systems to make guarantees on optimality loss. An integrated theory of optimization and tailored algorithms will be developed by casting NCO-tracking as a multi-parametric dynamic optimization problem.

Global Sensitivity Analysis and Metamodelling of Nonlinear Models **Sergei Kucherenko, Nilay Shah**

Modern industrial models contain a large number of parameters and are often highly non-linear. They also have large uncertainty ranges for the parameters and are computationally expensive to run. Traditional methods for uncertainty and sensitivity analysis are not suitable due to their computational expense, local nature and the difficulty in interpreting the results. Global sensitivity analysis evaluates the effect of an uncertain input while all other inputs are varied as well. It accounts for interactions between variables and the results do not depend on the stipulation of a nominal point. It can be used to identify key parameters whose uncertainty most strongly affects the output; rank variables in order of importance; fix unessential variables and reduce model complexity; identify functional dependencies; analyze efficiencies of numerical schemes.

We developed new advanced GSA methods ranging from improved estimates the variance based global sensitivity measures (the so-called Sobol' sensitivity indices) to new derivative based global sensitivity measures which are ideal for screening and model reduction.

A metamodel is a mathematical function which approximates the outputs of the model with a negligible CPU cost, which allows the user to make new output predictions with a good accuracy. It can be used to replace complex expensive explicit or black-box models which needs to be run on-line; for low cost screening and global sensitivity analysis; to replace expensive objective functions in global optimization. etc.

We have developed an efficient approach applying Quasi Random Sampling with Sobol' sequences for building High Dimensional Model Representation (HDMR) models for models with independent and dependent inputs. We also constructed high-dimensional Sobol' sequence generators with additional uniformity properties (Sobol' sequences are widely used for high-dimensional integration, experiment design, sampling in problem of global optimization, etc). The Quasi Random Sampling-High Dimensional Model Representation (QRS-HDMR) method exploits the fact that for many practical problems only low order interactions of the input variables are important. It can dramatically reduce the computational time for modeling such systems. The QRS-HDMR approach can be used for building meta-models with significantly reduced complexity in comparison with original models. This method also provides the values of the Sobol' sensitivity indices at no extra costs.

We developed a general purpose metamodeling software package called SobolHDMR. It is based on a number of metamodeling techniques including QRS-HDMR, the Radial Basis Function method and kriging. SobolHDMR can be used to construct metamodels either from explicitly known models or directly from data given by "black-box" models. Methods implemented in SobolHDMR can deal with models with independent and dependent input variables. SobolHDMR can be applied to both static and time-dependent problems. SobolHDMR can also be used for global sensitivity analysis. The set of available global sensitivity analysis techniques include variance and derivative based sensitivity measures. The software has a user friendly GUI interface for inputs and presenting results (Fig. 1). It can be linked to MATLAB and other packages. The produced metamodels are given as self-contained C++ or MATLAB files.

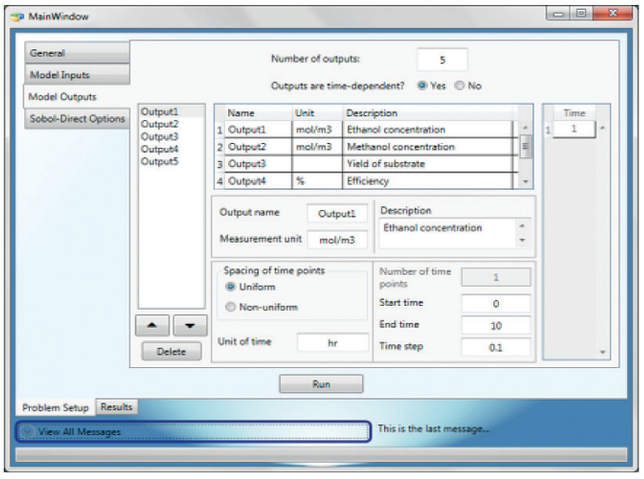


Figure (above). SobolHDRM software. One of the GUI input windows.

Stochastic methods for global optimization and Metamodel-based global optimization **Sergei Kucherenko, Nilay Shah**

The solution of nonconvex global optimization problems is one of the hardest fields of optimization. It presents many challenges in both practical and theoretical aspects. There are two types of commonly used techniques for solving such problems: deterministic and stochastic. Deterministic methods guarantee convergence to a global solution. However, for large-scale problems these methods may require a large CPU-time. Stochastic search methods yield an asymptotic (in a limit N going to infinity, where N is a number of randomly sampled points) guarantee of convergence. In reality problems can only be solved with limited number of points N, hence convergence to a global solution is not guaranteed. However, stochastic (although known as heuristic) methods have already shown their efficiency and usefulness in solving large scale practical problems.

We developed a novel method, which combines the advantages of deterministic and stochastic methods. It is based on application of Quasi Monte Carlo (QMC) sampling methods (Sobol' sequences) and multi-level linkage methods (MLSL). In comparison with pure stochastic methods employing random numbers, application of QMC sampling significantly decreases the number of points required to achieve the same tolerance of finding the global minimum. The MLSL method consists of three stages: I. Global: an objective function is evaluated on a set of sampled points. Objective: to obtain as much information as possible about the underlying problem with a minimum number of sampled points; II. Local: a deterministic local search method is applied to selected points. Objective: to solve a local constrained minimization problem; III. Multilevel: the clustering technique and stopping criteria are used. Objective: To find all global and local minima without finding the same local minima more than once.

We developed a general purpose global optimization solver SobolOpt based on the developed method. It is linked with modeling systems GAMS and MATLAB. The solver is capable of solving complex constrained global optimization problems with continuous or mixed-integer variables.

Optimization of complex products or processes can be very demanding from a computational point of view. In many cases there is a need for simplified models that could provide an accurate representation of the detailed and costly objective functions and/or set of constraints. These simplified models known as metamodels can be orders of magnitude cheaper to evaluate compared to the original models. Such an approach is also invaluable in cases when the model is not given explicitly but it exists only in a form of input-output maps or it is given as a "black box". Another advantage of using metamodel-based design optimization is that building metamodels may filter physical high frequency and numerical noise which can improve the quality of the optimization results. We showed that the global metamodelling approach based on the QRS – HDMR method is capable of dealing with high dimensional, multimodal problems of low or moderate complexity and its performance can be further enhanced by combining it with other metamodelling techniques such as Radial Basis Functions and kriging.

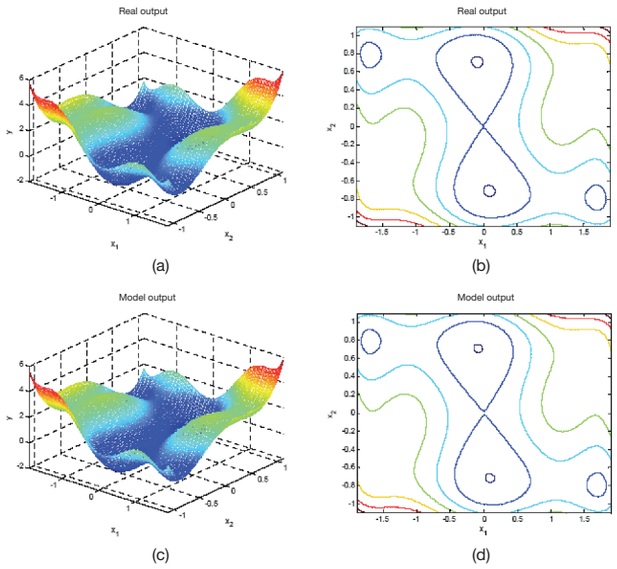


Figure (above). Comparison between the original (a,b) function with multiple minima and its metamodel (c,d)

The Branch-and-Sandwich algorithm for bilevel optimisation **Polyxeni-Margarita Kleniati, Claire S. Adjiman**

In many contexts, decision-making involves reconciling different objectives or the needs of different entities. For example, in production planning, one may aim to manufacture a series of products that come as close as possible to specified quality targets, with the overarching objective of minimising production costs. Alternatively, in the context of thermodynamic model development, the objective is to find a set of parameters that yield the best possible match between model and experimental data. The evaluation of the model performance often requires the determination of stable equilibrium phases, which entails the solution of Gibbs free energy minimisation(s). Problems of this type thus involve one or more optimisation problems embedded within a higher-level optimisation problem; they fall within the class of bilevel optimisation problems.

This class of problems is extremely challenging, especially when the functions involved are nonlinear and when integer variables are present, as is often the case in process systems engineering applications. Over the past few years, we have been developing an algorithm to address this class of problems: the Branch-and-Sandwich algorithm, which has recently been published in the Journal of Global Optimization, is guaranteed to identify correctly the global solution of nonlinear bilevel problems.

The incorporation of integer variables within the algorithmic framework has also been achieved. The algorithm is based on branch-and-bound framework in which an unusual branching scheme is introduced. This allows the simultaneous exploration of the two levels of optimisation and has led to promising results on a series of over 40 test cases.

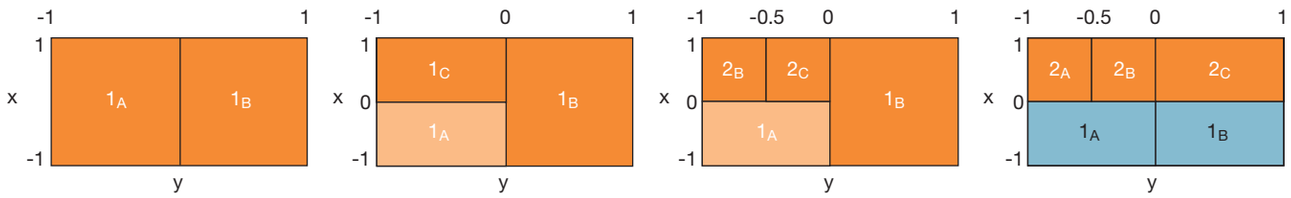


Figure (above). Branching scheme in the Branch-and-Sandwich algorithm. Contrary to usual practice, the inner (Y) space is partitioned and special lists (L) are used to ensure the whole inner space is considered so that a correct solution is found. The outer (X) space partitioning can lead to the creation of additional independent lists (panel (d)).

Global Optimisation of Dynamic Process Systems

Carlos Perez-Galvan, Bogle, CONACyT and UCL

In chemical process design it is often desired to know the optimal conditions for a given time-dependent process described by a system of ODEs. This is useful in applications such as parameter estimation, model predictive control and design of control systems, operating profiles of batch processes, etc.. The project aims to develop techniques that ensure that a globally optimal solution to problems such as maximising yield of a particular output variable or of minimising the cost associated with a particular disturbance also guarantees bounded performance across the whole dynamic trajectory.

For the dynamical optimisation problem there are several options to address the problem in a rigorous way. Three main steps are involved in the sequential approach in which finding efficient and tight bounds for the ODE system is the most challenging of them due to the fact that only low dimensional problems with small uncertainties can be solved with the available methods. Much work has been done in this aspect and improvements in methods such as Taylor models and McCormick relaxations have been devised. One of the main issues regarding the ODE integration is the overestimation generated in the so called validated methods. This overestimation is the product of the dependency problem and wrapping effect that arise in interval analysis. Consequently, this problem is preventing these methods to be used in higher dimensional problems besides it is also preventing the use of significant uncertainties in the ODE models.

We are exploring ways to reduce the overestimation when it has already been generated using interval analysis and interval contractors that help tackle the overestimation problem. Another alternative is the use of so-called consistency techniques. Alternatively we can deal with it before it happens by model reformulation, for example the dependency problem can be reduced by minimising the number of times a variable appears in a model. Having a tool able to systematically account for interval overestimation reduction strategies is a promising idea in the validated solutions of ODEs.

Improved Fleet Management Using Operations Research

Floudas, Gounaris, Repoussis, Tarantilis, Wiesemann

Fleet management is a business function that is concerned with the management of a company's transportation fleet, including trucks, rail cars, ships and planes. Amongst the many goals of fleet management are the prudent investment in company vehicles, as well as the continuous improvement of the efficiency, effectiveness and safety of the existing fleet. It is estimated that with an effective fleet management system in place, companies can on average reduce their fleet size by 15-25%, reduce their maintenance costs by 10-20% and improve fuel consumption by 8-12% (Accenture: Federal Fleet Management).

Similar to other business functions, fleet management decisions are taken under considerable uncertainty about the current conditions and future market developments. Informed decision-making in fleet management therefore requires the collection and analysis of data from multiple sources, such as inventory levels, customer demands, traffic conditions and the state of the current fleet. Using the data, (sets of) probability distributions can be constructed that truthfully reflect important characteristics of the involved business processes.

Decision-making under uncertainty has a long and distinguished history in operations research, with the origins dating back to the 50's (Markov decision processes) and 60's (stochastic programming). To date, the predominant paradigm is to model the uncertain data as random variables and then solve the decision problem by discretising the outcomes of these random variables. For multi-stage (i.e., dynamic) problems, this discretisation results in the classical curse of dimensionality, which implies that the computation times grow exponentially with problem size. This computational burden has been a major impediment to the applicability of these methods, and it became a wide-held belief that multi-stage decision-making under uncertainty is an inherently intractable endeavour.

Together with scientists from Athens University of Economics and Business, Carnegie Mellon University, Princeton University and Stevens Institute of Technology, researchers at the Centre for Processing Engineering are developing models and tools to determine prudent fleet management decisions that allow for probabilistic guarantees in view of the uncertainty about future customer demands and traffic conditions. The focus is on the development of methods that do not discretise the involved probability distributions. The resulting methods avoid the curse of dimensionality and thus scale to industry-size problems.

Multilevel Algorithms for Speeding up Molecular Dynamics Simulations **Chin Pang Ho, Cecilia Clementi, Charles Laughton, Panos Parpas**

It is often possible to exploit the structure of large scale optimization models to develop algorithms with lower computational complexity. A noteworthy example are composite convex optimization models that consist of the minimization of the sum of a smooth convex function and a non-smooth (but simple) convex function. Composite convex optimization models arise often in a wide range of applications from computer science (e.g. machine learning), statistics (e.g the lasso problem), and engineering (e.g. signal processing), and computational chemistry (e.g. molecular conformation problems)

In addition to the composition of the objective function, many of the applications described above share another common structure. The fidelity in which the optimization model captures the underlying application can often be controlled. Typical examples include the discretization of Partial Differential Equations in optimal control, the number of features in machine learning applications, the number of states in a Markov Decision Processes, or the number of collective variables in a molecular dynamics simulation. Indeed anytime a finite dimensional model arises from an infinite dimensional model it is straightforward to define such a hierarchy of optimisation models. In many areas it is common to take advantage of this structure by solving a low fidelity (coarse model) and using the solution as the starting point in the high fidelity (fine) model.

Together with colleagues we have been working on an algorithmic framework in order to take advantage of the availability of a hierarchy of models in a consistent manner for a variety of classes of optimisation models. Recent work includes developments in nonsmooth optimisation, semidefinite programming and global optimisation.

Mixed-Integer Optimisation **Vivek Dua**

The developments here include reformulation of mixed-integer optimisation problems has multi-parametric programs. This is achieved by relaxing the integer variables as continuous variables and then treating them as parameters. The optimal solution of the multi-parametric program is obtained as a function of the parameters. Fixing the parameters at the integer values provides a list of potential solutions from which the best or the set of best solutions is selected as the final solution. The main contribution is in not fully solving the multi-parametric programs and where possible exploiting the existence of specific types of nonlinearities.

Ion Transport Modelling for Cystic Fibrosis
Donal O'Donoghue, Vivek Dua, Guy Moss, Paola Vergani; CoMPLEX, UCL

Cystic fibrosis (CF) is genetic disease of the lung. We have developed a mathematical model of the ion transport for CF patients. This model shows that loss of apical chloride permeability alone can not explain the observed voltage data. An increased apical sodium permeability must also take place. This insight opens up new avenues for potential therapies for the CF.

Application Domains
Professor Paul Rutter

"The CPSE has a consistent record of attracting funding from UK Research Councils, UK and International industry, the European commission and other funding bodies. In the last five years this has amounted to grants of more than £30 million."

Application Domains
Chemical Manufacturing Systems

Chemical Manufacturing Systems form a key application domain of CPSE

Chemical Manufacturing Systems

Many of the fundamental tools developed in the three competence areas of Product & Process Design, Operations & Control and Modelling & Model Solution Tools are motivated by the challenges arising in this application domain. Through this domain, we serve several process industries such as bulk chemicals (including petrochemicals and oil & gas), pharmaceuticals & agrochemicals, specialty chemicals and biofuels.

The work of the Chemical Manufacturing Systems Engineering application area has several strands:

Multiscale Modelling of Biorefineries

There is a large body of literature regarding the choice and optimization of different processes for converting feedstock to biofuels and bio-commodities; moreover, there has been some reasonable technological development in bioconversion methods over the past decade. However, the eventual cost and other important metrics relating to sustainability of biofuels production will be determined not only by the performance of the conversion process, but also by the performance of the entire supply chain from feedstock production to consumption.

Moreover, in order to ensure world-class biorefinery performance, both the network and the individual components must be designed appropriately, and allocation of resources over the resulting infrastructure must effectively be performed. The goal of this project is to develop a framework and methodology for multi-scale modelling of flexible biorefineries, and the integration of process models with supply chain models to answer holistic supply chain questions, such as what are the prospects for second generation bioenergy crops, where are the main cost and efficiency bottlenecks, etc.

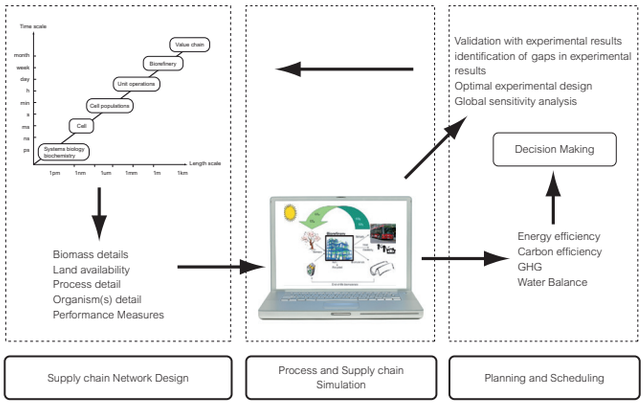


Figure (above). Integration of models for bioenergy/biofuels.

A variety of activities have been undertaken under this project. A particular advance has been the development of detailed models of hydrolysis of cellulose by different enzymes; this then enable the optimisation of the enzyme mix and process conditions for hydrolysis, which is one of the performance-limiting elements of the chain.

Synthesis of Chromatographic Strategies of Antibody Purification Processes

The strategies employed in chromatography steps play a key role in downstream processes for monoclonal antibody (mAb) manufacture. A key decision for mAb purification is the selection of the chromatography sequence. There usually exist multiple chromatography steps in the mAb purification process, and each step has a number of suitable candidate resins/types for selection. The candidate resins often have different characteristics, e.g., yield, price, dynamic binding capacities. Here an importation issue is how to choose the best combination of resins/types for all chromatography steps to be of most benefit to the whole downstream process. Also, at each chromatography step, another key decision is the column sizing strategy, e.g. opting to run a smaller column for several cycles so as to reduce resin costs or a large column for fewer cycles so as to save time and labour costs. Decisions on the chromatography column sizes include the selection, the bed height and diameter of each column and the number of cycles to run and the number of columns to use in parallel. In this project, an integrated optimisation-based framework

is proposed for chromatography step sequencing and column sizing in mAb purification processes. Chromatography sequencing decisions include the resin selection at each typical step, while the column sizing decisions include the number of columns, the column diameter and bed height, and number of cycles per batch (see figure 2). A mixed integer nonlinear programming (MINLP) model was developed and then reformulated as a mixed integer linear fractional programming (MILFP) model. A literature approach, the Dinkelbach algorithm, was adopted as the solution method for the MILFP model.

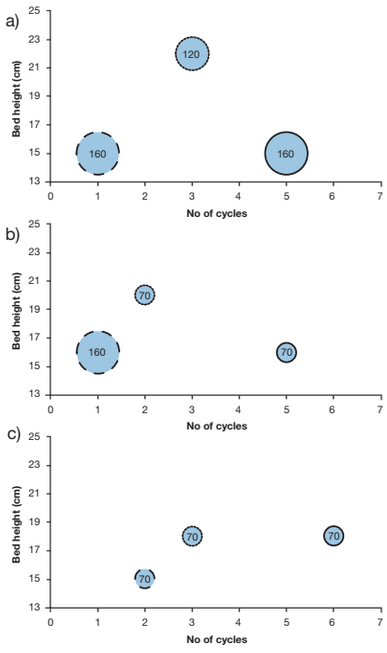


Figure (above). Optimal column sizing decisions: bed height (x-axis), number of cycles (y-axis), diameter (proportional to the bubble size, indicated at the centres of the circles), at a) capture step; b) intermediate purification step; c) polishing step, for 1USP:1DSP (solid circle lines), 2USP:1DSP (dotted circle lines) and 4USP:1DSP (dash circle lines) scenarios.

Sustainable Manufacturing of Transparent Conducting Oxide (TCO) Inks and Thin Films

This project seeks to develop processes and resources towards sustainable and inexpensive high quality transparent conducting oxide (TCO) films (and printed tracks) on float glass, plastics and steel. In particular replacement materials for Indium Tin Oxide (ITO) and F-doped Tin Oxide (FTO). In this project we will develop sustainable upscaled routes to TCO materials from precursors containing earth abundant elements (titanium, aluminium, zinc) with equivalent or better figures of merit to existing TCOs.

One the objectives of the project is to apply Life-cycle modelling and cost benefit analyses by taking a holistic approach to the considerations of energy, materials consumption and waste and, in consultation with key stakeholders and policy makers, identify best approaches to making improvement or changes, e.g. accounting for environmental legislation in nanomaterials, waste disposal or recyclability of photovoltaics.

Optimal Synthesis of Water Networks with Membrane Regenerators

Due to the high demand of water consumption together with the drive for achieving sustainable development, water network synthesis problems have received increasing attention in the PSE community. In the objective of minimizing freshwater use and wastewater generation, water can be reused by channelling 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.

The main objective in this project is to synthesize an optimal water network given the three elements of water sources with fixed flowrates and contaminant concentrations; water sinks with fixed flowrates and maximum allowable inlet concentration limits; and water regenerators. To this end, we have developed a source–regenerator–sink superstructure that allows all feasible interconnections of the elements to embed numerous alternative configurations for direct reuse/recycle, regeneration–reuse, and regeneration–recycle. The superstructure and regenerator models lead to a mixed-integer nonlinear program (MINLP) that optimizes the interconnections as described by total stream flows and concentrations. We successfully applied the MINLP model on a refinery case study that involves 28 sources including freshwater; 2 regenerators: mud trap-corrugated plate interceptor and a single-stage reverse osmosis network; and 14 sinks including two terminal sinks (effluent treatment plant and discharge to the environment). A globally optimal water network topology was attained with promising results of more than 50% annual savings in freshwater use.

Surrogate based Optimisation for Design of Pressure Swing Adsorption Systems

Pressure swing adsorption (PSA) is a cyclic adsorption process for gas separation and purification. PSA units have been installed in the process industry for applications such as air separation, hydrogen purification, and gas drying. Because of its low energy requirement it is considered to be a cheaper alternative to traditional absorption techniques.

In this study, a non-intrusive surrogate based optimisation procedure based on Kriging is suggested for design of PSA systems. The Kriging models are employed to guide the search more efficiently. To illustrate the significant improvement that could be achieved, we have compared surrogate based optimisation based on a genetic algorithm (GA) and multi-start sequential quadratic programming (SQP), and efficient global optimisation (EGO). The case study considered is the design of a dual piston PSA system. The general surrogate based optimization procedure with Kriging has been shown to suffice with GA and multi-start SQP, while it also allows the use of other optimization methods.

Application Domains
Molecular Systems Engineering

The integration of concepts from process systems engineering and molecular thermodynamics holds great promise to tackle today's engineering challenges

Molecular Systems Engineering

The first grant formalising the formation of our molecular systems engineering (MSE) area finished in 2013. At the Industrial Consortium Meeting of December 2013 the impressive achievements of the group were clear. In numbers, following the initial £3.6M awarded by the Engineering and Physical Sciences Research Council (EPSRC), we have secured £8M in complementary funding, have published over 50 papers and accumulated over 600 citations to our work in the duration of the grant. We had a very fruitful away day for the team in October 2013, to take stock on what has been achieved and to plan for an exciting and successful continuation of activities. We also have a new website: **http://molecularsystemsengineering.org/**, please visit it to see some of our recent papers and other work!

Our research continues, underpinned by a £1.8M Platform Grant (EPSRC) which supports our next generation of post-doctoral researchers, and with the support of BMS, Chemistry Innovation, GSK, P&G and Syngenta. The heading for this work is "Molecular Systems Engineering of High-Value Structured and Formulated Products". We are heading to tackle key fundamental challenges for the prediction of fundamental properties of pharmacological and biologically relevant compounds. Our plan is to advance the tools of molecular systems engineering to tackle some of the key molecular challenges associated with improving the productivity of drug discovery and processing by improving our predictive capability of the relevant physical properties. We are collaborating with industry across several sectors, including pharmaceuticals (e.g., Pfizer, Novartis, Dynamic Extractions, GSK, BMS) and oil & gas (e.g., Shell, BP, Qatar Petroleum).

We are tackling these challenges by bridging the scales from the sub-atomic (quantum) to the macroscopic, and developing state-of-the-art techniques at the atomic and coarse-grained level, which lead to robust methods for property prediction and molecular design. Three of our key recent publications are highlighted:

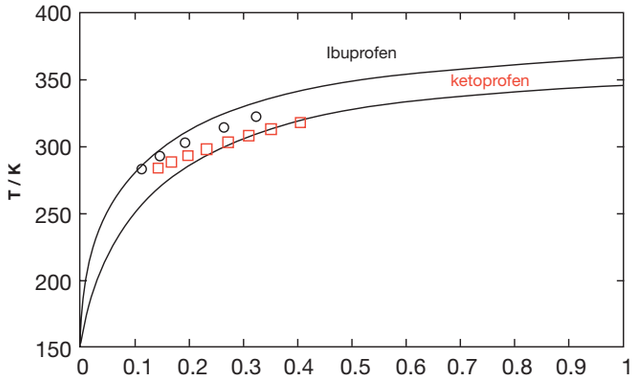


Figure (above). Prediction of the solubility (solid-liquid equilibrium) of ibuprofen and ketoprofen in acetone as temperature-composition (T-x) projection at p = 1bar. The symbols represent the experimental data and the continuous curves the corresponding predictions of the SAFT-γ Mie GC approach.

Physical property prediction for the 21st century: the SAFT-γ Mie group contribution approach
Vasileios Papaioannou, Simon Dufal, Thomas Pogiatzis, Claire S. Adjiman, George Jackson, Erich A. Müller, Amparo Galindo

Thermodynamic methodologies are continuously being developed and improved in order to meet the industrial requirements for accurate property prediction in an ever-expanding range of applications. An important consideration or application within integrated process and solvent design is the predictive capability of the platform, commonly perceived as the ability of a method to predict the properties of a system for which no experimental data is available. An important class of predictive thermodynamic models are group contribution (GC) approaches, where molecules are modelled based on their corresponding chemical moieties. The SAFT- γ Mie group contribution approach brings together the molecular rigour, accuracy and versatility of the SAFT formalism with the predictive capabilities intrinsic of the GC concept.

An exciting application of such predictive approaches is in the description of the solubility of complex molecules, such as active pharmaceutical ingredients (APIs), in solvents and solvent mixtures. The advantage of a predictive approach in this case is that the parameters required for the solubility prediction can be

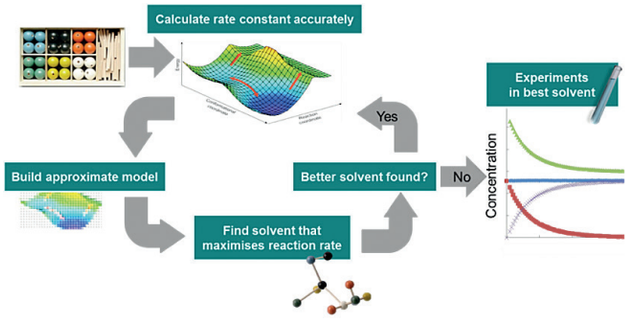
developed from experimental data for simple systems. Hence, the solubility of a given API is obtained in a fully predictive manner, without the requirement for API-specific experimental data for the parameterisation of the model. The potential of the SAFT-γ Mie approach in predicting the solubility of APIs in organic solvents is shown in Figure 1.

Sample publication: Papaioannou, V., Lafitte, T., Avendaño, C., Adjiman, C. S., Jackson, G., Müller, E. A. and Galindo, A., "Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments", J. Chem. Phys. 140, (2014) 054107.

Accelerating chemical reactions by computer-aided molecular design. **Heiko Strübing, Zara Ganase, Eirini Siougkrou, Aikaterini Diamanti, Amparo Galindo, Claire Adjiman**

What is the best solvent for a given chemical reaction? Given that the rate and selectivity of chemical reactions can vary by several orders of magnitude in different solvents, this question has important ramifications for the exploration of novel reaction routes and the development of industrial processes. We have been developing a methodology for optimal solvent design for enhanced reaction kinetics, QM-CAMD (cf. Figure 2), which relies on the integration of continuum solvation quantum mechanical calculations into a computer aided molecular design (CAMD) framework. This approach has been successfully applied to the SN2 reaction of phenacyl bromide and pyridine, leading to a 40% increase in the reaction rate. The results have been verified experimentally, using in-situ kinetic monitoring techniques.

Figure (below). The QM-CAMD approach to solvent design for accelerating reactions.



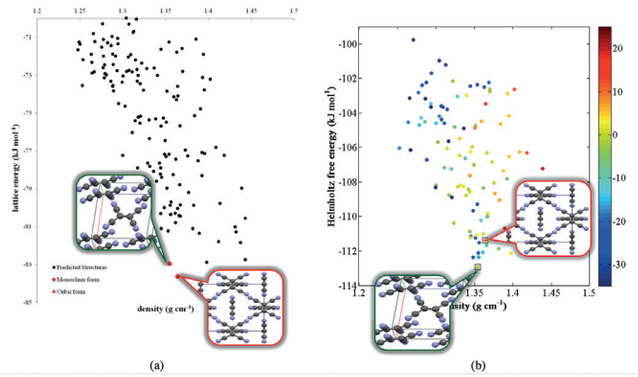
A central aspect of the proposed methodology is the use of a surrogate model. In initial work, we have used simple linear free energy relation, the solvatochromic equation. In more recent work, we have explored the use of more reliable surrogate models, in particular a kriging model, and found that it leads to further improvements in the solvents designed. On this basis, we have been extending the range of applicability of the approach by considering other reactions, including a Cope elimination reaction, in which the solvent can shift the equilibrium very significantly, and a Williamson reaction in which C-alkylation or O-alkylation products can be obtained preferentially depending on the solvent. We have also been further extending the methodology to include solubility and temperature effects on reaction kinetics.

Sample publication: Struebing, H, Ganase, Z., Karamertzanis, P.G., Siougkrou, E., Haycock, P. Piccione, P.M., Armstrong, A., Galindo, A., Adjiman, C.S., "Computer-aided molecular design of solvents for accelerated reaction kinetics", Nature Chem. 5 (2013) 952-957. Highlighted in News and Views article, D.G. Truhlar, "Chemical Reactivity: Inverse Solvent Design", Nature Chem. 5 (2013) 902-903.

Systematic methodologies for crystal structure predictions **Christina-Anna Gatsiou, Matthew Habgood, Isaac Sugden, Manolis Vasileiadis, Claire Adjiman, Costas Pantelides**

Methodologies for the systematic prediction of the polymorphs of organic molecules solely from the knowledge of the molecular connectivity diagram have undergone rapid improvements in the last few years. Following the success of our CrystalPredictor/ CrystalOptimizer codes in identifying the correct structure for the largest molecule considered to date in a Blind Test (molecule XX), we have been making further improvements to our algorithms in order to increase the range of molecules which can be investigated (in particular, molecular size), and to increase the accuracy of the relative energy calculations. Major areas of development include (i) the implementation of improved local approximate models within CrystalPredictor, which makes it feasible to treat larger molecules reliably; (ii) the development of a methodology to improve the accuracy of lattice energy calculations and to embed existing experimental knowledge within the Crystal Structure Prediction methodology (iii) the development of a methodology for the rapid evaluation of free energy, enabling temperature effects to be taken into account. This latter development has been applied successfully to small molecules. For example, in the case of tetracyanoethylene, it has been shown to lead to the successful prediction of reversal in stability of the cubic and monoclinic forms at higher temperatures, with the monoclinic form becoming more stable, as illustrated in Figure 3.

Figure (below). Crystal structure prediction calculations for tetracyanoethylene. (a) Lattice energy landscape at 0 K the cubic form is found to be most stable and the monoclinic is the second most stable structure. (b) Helmholtz free energy landscape at 300 K, the monoclinic structure is found to be the most stable



Sample publication: Pantelides, C.C., Adjiman, C.S., Kazantsev, A.V., "General computational algorithms for ab initio crystal structure prediction for organic molecules", Top. Curr. Chem., Springer Berlin Heidelberg (2014).

Application Domains
Biological Systems Engineering

The Biological Systems Engineering group within CPSE focuses on the development of mathematical models for biological systems

Biological Systems Engineering

The Biological Systems Engineering group within CPSE focuses on the development of mathematical models for biological systems. Topics of interest include industrial biotechnology, bioprocessing, systems biology and biomedical systems. Recent projects received significant funding from the Research Councils and the European Research Council and saw closer collaboration between Imperial and UCL in this research field.

Selected examples from the current project portfolio on biomedical systems are listed below:

Dr Vivek Dua is working on ion transport modelling for cystic fibrosis. Cystic fibrosis (CF) is genetic disease of the lung. Dr Dua's team have developed a mathematical model of the ion transport for CF patients, which shows that loss of apical chloride permeability alone cannot explain the observed voltage data, but an increased apical sodium permeability must also take place. This insight opens up new avenues for potential therapies for the CF.

Professor David Bogle is collaborating with researchers in UCL's Cancer Institute on network analysis of DNA damage response and cellular signalling in different KRAS mutated colorectal cancer cell lines. Personalized treatments have been postulated as the way forward in treating most types of cancer. This project has developed a systems analysis approach to the problem using gene expression microarray technology to explore the difference between different metastatic colorectal cancer cell lines in order to expose potential diagnostic measures and explain the response to different treatments.

The groups of Professors Pistikopoulos and Mantalaris are working on a number of biomedical systems, including cancer treatment and anaesthesia control. Specifically, Acute Myeloid Leukaemia (AML) is a subtype of blood cancer which only affects cells belonging to the myeloid lineage. The prescribed treatment is chemotherapy scheduled in several cycles. The mechanism behind drug action requires cell proliferation. AML cells are indeed highly proliferative and will be targeted by the drug; however, other stem cells that are actively duplicating in order to regenerate healthy cellular material will also be affected. It is thus critical to reach a trade-off between killing cancer cells and keeping a minimum number of healthy cells. In that direction, the research team is building a model based on patient- and disease- specific characteristics in order to design more rational chemotherapy protocols that are less risky and milder for the patient. In parallel, the group is developing modelling, optimisation and explicit model predictive control strategies for anaesthesia drug delivery systems. Closed-loop model predictive control strategies for anaesthesia are aimed at improving patient safety and to fine-tuning drug delivery, routinely performed by the anaesthetist.

Professor David Bogle is working with colleagues in UCL's Hepatology Department on understanding the function of the liver in health and disease. Firstly, they are following a combined computational modelling and experimental approach to assess the role of metabolic zonation across the sinusoid in healthy liver and the consequences of its dysregulation in disease. Their research focuses in particular on carbohydrate and lipid metabolism. Secondly, they are exploring the possibility of using a new bio-material as a cell support in bioartificial liver using the zonated model. They are investigating if cells can be grown throughout the cryogel support in the artificial organ, if they show signs of cell-cell communication, and whether they retain liver specific function over a period of time.

Dr Krishnan's group is working on the development of a multiscale/multilevel modelling framework for elucidating the effects of intrinsic and induced drug resistance in solid tumours at the cell and tissue scale, as well as developing an integrated framework for combined drug transport in the blood, interstitium and its effect on and interplay with cellular factors.

In Industrial Biotechnology and Bioprocessing, we have several projects including the following:

Professors Pistikopoulos and Mantalaris are developing population balance models for cell culture systems. The objective of their research is the development of a framework, experimental and mathematical, that facilitates the study of mammalian cell cultures as a sum of subpopulations with individual growth/metabolic and productivity characteristics. They are also involved in **model-based optimization and control for process intensification in chemical and biopharmaceutical systems**. Process Intensification (PI) is the response to world-wide changes in the chemical/biopharmaceutical industry for specific end-use product properties and stricter energy and

environmental constraints. In this framework, research aims to overcome the limitations on implementing PI by establishing a new methodological design approach for sustainable, intensified chemical/biopharmaceutical plant design.

Within this scope, four specific processes (Chromatography, Polymerization, Crystallization, Oxidation) are examined in detail.

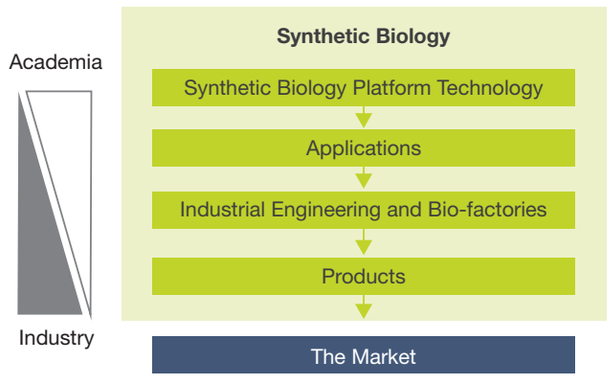
Research in Dr Krishnan's group has focussed on signal transduction and gene regulatory networks/processes and their control of cellular processes of basic and applied interest. It involves modelling in collaboration with experimentalists (cell biologists, biomedical scientists, synthetic biologists). Activities include modelling feedback regulation of protein synthesis at the translation stage, the development of new probabilistic Boolean networks based modelling approaches for modelling translation; tools for dissecting the complexity of translation in systems and synthetic biology, spatial control of signal transduction in signalling modules and networks and information processing in complex biochemical mechanisms: multi-site phosphorylation.

Dr Kontoravdi and colleagues in Life Sciences are examining the impact of bioprocess conditions on protein product quality using modelling and experimentation. Their most recent work focuses on developing dynamic metabolic flux analysis approaches in order to quantitatively determine the impact of nutrient availability on protein glycosylation. In parallel, they have developed algorithms for media and feed formulation for Chinese hamster ovary cell culture.

Professor Shah and Dr Kontoravdi are working with colleagues at UCL's Biochemical Engineering and Chemistry Departments on the manufacture of chemicals and pharmaceutical intermediates from sugar beet pulp. The research team is evaluating the process economics, energy and carbon balances for potential novel flowsheets, while setting up unit operations and process models to develop whole system models and perform life cycle analysis.

Finally, **Professor Shah and Dr Kontoravdi are involved in the recently awarded Frontier Manufacturing award in Synthetic Biology**. The goal is to drive a paradigm shift in the industrial scale production of chemicals, therapeutics, fuels and materials, revolutionising the translation and commercial exploitation

The Translation Process



of advances in biosciences and physical sciences through synthetic biology. At the heart of this approach is the application and integration of new synthetic biology production vectors into novel process technologies, thereby dovetailing cutting edge biological and chemical transformations.

Application Domains
Dr Benoit Chachuat

"The CPSE Industrial Consortium provides an ideal ground for applying state-of-the-art methods and tools to enhance industrial processes, and it is these applications that stimulate new theoretical developments in turn."

Application Domains
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

Supply Chains of the Future

These challenges include:

- 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

An example of such emerging supply chains is the concept of the biorenewables supply.

Biorenewable supply chains

Forecasts of fossil fuels price increases have been leading to the search for substitute carbon-based materials for chemical processes. This has led to the concept of a biobased economy. This concept is focused on the development of industrial biorefineries, where biomass conversion processes which produce fuels, power, and chemicals are integrated to minimise the environmental impacts and maximise the value derived from the biomass feedstock.

The overall biomass value chain is strongly related to the feedstock pre-treatment unit, which consists of a set of preliminary processes to fractionate the biomass and accounts for a large share of the total capital investment. As an example, the organosolv process is currently one of the most promising pre-treatment processes. The technology aims at efficiently solubilising lignins and providing high quality cellulose fibres and hemicellulose from which a wide variety of products can be derived (e.g. polyolefins, polyurethanes, polyvinyl chloride, second generation biofuels, adhesives, resins and feed ingredients.

The main strength of this technological solution is the wide variety of lignocellulosic feedstock being used (e.g. cereal straws, deciduous forestry residues, short rotation coppice (SRC) wood). However, the eventual bioproduct cost is determined not only by the performance of the conversion process, but also by the performance of the entire supply chain. In particular, a biorefinery requires a cost-effective biomass infrastructure where feedstock production, collection, storage and pre-processing are simultaneously optimised to guarantee a continuous all year round operation.

Process requirements are not only to be met in terms of biomass availability, but feedstock quality is to be guaranteed, too. Biomass transportation distance, storage needs and mass perishability reduction relies on optimal selection of densification technologies (e.g. chipping, pelletisation) and logistics infrastructure. In view of the above, quantitative design tools are useful to provide decision support assessing both financial and environmental performance of biorefineries in a holistic approach along the entire supply chain (SC) over the long-term.

This project, part of the BIOCORE programme (**http://www.biocore-europe.org**) aims at providing a Mixed Integer Linear Programming modelling framework to help define planning strategies for the development of sustainable biorefineries. The up-scaling of an Organosolv Biorefinery is addressed via optimisation of the whole system economics. Three real world cases studies are proposed to show the high-level flexibility and wide applicability of the tool to model different biomass typologies (i.e. forest fellings, cereal residues and energy crops) and supply strategies. Model outcomes reveal how supply chain optimisation techniques could help shed light on the development of sustainable biorefineries. Feedstock quality, quantity, temporal and geographical availability are crucial to determine biorefinery location and the cost-efficient way to supply the feedstock to the plant. Storage costs are relevant for biorefineries based on cereal stubble, while wood supply chains present dominant pretreatment operations costs.

A French Case study

The optimal Organosolv biorefinery SC in the French region is mainly supplied with wheat straw while residues from barley harvesting are used at a lower extent. The energy crop share of feedstock supply (i.e. miscanthus) as well as biomass supply differentiation increase over time, to face the straw competitive use rise over time.

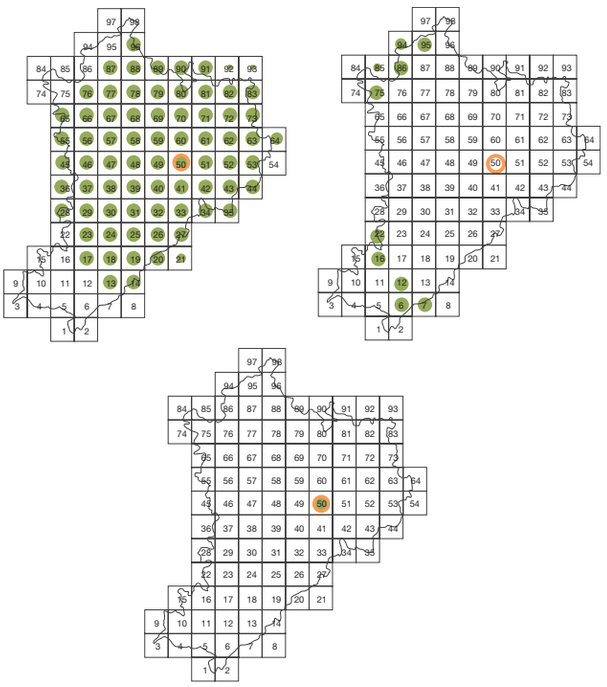
The pretreatment facility operates in cell 50, in the centre of an area devoted to the cultivation of the main crop (i.e. wheat straw). The land devoted to barley is located just around the area used

for wheat crop, while miscanthus is grown in the same cell as the Organosolv pretreatment plant (Figure 1.a-1.c). The biorefinery location optimisation is driven by the quality of the infrastructure: the region selected is characterized by more dense truck transportation links, used to deliver about 90% of the feedstock. The seasonal supply chain of biomass is affected by the availability of feedstock over a year: i.e. cereal straw can be only harvested in summer, while miscanthus only in winter.

The fluctuating nature of the biomass availability results in a high reliance of the supply network on storage facilities which are mainly located on the field border (Figure 2).

If the biorefinery is sustained only through cereal crop residues (i.e. barley and wheat straw), the optimal biomass SC configuration is rather similar to the one in Instance A, having an Organosolv facility in cell 50 within a large area devoted to wheat straw, the leading crop with rather low seasonal effects (Figure 3).

The higher reliance of wheat straw in Instance B widens the biomass collection area, up to a maximum in of 0.41 Mha, increasing transportation and storage cost share of total costs. **Figure (below).**



a) winter wheat straw b) winter barley straw
c) miscanthus (bottom)

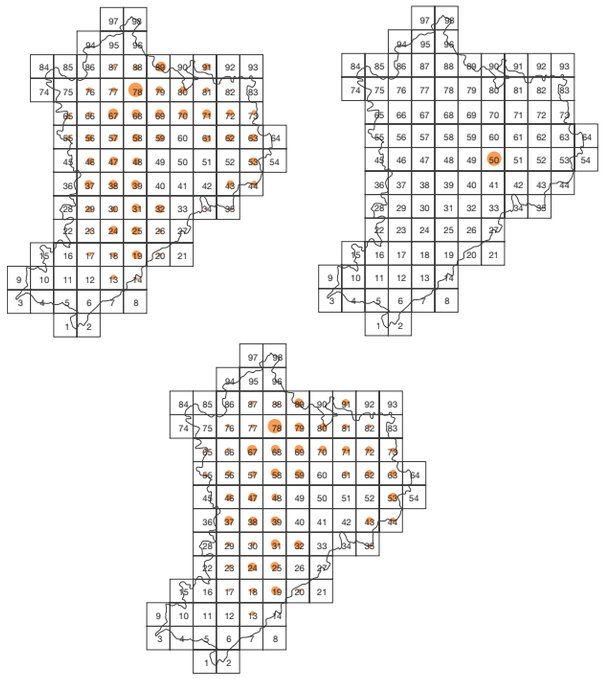


Figure (above).
a) Wheat straw (top left) b) Miscanthus (top right)
c) Barley straw (bottom)

Figure (above). French case: storage locations across the regions for a) wheat straw, b) miscanthus and c) barley straw. The circle size is scaled on the maximum storage capacity settled per each crops, across the region and over time).

French case (Instance B): Seasonal biomass supply to the Organosolv facility.

Application Domains
Energy Systems Engineering

The importance of Energy as a topic has if anything, increased over the last few years

Energy Systems Engineering

Introduction

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 intensesupply 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, Carbon Capture and Network systems.

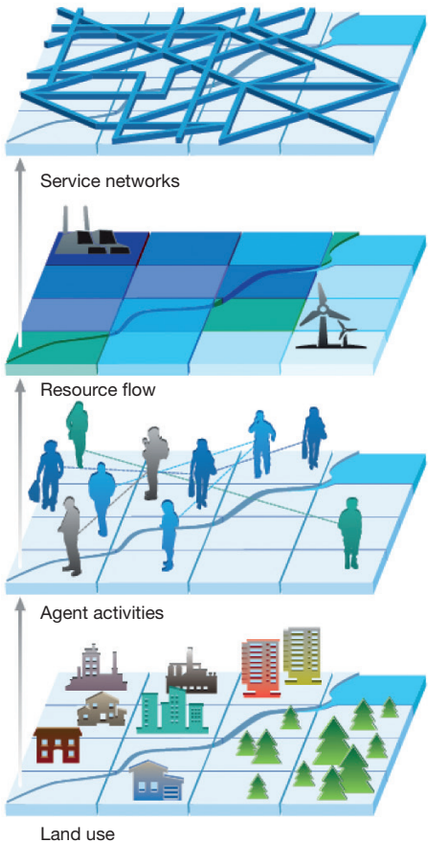
Urban Energy Systems

There has been significant progress in work on Urban Energy Systems. Dr James Keirstead and Professor Nilay Shah launched their book entitled 'Urban Energy Systems: An Integrated Approach.'

The book brings together the major lessons learnt from a £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.

Professor Shah made the following comments on the book: *"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. Our book features a mix of case studies, modelling techniques, and background material that can help the next generation of engineers and policy makers take new approaches to designing our urban energy infrastructure so that it is more efficient and has less impact on the environment."*

One outcome of the research has been a state of the art Urban Energy Systems Model (URBEN). This model 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.



The multiple layers in the UrbEn modelling system.

Within the urban environment, collaboration has continued with a major retail company allowing CPSE to study the energy demand of a large state of the art supermarket in considerable detail. This work has proved valuable in practice when looking at new store development. The possibility of a 'zero carbon store' has also been evaluated.

Mega Events: Urban Development Drivers
A quantitative methodology to optimise the sustainability performance of major international events
Olga Parkes, Bogle, Lettieri (UCL Chemical Engineering), Malcolm Preston and Dan Dowling (PwC), EPSRC)

Sustainability assessment of mega-events and post-event site redevelopment scenario planning is a complex task that involves detailed consideration of numerous social, environmental and economic factors and views. This project is developing a framework for sustainability assessment of mega-events to assist decision-makers with the evaluation of alternative design scenarios for the event and post-event site redevelopment. The framework will be for use early in the strategic planning process for the event so that both the event and its legacy can be considered together systematically. Our cases study is the London Olympic Park.

Design scenarios are assessed on the basis of a key indicator set that includes social, environmental and economic indicators. In terms of the environmental performance, the framework addresses the following issues: transport, construction and use of the buildings, water and energy use, and waste utilisation.

Scenario analysis is used to explore social impact. Life Cycle Analysis is a key tool for assessment of alternative environmental scenarios. For example LCA has been used to explore sustainable management of the municipal solid waste (MSW) which is a significant environmental issue. Using 10 integrated waste management scenarios we have shown that Advanced Thermal Treatment and incineration with energy recovery show the lowest Global Warming Potential (GWP). Economic assessment will use traditional methods.

The overall framework allows scenarios to be optimised across the life cycle under different assumptions. The results of the optimised scenarios can be used to assist in the long term planning and stakeholder consultation of the event and its legacy.

The optimisation of a future hydrogen infrastructure

Any future use of hydrogen as a significant fuel for power generation and transport will require a carefully designed supply chain capable of producing, distributing, storing and dispensing hydrogen to end users at the least possible cost. There are clearly many permutations of the ways hydrogen might be produced, transported and stored. The spatial distribution of these elements as well as demand and electricity cost profiles are critical parameters. Hydrogen has multiple uses including decarbonisation of transport and electricity storage.

Our approach was to build a MILP optimisation model to find the least cost supply network, subject to certain constraints. The model is based on a geographical grid of Great Britain and takes account of whether hydrogen is supplied as a liquid or gas, its primary source for example, natural gas, oil, coal, biomass, electrolysis using solar power etc. which determines the size, type and location of production plants together with the proximity of raw materials. Once produced, the model evaluates the various transport options; pipeline, truck or rail and the cost of transport mode compared to the establishment of a new production plant and decides on the number of fuelling stations in each grid square.

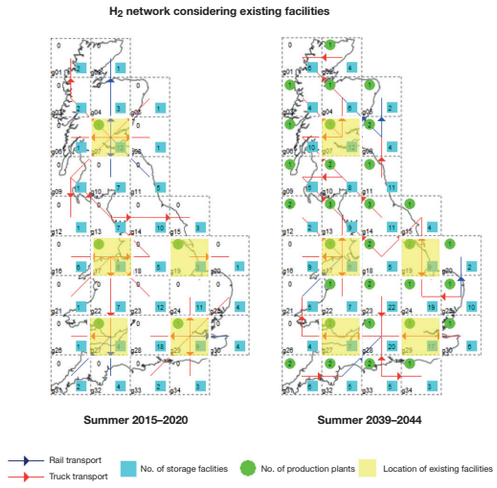


Figure (above). Possible future hydrogen system, indicating how existing facilities bias future infrastructure.

In one case study, we examined the possibility of hydrogen as a means of storing electricity and how advantage can be taken of daily price variations in grid electricity. This is illustrated below, where the relation between amount and cost of storage and hydrogen balances (surplus and deficit through a week are illustrated).

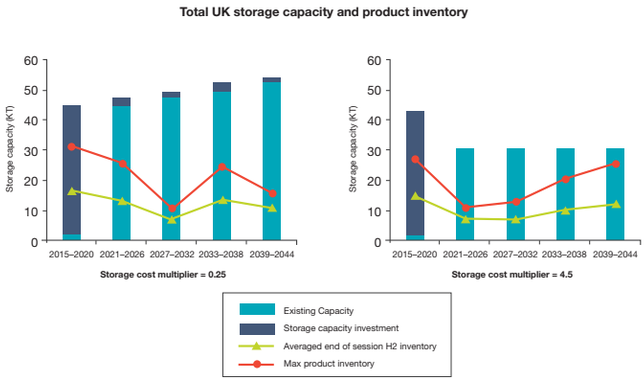


Figure (above). Relation between storage capacity growth and storage cost.

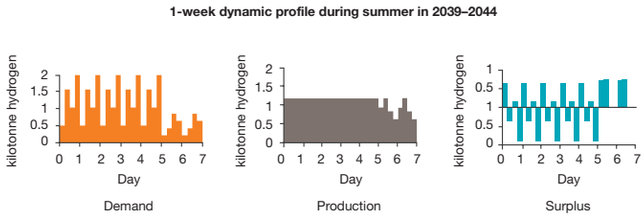


Figure (above). Hydrogen balance: demand, production and nett surplus/deficit (balanced by storage).

Application Domains
Environmental Systems Engineering

Environmental Systems Engineering is concerned with the development and application of mathematical models with the aim of improving the design, operation and control of existing environmental processes and also to develop the next generation of environmental systems

The world is facing a complex challenge – The International Energy Agency (IEA) has predicted a doubling of global energy demand by 2030, the UN's Food and Agriculture Organisation (FAO) predicts that the demand for foodstuffs will also double by 2030, and the International Food Policy Research Institute (IFPRI) has reported that the demand for water will increase by 30% in the same period. These increases in demand must be viewed against the backdrop of the latest report from the Intergovernmental Panel on Climate Change, which acknowledges human influence on the climate system. These interrelated issues provide a focus for CPSE's research on water recycling, wastewater treatment, and recovery of energy and material for waste or wastewater streams, with a particular emphasis on pushing the frontiers of microbial ecosystems for bioenergy production and waste treatment using systems thinking and methodologies. Current projects are concerned with the development and application of mathematical models with the aim of (i) improving the design, operation and control of existing environmental processes, and (ii) developing the next generation of environmental systems.

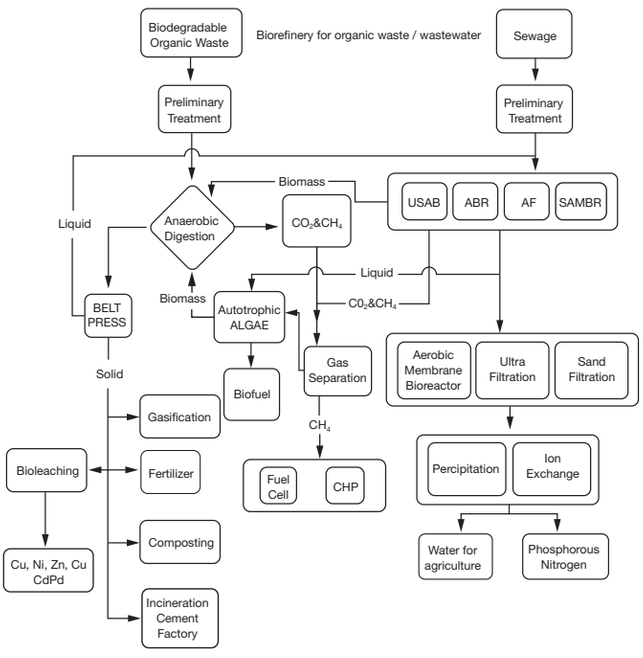


Figure (above). Treatment and separation technologies for polygeneration from wastewater.

Polygeneration from Wastewater

While there seems to be a general consensus that wastewater (and wastewater sludge) is a potential source of valuable resources, and that the technology needed for such resource recovery is maturing, it is the lack of decision-making tools and design methodologies that is the primary problem in identifying the most sustainable solutions in a given geographic and cultural context. CPSE is working on the development and application of systematic model-based methodologies for the synthesis of wastewater resource recovery systems that are both economically attractive and sustainable. With the array of available treatment and recovery options growing steadily, superstructure modeling and optimization approaches are investigated, which use surrogate models constructed from commercial wastewater simulators. State-of-the-art MINLP technology is applied to solve these problem, paying special attention to how uncertainty propagates throughout this methodology.

Integrated Water Networks for Freshwater Minimization

Due to the high demand of 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. In 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 is 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 also investigated the problem of integrated water network synthesis under uncertainty in with risk management using the Conditional Value-at-Risk (CVaR) metric, showing that rigorous, risk-averse solutions too can be computed in reasonable time.

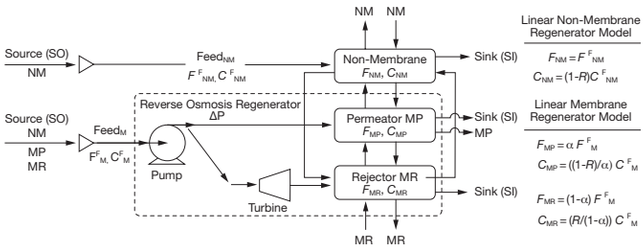


Figure (above). Superstructure (simplified) around the regenerators in water network synthesis problem Plant-wide Optimization of Existing Wastewater Treatment Plants.

Among the alternatives for the sewage industry to reduce their energy consumption without compromising effluent quality, improving operational and process control strategies holds much promise. 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) could be reduced by 10-40%. Nonetheless, 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 can even be detrimental overall.

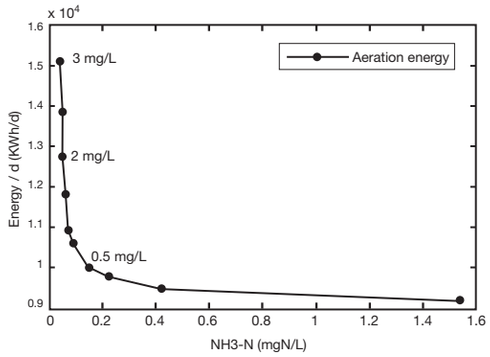


Figure (below, left). Interplay between power consumption, ammonia discharge and N2O emissions at various dissolved-oxygen set-points.

Multi-Scale Modeling of Microalgae Culture

Microalgae have long been identified 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 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 microlagae 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.

CPSE is working on the development of multiscale dynamic models of microalgae culture with applications to process monitoring, control and optimization. Particularly important in outdoor culture systems, where the light irradiance varies greatly, are the processes of photoinhibition and photoacclimation, which can affect photoproduction significantly. The former is caused by an excess of light and occurs on a fast time scale of minutes, whereas the latter results from the adjustment of the light harvesting capacity to the incoming irradiance and takes place on a slow time scale of days. Our recent focus has been on relating these key photosynthetic processes to characteristic fluorescence fluxes as measured by Pulsed Amplitude Modulation (PAM) fluorometers. In combination with classical photosynthetic observations, such as oxygen production and biomass growth, these advances allow for determination of reliable estimates for many model parameters, leading to more reliable short- and long-term predictions. Future work will involve combining the developed models with CFD models describing the hydrodynamics of raceway ponds and closed photobioreactors.

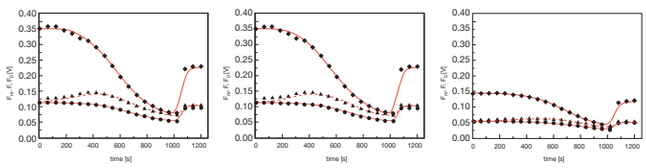
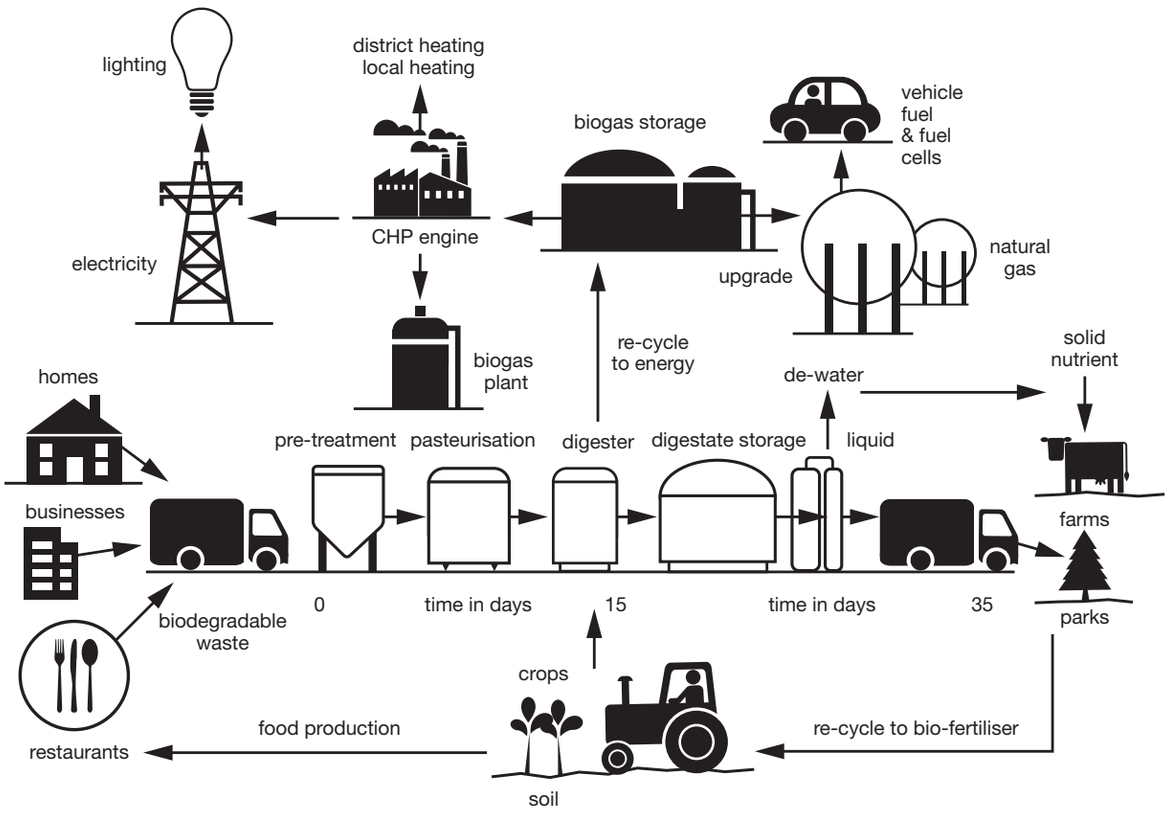


Figure (above). Experimental and predicted fluorescence fluxes in microalgae N. Salina at three different acclimation states.

Operational Improvements in Anaerobic Digestion Food Waste Plants.



Food waste is a serious problem. In the UK alone, some 18 million tonnes are produced every year, of which roughly 6 million tonnes have to be collected by local authorities. Treating food waste in an anaerobic digester is cost-competitive with landfill and other alternatives, and it is more environmentally sustainable. In anaerobic digesters, food waste breaks down into methane gas, which is captured and sent to super-efficient gas engines to generate renewable electricity and heat. All that remains is a liquid fertilizer, rich in nutrients, which goes back onto the land to grow crops, substituting for fossil fuel derived fertilizers.

Figure (above). Anaerobic digestion as part of food waste's life cycle.

Despite these promises, the operation of anaerobic digestion food waste plants presents many challenges. Contaminants and inorganic materials not eliminated by the pre-treatment can accumulate in the digester, potentially impairing mixing and causing operational failures in downstream pumps. Historical data reveal that such failure rates depend greatly on the schedule of degritting operations as well as the moisture content of the pretreated food waste slurry. In response to this, CPSE is investigating the application of systems methodologies and tools to improve the scheduling operations and waster management in food waste plants.

Academic Profiles
Professor Efstratios N Pistikopoulos

"Our long-term and well established collaboration with our industrial partners is vital to focus, enhance, expand and strengthen our research programme and portfolio while bringing engineering relevance and delivering value. Industrial companies participate with us in other European and research council projects as well as providing case studies to on-going research projects – activities that complement and leverage their Industrial Consortium participation."

Academic Profiles
A – Z

Claire S. Adjiman

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 Institution of Chemical Engineers
Chartered Engineer
EPSRC Leadership Fellowship, 2012–2017
Henry E. Armstrong Memorial Lecture of the Society of Chemical Industry, 2011
Philip Leverhulme Trust 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 Honorific Fellowship, Princeton University, 1997

Secondments
Process Systems Enterprise Ltd, September 2006–August 2007

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
AIChE Journal, Chemical Engineering Research and Design, Computers and Chemical Engineering, Molecular Physics, Journal of Power Sources, Energy & Fuels, Journal of Global Optimization, Industrial and Engineering Chemistry Research, Fluid Phase Equilibria, Chemical Engineering Science, Computers and Chemical Engineering, Imperial College Press, Mathematical Programming, Optimization and Engineering

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 (A * indicates open-access publication)

1. Pereira, F.E., Jackson, G., Galindo, A., Adjiman, C.S., "The HELD algorithm for multicomponent, multiphase equilibrium calculations with generic equations of state", *Computers and Chemical Engineering*, 36 (2012) 99-118.
2. Lafitte, T., Avendaño, C.,Papaioannou, V., Galindo, A., Adjiman, C.S., Jackson, G., Muller, E.A., "SAFT-γ force field for the simulation of molecular fluids: 3. Coarse-grained models of benzene and hetero-group models of n-decylbenzene", *Mol. Phys.*, 110 (2012) 1189-1203.
3. Rodriguez, J., Mac Dowell, N., Llovell, F., Adjiman, C.S., Jackson, G., Galindo, A., "Modelling the fluid phase behaviour of aqueous mixtures of multifunctional alkanolamines and carbon dioxide using transferable parameters with the SAFT-VR approach", *Mol. Phys.*, 110 (2012) 1325-1348.
4. Vasileiadis, M., Kazantsev, A.V., Karamertzanis, P.G., Adjiman C.S., Pantelides, C.C., "The polymorphs of ROY: application of a systematic crystal structure prediction technique", *Acta Cryst. B*, 68 (2012) 677-685.
5. Avendaño, C., Lafitte, T., Adjiman, C.S., Galindo, A., Müller, E.A., Jackson, G., "SAFT-γ Force Field for the Simulation of Molecular Fluids: 2. Coarse-Grained Models of Long Alkanes, Greenhouse Gases, and Refrigerants", *The Journal of Physical Chemistry B*, 117 (2013) 2717-2733.
6. Rhazaoui, K., Cai, Q., Adjiman, C.S., Brandon, N.P., "Towards the 3D modeling of the effective conductivity of solid oxide fuel cell electrodes. I. Model development", Chem. Eng. Sci., 99 (2013) 161-170 (http://dx.doi.org/10.1016/j.ces.2013.05.030).
7. Struebing, H, Ganase, Z., Karamertzanis, P.G., Siougkrou, E., Haycock, P. Piccione, P.M., Armstrong, A., Galindo, A., Adjiman, C.S., "Computer-aided molecular design of solvents for accelerated reaction kinetics", *Nature Chem*. 5 (2013) 952-957. *Highlighted in News and Views article, D.G. Truhlar, "Chemical Reactivity: Inverse Solvent Design", Nature Chem. 5 (2013) 902-903*.
8. Lafitte, T., Apostolakou, A., Avendaño, C., Galindo, A., Adjiman, C.S., Müller, E.A., Jackson, G., "Accurate statistical associating fluid theory for chain molecules formed from Mie segments", *J. Chem. Phys*.139(5) (2013) 154504.*
9. Siougkrou, E., Galindo, A., Adjiman, C.S., "On the optimal design of gas-expanded liquids based on process performance", *Chem. Eng. Sci.*, (2013) http://dx.doi.org/10.1016/j.ces.2013.12.025.*

Selected Refereed Conference Publications

1. Akula, P., Kleniati, P.-M., Adjiman, C.S., "On the Design of Optimal Solvent Mixtures using Generalised Disjunctive Programming", *Proc. of the 22nd ESCAPE*, London, June 2012.
2. Cai, Q., Haw, A.W.V., Adjiman, C.S., Brandon, N.P., "Hydrogen production through steam electrolysis: a model-based study", 22nd European Symposium on Computer-Aided Process Engineering, *Computer-aided Chemical Engineering*, (Bogle, I.D.L., Fairweather, M.., ed), vol. 30 (2012) 257-267
3. Brand, C.V., Rodriguez, J., Galindo, A., Jackson, G., Adjiman, C.S., "Validation of an absorber model of carbon dioxide capture in an aqueous amine solvent developed based on the SAFT-VR framework", 11th International Symposium on Process Systems Engineering, *Computer-aided Chemical Engineering*, (Karimi, I.A., Srinivasan, R., ed), vol. 31 (2012) 930-934.
4. Chremos, A., Forte, E.F., Papaioannou, V., Galindo, A., Jackson, G., Adjiman, C.S., "Modelling the fluid phase behaviour of multifunctional alkanolamines and carbon dioxide using the SAFT-γ approach", Proc. of the 16th Conf on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction, *Chem. Eng. Trans*. Vol. 35, (2013) 427-432. doi: 10.3303/CET1335071.
5. Brand, C.V., Rodriguez, J., Galindo, A., Jackson, G., Adjiman, C.S., "Validation of a process model of CO2 capture in aqueous solvent, using an implicit molecular based treatment of the reactions", *Energy Procedia*, 37 (2013) 1566-1571.

Invited lectures and Seminars

1. "Structure Optimisation: Crystals, Molecules and Processes", Foundations of Molecular Modeling and Simulation (FOMMS) 2012, Oregon, July 2012.
2. "Structure Optimisation: Crystals, Molecules and Processes", EQUIFASE, Chile, October 2012.
3. "Computer-Aided Design of Reaction Solvents", InPrompt, Berlin, November 2012.
4. "Structure optimization: crystals, molecules and processes", Francis Crick Institute retreat, Ashridge Business School, UK, 30 April 2013.
5. "Temperature effects in crystal structure prediction", PPEPPD, (one of a few contributed papers selected for presentation to whole conference), Iguazu Falls, Argentina, May 2013
6. "Integrated process and solvent design for physical CO2 absorption: using the SAFT-γ Mie equation of state and hierarchical optimization", Max Planck Institute Magdeburg, Germany, 25 June 2013.
7. "The expanding envelope of process design: from molecules to processes", University College London, UK, 27 Nov. 2013
8. "The expanding envelope of process design: from molecules to processes", University of Kaiserslautern, Germany, 13 Dec. 2013
9. "Bilevel Optimisation: From Phase Equilibria to General Mixed-Integer Problems", Global Optimization Workshop, UK, 19 December 2013

Edo Boek

Senior Lecturer, Department of Chemical Engineering, Imperial College London

Qualifications
MSc in Earth Sciences (Utrecht University)
PhD in Chemical Engineering (Twente University)

Awards and Distinctions
Principal Investigator, Qatar Carbonates and Carbon Storage Research Centre, 2009

Research Interests
My research is aimed at the flow of complex fluids in porous media. I study how the complex flow behaviour emerges from the underlying fluid and porous media properties using computer simulations and experiments. Applications include CO2 sequestration and hydrocarbon recovery. For this purpose, I have developed a range of multi-scale statistical mechanical simulation techniques, across length and time scales. These include lattice-Boltzmann (LB), Molecular Dynamics and Multi-Particle Collision Dynamics (MPCD / SRD). Since appointment at Imperial, I have broadened my activities to experimental work for direct comparison with and validation of the computer simulations. Thanks to generous support from sponsors and IC, I have been able to establish the Qatar Complex Fluids lab (ACEX 504), including micro-fluidic experiments for CO2 storage and asphaltene fouling, confocal laser scanning microscopy; and HPHT rheology of complex fluids. In addition, I am responsible for the Qatar Multi-Scale Imaging lab, including a state of the art micro-CT scanner. Using this equipment, we obtain high resolution 3D pore space images of complex porous media. These images are used directly in massively parallel LB simulations to predict flow properties. In addition, we are currently carrying out multi-phase and reactive flow experiments under HPHT reservoir conditions to study CO2 storage efficiency and multi-phase flow properties, including relative permeability. The experiments are directly compared with LB simulations on the pore space images obtained.

Other Activities
Committee member, Liquids and Complex Fluids, Institute of Physics Member, Editorial board Journal of Chemical Engineering & Process Technology

Reviewer for
Energy and Fuels , member of editorial advisory board
Journal of Chemical Engineering & Process Technology, member of editorial board
J. Fluid Mechanics, Langmuir, Transport in Porous Media, J. Am. Chem. Soc.,
J. Colloid Interface Sci., J. Phys. Chem., J. Chem. Phys., Europhys. Letters, Energy & Fuels, J. Non-Newt. Fluid Mech., Mol. Phys.,

Academic Collaborations
Visiting scientist, Centre for Computational Chemistry (CUC3), Dept. of Chemistry, University of Cambridge, Lensfield Road Cambridge U.K., prof. Daan Frenkel visiting scientist, BP Institute University of Cambridge.Eindhoven University, NL

Industrial Collaborations
Shell, Qatar Petroleum

Consultancies
Schlumberger Cambridge Research, MI-SWACO, Shell

Publications
Journal Articles

1. Yang J, Crawshaw J, Boek ES, 2013, Quantitative determination of molecular propagator distributions for solute transport in homogeneous and heterogeneous porous media using lattice Boltzmann simulations, *Water Resources Research*, Vol:49, ISSN:0043-1397, Pages:8531-8538
2. Seifried CM, Crawshaw J, Boek ES, 2013, Kinetics of Asphaltene Aggregation in Crude Oil Studied by Confocal Laser-Scanning Microscopy, *Energy & Fuels*, Vol:27, ISSN:0887-0624, Pages:1865-1872
3. Mikami Y, Liang Y, Matsuoka T, et al., 2013, Molecular Dynamics Simulations of Asphaltenes at the Oil-Water Interface: From Nanoaggregation to Thin-Film Formation, *Energy & Fuels*, Vol:27, ISSN:0887-0624, Pages:1838-1845
4. Li X, Ross DA, Trusler JPM, et al., 2013, Molecular Dynamics Simulations of CO2 and Brine Interfacial Tension at High Temperatures and Pressures, *Journal of Physical Chemistry B*, Vol:117, ISSN:1520-6106, Pages:5647-5652
5. Yang J, Boek ES, 2013, A comparison study of multi-component Lattice Boltzmann models for flow in porous media applications, *Computers & Mathematics with Applications*, Vol:65, ISSN:0898-1221, Pages:882-890
6. Al Halwachi HK, Yakovlev DS, Boek ES, 2012, Systematic Optimization of Asphaltene Molecular Structure and Molecular Weight Using the Quantitative Molecular Representation Approach, *Energy & Fuels*, Vol:26, ISSN:0887-0624, Pages:6177-6185
7. Stukan MR, Ligneul P, Boek ES, 2012, Molecular Dynamics Simulation of Spontaneous Imbibition in Nanopores and Recovery of Asphaltenic Crude Oils Using Surfactants for EOR Applications, *Oil & Gas Science and Technology-Revue d'IFP Energies Nouvelles*, Vol:67, ISSN:1294-4475, Pages:737-742
8. Suter JL, Sprik M, Boek ES, 2012, Free energies of absorption of alkali ions onto beidellite and montmorillonite surfaces from constrained molecular dynamics simulations, *Geochimica et Cosmochimica Acta*, Vol:91, ISSN:0016-7037, Pages:109-119

9. Boek ES, 2012, 12th International Conference on Petroleum Phase Behavior and Fouling, *Energy & Fuels*, Vol:26, ISSN:0887-0624, Pages:2547-2547
10. Li X, Boek ES, Maitland GC, et al., 2012, Interfacial Tension of (Brines+CO2): CaCl2(aq), MgCl2(aq), and Na2SO4(aq) at Temperatures between (343 and 423) K, Pressures between (2 and 50) MPa, and Molalities of (0.5 to 5) mol.kg-1, *Journal of Chemical and Engineering Data*, Vol:57, ISSN:0021-9568, Pages:1369-1375
11. Lawal KA, Crawshaw JP, Boek ES, et al., 2012, Experimental Investigation of Asphaltene Deposition in Capillary Flow, *Energy & Fuels*, Vol:26, ISSN:0887-0624, Pages:2145-2153
12. Li X, Boek E, Maitland GC, et al., 2012, Interfacial Tension of (Brines + CO2): (0.864 NaCl+0.136 KCl) at Temperatures between (298 and 448) K, Pressures between (2 and 50) MPa, and Total Molalities of (1 to 5) mol.kg(-1), *Journal of Chemical and Engineering Data*, Vol:57, ISSN:0021-9568, Pages:1078-1088
13. Sengupta A, Hammond PS, Frenkel D, et al., 2012, Error analysis and correction for Lattice Boltzmann simulated flow conductance in capillaries of different shapes and alignments, *Journal of Computational Physics*, Vol:231, ISSN:0021-9991, Pages:2634-2640
14. Boek ES, Hall C, Tardy PMJ, 2012, Deep Bed Filtration Modelling of Formation Damage Due to Particulate Invasion from Drilling Fluids, *Transport in Porous Media*, Vol:91, ISSN:0169-3913, Pages:479-508

I David L. Bogle FREng

Professor of Chemical Engineering and Head of the Graduate School, University College London

Qualifications

BSc (Eng) Hons MSc PhD DIC CEng FREng FIChemE

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

Head of the UCL Graduate School.
Chair of 22nd European Symposium on Computer Aided Process Engineering (ESCAPE22).
Member of College of Engineering for the Engineering & Physical Sciences Research Council (EPSRC).
University of Sheffield Chemical Engineering at the Life Science Interface International Advisory Board.
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 Committees on Chemical Process Control and on Control of Environmental Systems.
Member of Royal Academy International Committee.
Chair Royal Academy of Engineering Distinguished Visiting Fellowship Scheme.
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.

Reviewer for
EPSRC, Royal Academy of Engineering, Industrial and Engineering Chemistry Research, Computers and Chemical Engineering, AIChEJournal, Engineering in the Life Sciences, Hepatology

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

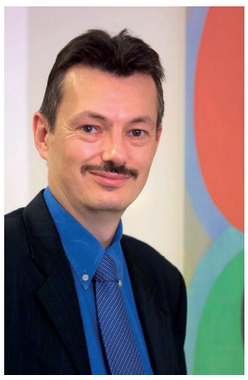
Publications
Book Chapters
Bogle I.d.l., Jalan R., Shephard E., Seymour R.m., Finkelstein A., Sumner, Warner A. (2012) Systems Biology of the Liver. In "System Biology, Encyclopedia of Molecular Cell Biology and Molecular Medicine", John Wiley & Son.

Book Editor
Computer Aided Chemical Engineering Vol 30 ed. I.D.L. Bogle and M. Fairweather, Elsevier, 2012

Journal Articles
1. HETHERINGTON J., SUMNER T., SEYMOUR R.M., LI L., VARELA REY M., MARGONINSKI O., BOGLE I.D.L., FINKELSTEIN A., and WARNER A. (2012) A composite computational model of liver glucose homeostasis. Part 1: Building the composite model. J Roy Soc Interface 9 69 689-700 doi: 10.1098/rsif.2011.0141
2. SUMNER T., HETHERINGTON J., SEYMOUR R.M., LI L., VARELA REY M., MARGONINSKI O., BOGLE I.D.L., FINKELSTEIN A., and WARNER A. (2012) A composite computational model of liver glucose homeostasis. Part 2: Exploring system behaviour. J Roy Soc Interface 9 69 701-706, doi: 10.1098/rsif.2011.0783
3. Al FULAIJ H., CIPPOLINA A., BOGLE I.D.L. and ETTOUNEY H. (2011) Simulation of Stability and Dynamics of Multistage Flash Desalination. Desalination 281 404-412 http://dx.doi.org/10.1016/j.desal.2011.08.012
4. SUMNER T., SHEPHARD E., BOGLE I.D.L. (2012) A methodology for global sensitivity analysis of time-dependent outputs in systems biology modelling. J Roy Soc Interface 9 74 2156-2166, doi: 10.1098/rsif.2011.0891
5. PARKES O., BOGLE I.D.L. and LETTIERI P. (2012) Towards defining a quantitative methodology to enhance the sustainability performance of major international events. Computer Aided Chemical Engineering Vol. 30 pp46-50. Elsevier
6. BOGLE I.D.L. (2012) Recent Developments in Process Systems Engineering as Applied to Medicine. Current Opinion in Chemical Engineering 2012 1: 453-458

Conference Contributions:
1. PARKES O., BOGLE I.D.L. and LETTIERI P. (2012) Towards defining a quantitative methodology to enhance the sustainability performance of major international events. ESCAPE22
2. Perez-Galvan C, Bogle I.D.L. and Dua V., Global Optimisation of Dynamic Process Systems. 6th Small Workshop on Interval Methods, Brest, 2013.

Invited Lectures and Seminars
1. The Role for Process Systems Engineering in Physiology and Clinical Medicine ETH Zurich
2. Planning Sustainable Process Businesses with Process Systems Engineering Ecochem, Basel 2013.



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
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

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 as, with other research centres and universities around the world, as 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

1. Maher RC, Duboviks V, Offer GJ, et al., 2013, Raman Spectroscopy of Solid Oxide Fuel Cells: Technique Overview and Application to Carbon Deposition Analysis, *Fuel Cells*, Vol:13, ISSN:1615-6846, Pages:455-469
2. Wu B, Yufit V, Marinescu M, et al., 2013, Coupled thermal-electrochemical modelling of uneven heat generation in lithium-ion battery packs, *Journal of Power Sources*, Vol:243, ISSN:0378-7753, Pages:544-554
3. Rhazaoui K, Cai Q, Adjiman CS, et al., 2013, Towards the 3D modeling of the effective conductivity of solid oxide fuel cell electrodes: I. Model development, *Chemical Engineering Science*, Vol:99, ISSN:0009-2509, Pages:161-170
4. Yufit V, Hale B, Matian M, et al., 2013, Development of a Regenerative Hydrogen-Vanadium Fuel Cell for Energy Storage Applications, *Journal of the Electrochemical Society*, Vol:160, ISSN:0013-4651, Pages:A856-A861
5. Shearing PR, Brandon NP, Gelb J, et al., 2012, Multi Length Scale Microstructural Investigations of a Commercially Available Li-Ion Battery Electrode, *Journal of the Electrochemical Society*, Vol:159, ISSN:0013-4651, Pages:A1023-A1027
6. Lorente E, Millan M, Brandon NP, 2012, Use of gasification syngas in SOFC: Impact of real tar on anode materials, *International Journal of Hydrogen Energy*, Vol:37, ISSN:0360-3199, Pages:7271-7278
7. Offer GJ, Yufit V, Howey DA, et al., 2012, Module design and fault diagnosis in electric vehicle batteries, *Journal of Power Sources*, Vol:206, ISSN:0378-7753, Pages:383-392
8. Somalu MR, Brandon NP, 2012, Rheological Studies of Nickel/Scandia-Stabilized-Zirconia Screen Printing Inks for Solid Oxide Fuel Cell Anode Fabrication, *Journal of the American Ceramic Society*, Vol:95, ISSN:0002-7820, Pages:1220-1228

Invited Lectures

1. A UK academic perpective on low carbon vehicles, Invited lecture, US-UK Low Carbon Vehicle Workshop, Atlanta, Georgia, USA, March 2nd, 2012.
2. Characterising battery microstructure in three dimensions at a range of length scales, Invited lecture, Gordon conference on Batteries, Ventura, California, USA, March 4-9th 2012.
3. The prospects for fuel cells and batteries in low carbon transport, Invited lecture, Uk-Israel BIRAX programme, Tel Aviv University, Israel, March 27th, 2012.
4. The role of fuel cell technology in low carbon energy systems, Invited lecture, I-SEE lecture series, University of Calgary, Canada, April 23rd, 2012.
5. Solid Oxide Fuel Cells for Power and Heat, Invited lecture, SOFC Industry day, Petroleum Club, Calgary, Canada, April 24th 2012.
6. UK and China working together in Energy Research, Invited lecture, RCUK China 5 years and beyond, Beijing, China, 24th September 2012.
7. The Role of fuel cell and energy storage technologies in low carbon energy future, 505th Nanqiang Lecture, Xiamen University, Xiamen, China, Sep 27th 2012.
8. Opportunities for innovation in grid scale energy storage, Invited lecture, Symposium on Emerging technologies and Industries, Beijing, China, 19-20th Nov 2012.
9. Towards the in-situ characterisation of SOFCs, Invited lecture, Fuel Cell and Hydrogen Production Symposium, Kyushu, Japan, 28th January 2013.
10. Regenerative liquid-gas fuel cells for energy storage applications, Invited lecture, US-UK workshop on grid-scale energy storage, Lawrence Berkeley National Lab, California, USA, Mar 5-6th 2013.
11. Measurement and modelling of solid oxide fuel cell and lithium battery electrode microstructure in three dimensions, Plenary lecture, 10th Symposium on fuel cell and battery modelling and experimental validation, Bad Boll, Germany, March 19-20th, 2013.
12. The role of fuel cell and energy storage technology in a low carbon energy future, Keynote lecture, Global Green Energy Hub, Incheon, Korea, 29-20th April, 2013.
13. Trends in fuel cell mCHP, Invited lecture, All-Energy, Aberdeen, 22-23rd May, 2013.
14. Understanding performance and failure in Solid Oxide Fuel Cells and Electrolysers, Invited lecture, Aachen University, Germany, 5th July 2013.
15. Developments in Long-term Sustainable Energy, Invited lecture, 100 Years and Beyond: Future Petroleum Science and Technology Drivers, Imperial College, London, 23-24th September, 2013.
16. The Hydrogen and Fuel Cell SUPERGEN Hub, Invited lecture, Royal Academy of Engineering - Chinese Academy of Engineering joint symposium on innovation in low carbon technologies, RAE, London, 26-27 November, 2013.
17. The role of hydrogen and fuel cell technology in low carbon energy systems, Invited lecture, H2FC Supergen research conference, University of Birmingham, Dec 16-18th, 2013.

Benoit Chachuat

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

Qualifications

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

Awards and Distinctions

Certificate of Excellence in Reviewing, Computers & Chemical Engineering, 2013
Automatica Outstanding Reviewer Award, 2007
Lavoisier Postdoctoral Fellowship, 2003–2004
Outstanding PhD Thesis Award, INPL, 2002

Research Interests

Environmental systems engineering, especially design and operation of wastewater treatment and recovery plants; integrated design and operation of miroalgae photobioreactors
Systematic methodologies for design and operation under uncertainty
Real-time optimization of dynamic and large-scale processes
Development of new methods and tools for deterministic global optimization

Other Activities

International Programming Committee, 11th IWA Conference on Instrumentation Control and Automation (ICA), 2013
International Advisory Board, 3rd International Conference on Engineering Optimization (EngOpt), 2012
International Programming Committee, 8th IFAC Symposium on Advanced Control of Chemical Processes (ADCHEM), 2012
International Scientific Committee, 22nd European Symposium on Computer Aided Process Engineering (ESCAPE), 2012
Adjunct Professor, Department of Chemical Engineering, McMaster University, Canada

Reviewer Activities

Associate Editor, Journal of Process Control, Elsevier
Associate Editor, Journal of Optimization Theory & Applications, Springer
Regular reviewer for: AIChE Journal; Annual Reviews in Control; Applied Energy; Applied Mathematics & Computations; Applied Numerical Mathematics; Automatica; Computers & Chemical Engineering; IEEE Control Systems Magazine; IEEE Transactions on Automatic Control; Industrial & Engineering Chemistry Research; Journal of Global Optimization; Journal of Optimization Theory & Applications; Journal of Process Control; Mathematical Programming; Optimization & Engineering; Optimization Letters; Optimization Methods & Software

Academic Collaborations

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

Industrial Collaborations

Actility; Arup; Petrobras; Praxair, Sydney Water

Publications

Journal Articles

1. C.S. Khor, B. Chachuat, N. Shah, “Fixed-Flowrate Total Water Network Synthesis under Uncertainty with Risk Management,” *Journal of Cleaner Production* (DOI 10.1016/j.jclepro.2014.01.023)
2. B. Houska, B. Chachuat, “Branch-and-Lift Algorithm for Deterministic Global Optimization in Nonlinear Optimal Control,” *Journal of Optimization Theory & Applications* (DOI 10.1007/s10957-013-0426-1)
3. S. Gros, B. Chachuat, “Optimization-based Load Reduction during Emergency Shut-down of Multi-Megawatt Wind Turbine Generators,” *Wind Energy* (DOI 10.1002/we.1618)
4. A. Bompadre, A. Mitsos, B. Chachuat, “Convergence Analysis of Taylor Models and McCormick-Taylor Models,” *Journal of Global Optimization*, 57(1):75-114, 2013
5. M. Podmajersky, M. Fikar, B. Chachuat, “Measurement-based Optimization of Batch and Repetitive Processes using an Integrated Two-Layer Architecture,” *Journal of Process Control*, 23(7):943-955, 2013
6. J.K. Scott, B. Chachuat, P.I. Barton, “Nonlinear Convex and Concave Relaxations for the Solutions of Parametric ODEs,” *Optimal Control Applications & Methods*, 34(2):145-163, 2013
7. A. Radivojevic, A., B. Chachuat, D. Bonvin, V.H. Hatzimanikatis, “Exploration of Trade-offs between Steady-State and Dynamic Properties of Signaling Cycles,” *Physical Biology*, 9(4):045010, 2012
8. S.A. Deshpande, D. Bonvin, B. Chachuat, “Directional Input Adaptation in Parametric Optimal Control Problems,” *SIAM Journal on Control & Optimization*, 50(4):1995-2024, 2012

9. C.S. Khor, B. Chachuat, N. Shah, “A Superstructure Optimization Approach for Water Network Synthesis with Membrane Separation-based Regenerators,” *Computers & Chemical Engineering*, 42:48-63, 2012
10. F. Mairet, O. Bernard, E.T. Cameron, M. Ras, L. Lardon, Steyer J.P., B. Chachuat, “Three Reaction Model for the Anaerobic Digestion of Microalgae,” *Biotechnology & Bioengineering*, 109:415-425, 2012

Peer Reviewed International Conference Papers

1. A. Nikolaou, A. Bernardi, F. Bezzo, T. Morosinotto, B. Chachuat, “A Dynamic Model of Photoproduction, Photoregulation and Photoinhibition in Microalgae using Chlorophyll Fluorescence,” 19th IFAC World Congress (IFAC’14), 24-29 Aug 2014, Cape Town, South Africa
2. M.E. Villanueva, B. Houska, B. Chachuat, “On the Stability of Set-Valued Integration for Nonlinear Parametric ODEs,” 24th European Symposium on Computer Aided Process Engineering (ESCAPE24), 15-18 June 2014, Budapest, Hungary
3. B. Houska, M.E. Villanueva, B. Chachuat, “A Validated Integration Algorithm for Nonlinear ODEs using Taylor Models and Ellipsoidal Calculus,” 52nd IEEE Conference on Decision and Control (CDC), 10-13 Dec 2013, Florence, Italy
4. R. Paulen, M.E. Villanueva, B. Chachuat, “Optimization-based Domain Reduction in Guaranteed Parameter Estimation of Nonlinear Dynamic Systems,” 9th IFAC Symposium on Nonlinear Control Systems (NOLCOS), 4-6 Sep 2013, Toulouse, France
5. C.S. Khor, B. Chachuat, N. Shah, “Optimal Water Network Synthesis under Uncertainty with Detailed Membrane-based Regenerator Models,” 6th International Symposium on Process Systems Engineering Asia (PSE Asia)}, 25-27 June 2013, Kuala Lumpur, Malaysia
6. P. Hartmann, A. Nikolaou, B. Chachuat, O. Bernard, “A Dynamic Model coupling Photoacclimation and Photoinhibition in Microalgae,” European Control Conference (ECC), 17-19 July 2013, Zürich, Switzerland
7. R. Paulen, M.E. Villanueva, M. Fikar, B. Chachuat, “Guaranteed Parameter Estimation in Nonlinear Dynamic Systems using Improved Bounding Techniques,” European Control Conference (ECC), 17-19 July 2013, Zürich, Switzerland
8. M.E. Villanueva, R. Paulen, B. Houska, B. Chachuat, “Enclosing the Reachable Set of Parametric ODEs using Taylor Models and Ellipsoidal Calculus,” 23rd European Symposium on Computer Aided Process Engineering (ESCAPE23), 9-12 June 2013, Lappeenranta, Finland
9. J. Rajyaguru, B. Chachuat, “Taylor Models in Deterministic Global Optimization for Large-Scale Systems with Few Degrees of Freedom,” 23rd European Symposium on Computer Aided Process Engineering (ESCAPE23), 9-12 June 2013, Lappeenranta, Finland
10. C.S. Khor, B. Chachuat, N. Shah, “Optimal Water Network Synthesis with Mechanistic Membrane Separation-based Regenerator Models,” 11th International Symposium on Process Systems Engineering (PSE), 15-19 July 2012, Singapore
11. S. Gros, B. Chachuat, “Methodology for Emergency Shut-Down of Multi-Megawatt Wind Turbine Generators,” 11th International Symposium on Process Systems Engineering (PSE), 15-19 July 2012, Singapore
12. C. Gomez-Mont, C. Puchonkawarin, D.C. Stuckey, Chachuat B., “Optimization-based Methodology for the Synthesis of Biorefinery Treatment Plants for Energy and Nutrient Recovery,” IWA Specialist Conference on Ecotechnologies for Wastewater Treatment (ECOSTP)},25-27 June 2012, Santiago de Compostela, Spain
13. B. Chachuat, M.E. Villanueva, “Bounding the Solutions of Parametric ODEs: When Taylor Models Meet Differential Inequalities,” 22nd European Symposium on Computer Aided Process Engineering (ESCAPE22), 17-20 June 2012, London, UK
14. C.S. Khor, B. Chachuat, N. Shah, “Optimal Water Network Synthesis for Process Industry using Mixed-Integer Nonlinear Programming (MINLP) with Logical Constraints,” 22nd European Symposium on Computer Aided Process Engineering (ESCAPE22), 17-20 June 2012, London, UK
15. C. Puchonkawarin, C. Gomez-Mont, D.C. Stuckey, B. Chachuat, “Optimization-based Methodology for the Synthesis of Wastewater Facilities for Energy and Nutrient Recovery,” 9th IWA Leading-Edge Conference on Water and Wastewater Technologies (LET), 3-7 June 2012, Brisbane, Australia
16. C.S. Khor, B. Chachuat, N. Shah, “Optimal Process Planning under Uncertainty with Risk Management,” Foundations of Computer-Aided Process Operations (FOCAPO), 8-12 Jan 2012, Savannah, GA

Invited Lectures and Seminars

1. “Branch-and-Lift Algorithm for Deterministic Global Optimization in Nonlinear Optimal Control,” Invited Lecture, 4th International Conference on Continuous Optimization (ICCOPT), 27 July-1 Aug 2013, Lisbon, Portugal
2. “Systems Thinking and Tools Applied to Water and Environmental Engineering,” ChemEngDayUK 2013, 25-26 Mar 2013, London, UK
3. “Real-Time Dynamic Optimization: Current Trends and Future Perspectives,” Keynote Address, 19th Brazilian Congress of Chemical Engineering (COBEQ), 9-12 Sep 2012, Buzios (RJ), Brazil
4. “Optimization-based Methodology for the Synthesis of Wastewater Facilities for Energy and Nutrient Recovery,”, Keynote Lecture, 9th IWA Leading-Edge Conference on Water and Wastewater

Peter DiMaggio

Lecturer, Department of Chemical Engineering,
Imperial College London

Qualifications:

BSc in Chemical Engineering (Summa Cum Laude – University of Rhode Island, Kingston, RI, USA). PhD in Chemical Engineering (Princeton University, Princeton, NJ, USA).

Awards and Distinctions

Ruth L. Kirschstein National Research Service Award: NIH Postdoctoral Research
Fellowship, Princeton U., 2010-2012.
Porter Ogden Jacobus Honorific Fellowship, Princeton U., 2008–09.
Kristine M. Layn Award for Outstanding Achievement in Research, Princeton U., 2007.
Engineering Council Excellence in Teaching Award, Princeton U., 2006.
Ticona Excellence in Teaching Assistantship Award, Princeton U., 2006.
President's Student Excellence Award, URI, 2004.

Research Interests

High-throughput proteomics and genomics technologies for discovering the epigenetic mechanisms involved in disease regulation
Multivariate optimisation-based tools for the interpretation and integration of large-scale omics datasets
Methods for optimal design in synthetic biology

Reviewer for

Analytical Chemistry, Journal of Proteome Research, Computers & Chemical Engineering, Journal of Global Optimisation, Chemical Engineering Research and Design

Academic Collaborations

MRC Clinical Sciences Centre (London), Hammersmith Hospital (London), University of Pennsylvania (USA), National High Magnetic Field Laboratory (FSU, USA).

Industrial Collaborations

Pfizer/Neusentis, Constellation Pharmaceuticals (USA)

Publications

Journal Articles

1) Baliban R.C., Sakellari D., Li Z.K., et al., Novel Protein Identification Methods for Biomarker Discovery via a Proteomic Analysis of Periodontally Healthy and Diseased Gingival Crevicular Fluid Samples, *Journal of Clinical Periodontology*, 2012, Vol: 39(3), Pages: 203-212.
2) Yu, Y., Song C., Zhang Q., et al., Histone H3 Lysine 56 Methylation Regulates DNA Replication through its Interaction with PCNA, *Molecular Cell*, 2012, Vol: 46(1), Pages: 7-17.
3) LeRoy G., Chepelev I., DiMaggio P.A. et al., Proteogenomic Characterization and Mapping of Nucleosomes Decoded by Brd and HP1 Proteins, *Genome Biology*, 2012, Vol: 13(8), Page: R68.
4) DiMaggio P.A., Wu Y., Perlman D.H. et al., Novel Phosphorylation Sites in the S. Cerevisiae Cdc13 Protein Reveal New Targets for Telomere Length Regulation, *Journal of Proteome Research*, 2012, Vol: 12(1), Pages: 316-327.
5) Evertts A.G., Zee B.M., DiMaggio P.A. et al., Quantitative Dynamics of the Link Between Cellular Metabolism and Histone Acetylation, *Journal of Biological Chemistry*, 2013, Vol: 288(17), Pages: 12142-12151.
6) Bartke T., Borgel J., and P.A. DiMaggio, Proteomics in Epigenetics: New Perspectives for Cancer Research, *Briefings in Functional Genomics*, 2013, Vol: 12(3), Pages: 205-218.
7) LeRoy G., DiMaggio P.A., Chan E.Y. et al., A Quantitative Atlas of Histone Modification Signatures from Human Cancer Cells, *Epigenetics and Chromatin*, 2013, Vol: 6(20), doi: 10.1186/1756-8935-6-20.
8) Cherblanc F.L., Chapman K.L., Reid J. et al., On the Histone Lysine Methyltransferase Activity of Fungal Metabolite Chaetocin, *J. Med. Chem*., 2013, Vol: 56(21), Pages: 8616-8625.

Invited Lectures and Seminars

Chemical Engineering at the Life Science Interface (CheLSI), November 2012, U Sheffield.
26th London Biological Mass Spectrometry Discussion Group, March 2013, UCL School of Pharmacy.
Proteomics Methods Forum Meeting, June 2013, University of York.

Vivek Dua

Senior Lecturer in Chemical Engineering,
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
AIChE Journal, Industrial and Engineering Chemistry Research, Computers and Chemical Engineering, Journal of Global Optimization, Automatica, IEEE Transactions Neural Networks, IFAC Conferences

Publications
Journal Articles

1. Gueddar, T and Dua, V (2012) Approximate multi-parametric programming based B&B algorithm for MINLPs. Computers & Chemical Engineering, 42, 288 - 297.
2. O'Donoghue DL, Dua V, Moss GW, Vergani P (2013). Increased apical Na+ permeability in cystic fibrosis is supported by a quantitative model of epithelial ion transport. The Journal of Physiology 591.15, 3681-3692.
3. Gueddar, T. and Dua, V. (2012). Novel model reduction techniques for refinery-wide energy optimisation. Applied Energy 89, 117–126.
4. Dua, V. and Dua, P. (2012). A simultaneous approach for parameter estimation of a system of ordinary differential equations, using artificial neural approximation, Industrial and Engineering Chemistry Research, 51(4), 1809-1814.

Conference Contributions

1. Bhatti, A. and Dua, V. (2013) Model-Based Optimal Design of a Gene Metabolator System, AIChE Annual Meeting, San Francisco.
2. Polykarpou, E.M. and Dua, V. (2013) Optimisation of a liquid-liquid extraction based sustainable water desalination process, Proceedings of the 6th International Conference on Process Systems Engineering (PSE ASIA), Kuala Lumpur, Malaysia.
3. Polykarpou, E.M. and Dua, V. (2012) Sustainable water desalination: Model-based optimisation of a low-temperature liquid-liquid extraction process, 22nd European Symposium on Computer-Aided Process Engineering.
4. Dua, V. (2012) Model-Based Optimal Control of Non-Viral Gene Delivery, 22nd European Symposium on Computer-Aided Process Engineering.

Eric S Fraga

Professor of Process Systems Engineering,
Department of Chemical Engineering, UCL

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 Information Technology and Control journal, the Journal of Optimization and Revista Scientia Alimentaria.
Member of the Scientific review committee for the Congress on Evolutionary Computing and on the Program Committee for the 5th World Congress on Nature and Biologically Inspired Computing.

Reviewer for

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

Academic Collaborations

University of Edinburgh, UK; University of Essex, UK

Publications

Journal Articles

1. Noorkami, M., Robinson, J., Meyer, Q., Obeisun, O., Fraga, E. S., Reisch, T., Brett, D. J. L. (2014), Effect of temperature uncertainty on polymer electrolyte fuel cell performance, International Journal of Hydrogen Energy 39, 1439-1448, doi:10.1016/j.ijhydene.2013.10.156.
2. Brown, S., Mahgerefteh, H., Beck, J., & Fraga, E. S. (2013). Global sensitivity analysis of the impact of impurities on CO pipeline failure. Reliability Engineering and System Safety, 115, 43-54. doi:10.1016/j.ress.2013.02.006
3. Yang, L., Fraga, E. S., & Papageorgiou, L. G. (2013). Mathematical programming formulations for non-smooth and non-convex electricity dispatch problems. Electric Power Systems Research, 95, 302-308.
4. Fraga, E. S., Yang, L., & Papageorgiou, L. G. (2012). On the modelling of valve point loadings for power electricity dispatch. Applied Energy, 91 (1), 301-303. doi:10.1016/j.apenergy.2011.10.001
5. Beck, J., Friedrich, D., Brandani, S., Guillas, S., & Fraga, E. S. (2012). Surrogate based Optimisation for Design of Pressure Swing Adsorption Systems. Computer Aided Chemical Engineering, 30, 1217-1221. Amsterdam, The Netherlands: Elsevier.

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 an 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 truly predict complex phase behaviour. The types of problems I am interested in at the moment include charged systems, near-critical and supercritical separations, mixtures of polymers and liquid crystals, and solid phases of chain molecules. 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).
Chairman of the Statistical Mechanics and Thermodynamics Group of the RSC. Member of the peer review college of the Engineering and Physical Sciences Research Council (EPSRC).
Member of the Advisory Board of the Chemical Database Service of the UK. Member of the International Scientific Advisory Committee of the European Symposium on Applied Thermodynamics (ESAT).

Editorial Activity

Associate Editor of the Journal of Chemical Engineering Data
Molecular Physics, Member of the advisory board

Academic Collaborations

Vanderbilt University (USA), UCM (Spain), U. Vigo (Spain),
U. Huelva (Spain)

Industrial Collaborations

IFP, BMS, Dynamic Extractions, P&G, Pfizer, PSE Ltd., Qatar Petroleum, Shell, Syngenta, Total.

Publications

Journal Articles

1. Lafitte T, Apostolakou A, Avendano C, et al., 2013, Accurate statistical associating fluid theory for chain molecules formed from Mie segments, *Journal of Chemical Physics*, Vol:139, ISSN:0021-9606, Pages:-
2. Struebing H, Ganase Z, Karamertzanis PG, et al., 2013, Computer-aided molecular design of solvents for accelerated reaction kinetics, *Nature Chemistry*, Vol:5, ISSN:1755-4330, Pages:952-957
3. Horton RM, Haslam AJ, Galindo A, et al., 2013, New methods for calculating the free energy of charged defects in solid electrolytes, *Journal of Physics – Condensed Matter*, Vol:25, ISSN:0953-8984, Pages:-
4. Rozmus J, de Hemptinne J-C, Galindo A, et al., 2013, Modeling of Strong Electrolytes with ePPC-SAFT up to High Temperatures, *Industrial & Engineering Chemistry Research*, Vol:52, ISSN:0888-5885, Pages:9979-9994
5. Cristino AF, Rosa S, Morgado P, et al., 2013, High-temperature vapour-liquid equilibrium for the (water plus alcohol) systems and modelling with SAFT-VR: 2. Water-1-propanol, *Journal of Chemical Thermodynamics*, Vol:60, ISSN:0021-9614, Pages:15-18
6. Forte E, Galindo A, Trusler JPM, 2013, Experimental and molecular modelling study of the three-phase behaviour of (propane plus carbon dioxide plus water) at reservoir conditions, *Journal of Supercritical Fluids*, Vol:75, ISSN:0896-8446, Pages:30-42
7. Forte E, Llovell F, Trusler JPM, et al., 2013, Application of the statistical associating fluid theory for potentials of variable range (SAFT-VR) coupled with renormalisation-group (RG) theory to model the phase equilibria and second-derivative properties of pure fluids, *Fluid Phase Equilibria*, Vol:337, ISSN:0378-3812, Pages:274-287
8. Avendano C, Lafitte T, Adjiman CS, et al., 2013, SAFT-gamma Force Field for the Simulation of Molecular Fluids: 2. Coarse-Grained Models of Greenhouse Gases, Refrigerants, and Long Alkanes, *Journal of Physical Chemistry B*, Vol:117, ISSN:1520-6106, Pages:2717-2733
9. Solanki R, Mathie R, Galindo A, et al., 2013, Modelling of a two-phase thermofluidic oscillator for low-grade heat utilisation: Accounting for irreversible thermal losses, *Applied Energy*, Vol:106, ISSN:0306-2619, Pages:337-354
10. Chremos A, Forte E, Papaioannou V, et al., 2013, Modelling the fluid phase behaviour of multifunctional alkanolamines and carbon dioxide using the SAFT-γ approach, *Chemical Engineering Transactions*, Vol:35, ISSN:1974-9791, Pages:427-432
11. Llovell F, Mac Dowell N, Bias FJ, et al., 2012, Application of the SAFT-VR density functional theory to the prediction of the interfacial properties of mixtures of relevance to reservoir engineering, *Fluid Phase Equilibria,* Vol:336, ISSN:0378-3812, Pages:137-150
12. Jover J, Haslam AJ, Galindo A, et al., 2012, Pseudo hard-sphere potential for use in continuous molecular-dynamics simulation of spherical and chain molecules, *Journal of Chemical Physics*, Vol:137, ISSN:0021-9606, Pages:-
13. Dufal S, Galindo A, Jackson G, et al., 2012, Modelling the effect of methanol, glycol inhibitors and electrolytes on the equilibrium stability of hydrates with the SAFT-VR approach, *Molecular Physics*, Vol:110, ISSN:0026-8976, Pages:1223-1240
14. Rodriguez J, Mac Dowell N, Llovell F, et al., 2012, Modelling the fluid phase behaviour of aqueous mixtures of multifunctional alkanolamines and carbon dioxide using transferable parameters with the SAFT-VR approach, *Molecular Physics*, Vol:110, ISSN:0026-8976, Pages:1325-1348
15. Lafitte T, Avendano C, Papaioannou V, et al., 2012, SAFT-gamma force field for the simulation of molecular fluids: 3. Coarse-grained models of benzene and hetero-group models of n-decylbenzene, *Molecular Physics*, Vol:110, ISSN:0026-8976, Pages:1189-1203
16. Solanki R, Galindo A, Markides CN, 2013, The role of heat exchange on the behaviour of an oscillatory two-phase low-grade heat engine, *Applied Thermal Engineering*, Vol:53, ISSN:1359-4311, Pages:177-187
17. Morales-Anda L, Wensink HH, Galindo A, et al., 2012, Anomalous columnar order of charged colloidal platelets, *Journal of Chemical Physics*, Vol:136, ISSN:0021-9606, Pages:-
18. Pereira FE, Jackson G, Galindo A, et al., 2012, The HELD algorithm for multicomponent, multiphase equilibrium calculations with generic equations of state, *Computers & Chemical Engineering*, Vol:36, ISSN:0098-1354, Pages:99-118
19. Avaullee L, Duchet-Suchaux P, Adjiman CS, et al., 2012, Gsaft: Application of the SAFT-γ mie group contribution EoS in the Oil/Gas Industry - From academic research to industrial deployment, AIChE 2012 - 2012 AIChE Annual Meeting, Conference Proceedings
20. Brand CV, Rodriguez-Perez J, Galindo A, et al., 2012, Validation of a process model of CO capture in an aqueous solvent, using an implicit molecular based treatment of the reactions, AIChE 2012 - 2012 AIChE *Annual Meeting, Conference Proceedings*
21. Brand CV, Rodriguez J, Galindo A, et al., 2012, Validation of an absorber model of carbon dioxide capture in an aqueous amine solvent developed based on the SAFT-VR framework, *11TH International Symposium on Process Systems Engineering,* PTS A AND B, Vol:31, ISSN:1570-7946, Pages:930-934

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
Fellow of the Royal Society of Chemistry (RSC), Chartered Chemist (FRSC, CChem)

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: as 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
Member of Executive Committee and Special Issue Editor of Molecular Physics
Member of Editorial Board of Fluid Phase Equilibria
Fellow of the Mexican Academy of Molecular Engineering
Chairman of the Statistical Mechanics and Thermodynamics Group (SMTG) of the Faraday Division of the RSC
Council Member of the Faraday Division of the RSC
Member of the Faraday Standing Committee on Conferences (FSCC)
Member of Management Committee of the Complex Fluids Group of the Institute of Physics (IOP)
External Examiner for Physical Chemistry, University of the West Indies, (Barbados, Jamaica, and Trinidad and Tobago)

Reviewer for
AIChE Journal
Chemical Physics Letters
Fluid Phase Equilibria
Industrial and Engineering Chemistry Research
Journal of the American Chemical Society
Journal of Chemical Physics
Journal of Physical Chemistry
Journal of Physics: Condensed Matter
Macromolecules
Molecular Physics
Molecular Simulation
Nature
Physical Chemistry, Chemical Physics
Physical Review Letters
Physical Review E

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
Schlumberger
Syngenta
Total
Unilever Research

Publications
Journal Articles
1. Lafitte, T., Avendaño, C., Papaioannou, V., Galindo, A., Adjiman, C. S., Jackson, G., and Müller, E. A., “SAFT-γ force field for the simulation of molecular fluids. 3. Coarse-grained models of benzene and hetero-group models of n-decylbenzene,” Molec. Phys., 110, (2012), 1189-1203. 3

2. Dufal, S., Galindo, A., Jackson, G., and Haslam, A. J., "Modelling the effect of methanol, glycol inhibitors and electrolytes on the equilibrium stability of hydrates with the SAFT-VR approach," Molec. Phys., 110, (2012), 1223-1240. 2
3. Wu, L., Wensink, H. H., Jackson, G., and Müller, E. A., "A generic equation of state for liquid crystalline phases of hard-oblate particles," Molec. Phys., 110, (2012), 1269-1288. 2
4. Rodríguez, J., Mac Dowell, N., Llovell, F., Adjiman, C. S., Jackson, G., and Galindo, A., "Modelling the fluid phase behaviour of aqueous mixtures of multifunctional alkanolamines and carbon dioxide using transferable parameters with the SAFT-VR approach," Molec. Phys., 110, (2012), 1325-1348. 5
5. Pereira, F. E., Jackson, G., Galindo, A., and Adjiman, C. S., "The HELD algorithm for multicomponent, multiphase equilibrium calculations with generic equations of state," Computers Chem. Eng., 36, (2012), 99-118. 3
6. de Wijn, A. S., Riesco, N., Jackson, G., Trusler, J. P. M., and Vesovic, V., "Viscosity of liquid mixtures: The Vesovic-Wakeham method for chain molecules," J. Chem. Phys., 136, (2012), 074514 (1-10). 2
7. Horsch, M., Hasse, H., Shchekin, A. K., Agarwal, A., Eckelsbach, S., Vrabec, J., Müller, E. A., and Jackson, G., "Excess equimolar radius of liquid drops," Phys. Rev. E, 85, (2012), 031605 (1-12). 7
8. Jover, J., Haslam, A. J., Galindo, A., Jackson, G., and Müller, E. A., "Pseudo hard-sphere potential for use in continuous molecular-dynamics simulation of spherical and chain molecules," J. Chem. Phys., 137, (2012), 144505 (1-13). 1
9. Malijevský, A., and Jackson, G., "A perspective on the interfacial properties of nanoscopic liquid drops," J. Phys.: Cond. Matt., 24, (2012), 464121 (1-28). 4
10. Llovell, F., Mac Dowell, N., Blas, F. J., Galindo, A., and Jackson, G., "Application of the SAFT-VR density functional theory to the prediction of the interfacial properties of mixtures of relevance to reservoir engineering," Fluid Phase Equil., 336, (2012), 137-150. 0
11. Avendaño, C., Lafitte, T., Adjiman, C. S., Galindo, A., Müller, E. A., and Jackson, G., "SAFT-γ force field for the simulation of molecular fluids. 2. Coarse-grained models of greenhouse gases, refrigerants, and long alkanes," J. Phys. Chem. B., 117, (2013), 2717-2733. 0
12. Domínguez, H., Haslam, A. J., Jackson, G., and Müller, E. A., "Modelling and understanding of the vapour-liquid and liquid-liquid interfacial properties for the binary mixture of n-heptane and perfluoro-n-hexane," J. Molec. Liq., 185, (2013), 36-43. 0
13. Horton, R. M., Haslam, A. J., Galindo, A., Jackson, G., and Finnis, M. W., "New methods for calculating the free energy of charged defects in solid electrolytes," J. Phys.: Cond. Matt., 25, (2013), 395001 (1-9). 0
14. Wu, L., Jackson, G., and Müller, E. A., "Liquid crystal phase behaviour of attractive disc-like particles," Int. J. Molec. Sci., 14, (2013), 16414-16442. 039
15. Lafitte, T., Apostolakou, A., Avendaño, C., Galindo, A., Adjiman, C. S., Müller, E. A., and Jackson, G., "Accurate statistical associating fluid theory for chain molecules formed from Mie segments," J. Chem. Phys., 139, (2013), proofs (1-37). DOI: http://dx.doi.org/10.1063/1.4819786 0
16. Wu, L., Müller, E. A., and Jackson, G., "Understanding and describing the liquid crystalline states of polypeptide solutions: a coarse grained model of PBLG in DMF," Macromolecules, in press, (2013).

Keynote/plenary talks given at international conferences
2012 "*Fluctuations in nanoscale drops*," Colloidal Dispersions in External Fields III (CODEF III), Bonn, Germany;
2012 "*The SAFT-γ force field,*" SciMeeting2012 - Molecular Simulations for Product and Process Design, Paris, France;
2013 "*Drops and confined anisotropic phases,*" Max Planck Institute, Soft Matter at Interfaces, Schloss Ringberg, Germany;
2013 "*Plenarvorträge: The use of SAFT in obtaining force fields for molecular simulation,*" Annual DECHEMA Conference, Würzburg, Germany.

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

Other Activities
Elected board member, Sustainable Urban Systems section,

International Society for Industrial Ecology. Technical committee member, ISIE and ATES conferences. Proposal peer review for EPSRC, ESRC, US National Science Foundation, Natural Sciences and Engineering and Social Sciences and Humanities Research Councils of Canada.

Reviewer Activities

Energy Policy, Proceedings of the National Academy of Sciences, Building Research and Information, Technological Forecasting and Social Change, Energy, Energy Economics, Journal of Artificial Societies and Social Simulation, Energy Efficiency, The Energy Journal, Journal of Industrial Ecology, Computers, Environment and Urban Systems, Journal of Urban Technology, International Journal of Sustainable Transportation, Climatic Change, Urban Design and Planning, Environmental Science & Technology, IET Renewable Power Generation, Environment and Planning B, Ecological Modelling, Environmental Research Letters, and others.

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

Publications

Book Chapters

1. Keirstead, J., Shah, N., eds. 2013. *Urban Energy Systems: An Integrated Approach*. Earthscan: London.
2. Shah, N, et al. 2013. “Halving global CO2 by 2050: Technologies and Costs”, Grantham Institute report, Imperial College London.
3. Keirstead, J., Shah, N. 2013 “The changing role of optimization in urban planning” in *Optimization, Simulation and Control*, edited by A. Chinchuluun et al. Springer Series in Optimization and Its Applications. Springer.
4. Keirstead, J., Shah., N. 2012 “Urban energy systems planning, design and implementation” in *Energizing Sustainable Cities: Assessing Urban Energy*, edited by A. Grubler and D. Fisk, Earthscan: London.
5. Grubler, A. et al. 2012 “Urban Energy Systems” in *The Global Energy Assessment*. Cambridge: Cambridge University Press.

Journal Articles

1. Keirstead, J. 2013. “Benchmarking urban energy efficiency in the UK” *Energy Policy,* 63: 575-587
2. Morlet, C., Keirstead, J. 2013 “A comparative analysis of urban energy governance in four European cities” *Energy Policy*, 61: 852-863.
3. Keirstead, J., Sivakumar, A. 2013. “Using activity-based modeling to simulate urban resource demands at high spatial and temporal resolutions”. *Journal of Industrial Ecology*, 16(6): 889-900.
4. Rutter, P., Keirstead, J. 2012. “A brief history and the possible future of urban energy systems.” *Energy Policy*, 50: 72-80.
5. Calderon, C., Keirstead, J. 2012. “Modelling frameworks for delivering low carbon cities: advocating a normalised practice.” *Building Research and Information*, 40(4): 504-517.
6. Keirstead, J., Calderon, C. 2012. “Capturing spatial effects, technology interactions, and uncertainty in urban energy and carbon models: retrofitting Newcastle as a case-study.” *Energy Policy*, 46: 253-267.
7. Keirstead, J., Jennings, M., Sivakumar, A. 2012 “A review of urban energy system models: approaches, challenges, and opportunities.” *Renewable and Sustainable Energy Reviews*, 16(6): 3847-3866.
8. Keirstead, J., Samsatli, N., Shah, N., Weber, C. 2012 “The impact of CHP (combined heat and power) planning restrictions on the efficiency of urban energy systems.” *Energy*, 41(1): 93-103.
9. Keirstead, J., Samsatli, N., Pantaleo, A.M., Shah, N. 2012. “Evaluating biomass energy strategies for a UK eco-town with an MILP optimization model.” *Biomass and Bioenergy*, 39: 306-316.
10. Liang, H, Long, W., Keirstead, J., Samsati, N., Shah, N. 2012. “Urban Energy Systems Planning and Chinese Low-Carbon Eco-City Case Study” *Advanced Materials Research*, 433-440.

Conference Contributions

1. Keirstead, J. 2013. “Introducing sustainable development to engineers with a simple mathematical model”. Engineering Education for Sustainable Development conference. Cambridge.
2. N J D Graham, K Hellgardt, K S Wong, J Keirstead, Q Majali. 2013. “Combining H2 Generation and Grey Water Recycling at Household Scale” 12th International Conference on Sustainable Energy Technologies, Hong Kong.
3. S Giarola, A.M. Pantaleo, J. Keirstead, N. Shah. 2013 “Biomass and Natural Gas Cofiring Strategies for Optimal Integration into Urban Energy Systems”. European Biomass Conference, Copenhagen.
4. C. Calderon, J. Keirstead. 2012. “Modelling approaches for retrofitting energy systems: Newcastle as a case study”. Applied Urban Modelling 2012, Cambridge.

Invited Lectures and Seminars

“How do models of urban energy systems account for climate change?” RCN Virtual Collaboratory call, October 2013. “Technologies and policies for urban energy systems” Global Sustainability Summer School, Potsdam Institute for Climate Impact Research, July 2013.Fit for purpose? A comparison of urban resource demand simulation techniques.” ISIE Conference, Ulsan, Korea, June 2013. “What can dynamical systems tell us about urban energy systems?” SIAM Conference on the Application of Dynamical Systems, Utah, May 2013. “What next for urban energy systems?” Flexible Energy Delivery Systems seminar series, Cardiff University, October 2012.“Modelling urban energy systems with SynCity” RCN Workshop on Sustainable Cities, Denver, USA. August 2012. “Modelling urban energy systems” GreenBridge seminar series, University of Cambridge, UK. March 2012. “Modelling approaches to urban energy systems: optimization, simulation, and more” Martin Centre seminar series, University of Cambridge, February 2012.

Cleo Kontoravdi

Lecturer (Lonza/RCUK Academic Fellowship), 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

Collaborations

Lonza Biologics
MedImmune

Publications

Journal Articles

1. Kyriakopoulos S., Polizzi K.M., Kontoravdi C., “Comparative analysis of amino acid metabolism and transport in CHO variants with different levels of productivity” J. Biotechnol. 168, (2013), 543–551.
2. Jimenez del Val I., Kyriakopoulos S., Polizzi K.M., Kontoravdi C., “An optimised method for extraction and quantification of nucleotides and nucleotide sugars from mammalian cell cultures” Anal. Biochem. 443, (2013), 172–180
3. Chen N., Bennett M.H., Kontoravdi C., “Analysis of Chinese hamster ovary cell metabolism through a combined computational and experimental approach”, Cytotechnology (2013), DOI: 10.1007/s10616-013-9648-1.
4. Behjousiar A., Constantinou A., Polizzi K.M., Kontoravdi C., “FIBS-enabled non-invasive metabolic profiling”, J Vis Exp 84, (2014), e51200.
5. Kontoravdi C., Samsatli N.J., Shah N., “Development and design of bio-pharmaceutical processes”, Curr. Opin. Chem. Eng. 2, (2013), 435–441.
6. Royle K.E., Jimenez del Val I., Kontoravdi C., “Integration of models and experimentation to optimise the production of potential biotherapeutics”, Drug Discov. Today 18, (2013), 1250–1255.
7. Sou S.N., Polizzi K.M., Kontoravdi C., “Evaluation of transfection methods for transient gene expression in Chinese hamster ovary cells”, Adv. Biosc. Biotechnol. 4, (2013), 1013-1019
8. Kontoravdi C., ”Systematic methodology for the development of mathematical models for biological processes”, Methods Mol. Biol. 1073, (2013), 177-190.
9. Kyriakopoulos S., Kontoravdi C., “Analysis of the landscape of biologically-derived pharmaceuticals in Europe: dominant production systems, molecule types on the rise and approval trends”, Eur. J. Pharm. Sci. 48, (2013), 428-441.
10. Royle K., Kontoravdi C., “A systems biology approach to optimising hosts for industrial protein production”, Biotechnol. Lett. 35, (2013) 1961-1969.
11. Jedrzejewski P.M., Jimenez del Val I., Polizzi K.M., Kontoravdi C., “Applying quality by design to glycoprotein therapeutics: experimental and computational efforts of process control”, Pharm. Bioproc. 1, (2013), 51-69.
12. Behjousiar A., Kontoravdi C., Polizzi K.M., “In Situ Monitoring of Intracellular Glucose and Glutamine in CHO Cell Culture”, PLOS ONE 7(4), (2012), e34512.
13. Chen N., Koumpouras G.C., Polizzi K.M., Kontoravdi C., “Genome-based kinetic modeling of cytosolic glucose metabolism in industrially relevant cell lines - Saccharomyces cerevisiae and Chinese hamster ovary cells”, Bioproc. Biosystems Eng. 35, (2012), 1023-1033.
14. Kontoravdi C., “From Systems Biology to Systems Medicine”, The Bentham Science Newsletter 4, (2012), 1.
15. Koumpouras G.C., Kontoravdi C., “Dynamic Optimization of Bioprocesses”, Appl. Math. 3, (2012), 1487-1495.
16. Stefani I.C., Wright D., Polizzi K.M., Kontoravdi C., “The role of ER stress-induced apoptosis in neurodegeneration”, Curr. Alzheimer Res. 9(3), (2012), 373-387.
17. Jimenez del Val I., Nagy J.M., Kontoravdi C., “A dynamic mathematical model for monoclonal antibody N-linked glycosylation and nucleotide sugar donor transport within a maturing Golgi apparatus”, Biotechnol. Prog. 27, (2011), 1730-1743.
18. Chen N., Jimenez del Val I., Kyriakopoulos S., Polizzi K.M., Kontoravdi C., “Metabolic network reconstruction: advances in in silico interpretation of analytical information”, Curr. Opin. Biotechnol. 23, (2011), 1-6.

Refereed Conference Publications

1. Kyriakopoulos S., Polizzi K.M., Kontoravdi C. (2013), Dynamic profiling of amino acid transport and metabolism in Chinese hamster ovary cell culture, Forthcoming in BMC Proceedings of 23rd European Society for Animal Cell Technology (ESACT) Meeting.
2. Jiménez del Val I., Constantinou A., Dell A., Haslam S., Polizzi K.M., Kontoravdi C. (2013), A quantitative and mechanistic model for monoclonal antibody glycosylation as a function of nutrient availability during cell culture, Forthcoming in BMC Proceedings of 23rd European Society for Animal Cell Technology (ESACT) Meeting.
3. Stefani I., Kontoravdi C., Polizzi K. (2013), Analysis of the profile of unfolded protein response (UPR) markers in model-systems of Alzheimer’s disease, Alzheimer’s & Dementia: The Journal of the Alzheimer’s Association 9(4): P143-P144.

4. Chen N, Polizzi KM, Kontoravdi C 2011, Kinetic modelling of cytosolic glucose metabolism, 21st European Symposium on Computer Aided Process Engineering, ELSEVIER, Supplementary Volume.
5. Jimenez del Val I, Nagy JM, Kontoravdi C 2011, Quantification of intracellular nucleotide sugars and formulation of a mathematical model for prediction of their metabolism, BMC Proceedings of 22nd European Society for Animal Cell Technology (ESACT) Meeting on Cell Based Technologies, Pages:P10-, 1753-6561

Referee for

Biotechnology Progress
Biotechnology and Bioengineering
Analytical Biochemistry
Biochemical Engineering Journal
Current Alzheimer Research
Journal of Neurochemistry
PLoS ONE
Cytotechnology
Biotechnology and Applied Biochemistry
Bioprocess and Biosystems Engineering
Chemical Engineering Science
Computer Applications in Biotechnology
European Symposium on Computer Aided Process Engineering

Invited talks

Cell Line Development & Engineering 2014, Vienna, Austria, February 2014
Advanced in Recombinant Protein Technology, ELRIG Conference organised by AstraZeneca, Manchester, U.K., November 2013
BioProduction 2013, Dublin, Ireland, October 2013
Loughborough University, Department of Chemical Engineering, February 2013
ESACT UK meeting, January 2012
R&D Seminar, MedImmune, October 2011
'High value compounds- the role of molecular processing' conference at the Centre for Molecular Processing, University of Kent, July 2011

J Krishnan

Lecturer, Department of Chemical Engineering, Centre for Process Systems 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

Mathematical/computational modelling and theoretical/systems approaches for elucidating, manipulating and controlling cellular processes (especially signal transduction and gene regulation) with two main strands (i) mathematical modelling, both cellular and multilevel/multiscale, in collaboration with cell biologists, biomedical scientists, synthetic biologists, in a number of processes of basic and applied interest. Modelling includes deterministic temporal, spatial and stochastic descriptions (ii) theoretical and systems approaches and development of tools for elucidating signal transduction and cellular information processing: approaches from dynamical systems, control and systems engineering, network analysis employed. A secondary strand involves non-biological analogues and extensions of such work and non-linear dynamics and self-organization in engineered and related physicochemical systems.

Reviewer for

Journals:

Systems and Synthetic Biology: PLOS Computational Biology, Journal of Theoretical Biology, Interface Journal of the Royal Society, Wiley Interdisciplinary Reviews in Systems Biology and Medicine, Biochemical Engineering Journal, IET Systems Biology, BMC Systems Biology, BMC Research Notes, Physical Biology, Advances in Systems Biology (book), Biophysical Journal.
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
Funding agencies: BBSRC, MRC, French National Alliance for the Life and Health Sciences.

Academic Collaborations

Collaborations with experimental groups (cellular biology, biomedical science and engineering, synthetic biology) at Imperial, UCL, Aberdeen, Warwick. Collaborations with computational and systems biology groups with complementary expertise (eg. fluid dynamics, Bayesian inference).

Publications

Journal Articles

1. Liu, C., Krishnan, J.* and Xu, X.-Y. *A systems-based modelling framework for understanding interstitial drug transport and cellular response in solid tumours*. Theor. Bio. Med. Modelling ,8:45, 2011
2. Krishnan, J. *Chemical Engineering at the cellular scale: cellular signal processing*, Ind. Engg. Chem. Res.,50, 13236-43, 2011
3. Alam-Nazki, A., and Krishnan, J.* *An investigation of spatial signal transduction in cellular networks*, BMC Sys Bio. 6:83,, 2012 (BMC Syst. Bio. Highly accessed).
4. Seaton, D., and Krishnan, J.* *Effect of multiple enzyme-substrate interactions in a basic unit of cellular processing*, Physical Biology, 045009, 2012
5. Betney, R., De Silva, E., Mertens, C., Knox, Y., Krishnan, J and Stansfield, I. *Regulation of release factor expression using a translational negative feedback loop: a systems analysis*, RNA, 18, 2320-34, 2012.
6. Liu, C., Krishnan, J.* and Xu, X.-Y.. *An investigation of drug resistance mechanisms at the cell and tissue scale*, Integrative Biology, 5, 555-568, 2013.
7. Liu, C., Krishnan, J. and Xu, X.-Y.. *Towards an integrative model of drug transport and its effect on solid tumours*, J. Bio. Engg, 2013
8. Krishnan, J.* and Liu, C. *An investigation of design principles underlying irreversible decision making in monostable and bistable circuits*, Systems and Synthetic Biology : A Systematic View, Springer Verlag, 2013
9. Alam-Nazki, A., and Krishnan, J.* Covalent modification cycles through the spatial prism, Biophys. J., 105, 1720-1731, 2013
10. Suwanmajo, T. and Krishnan, J.*. Biphasic responses in multisite phosphorylation systems, J. Roy. Soc. Interface: 10:20130742, 2013.
11. Zhao, Y.B and Krishnan, J*. mRNA translation and protein synthesis: An analysis of modelling approaches and a new PBN based method. BMC Systems Biology, 2014.

Invited Lectures and Seminars

Oxford University, Cambridge University, Indian Institute of Science, Systems Biology Network, University of Sheffield, Angionet Conference, National Centre for Biological Sciences, Bangalore, TIFR, Syngenta Systems Biology Workshop.
Lectures at Cold Spring Harbor Computational Cell Biology, Engineering principles of biological systems, International Conference in Systems Biology (ICSB), 2013, Copenhagen, EMBO (European Molecular Biology Organization) Spatial Biology, 2013, Dead Sea.

Invitation to lectures at Harvard University, Univ. of Pennsylvania, Purdue University, Univ. of Michigan, Columbia University, Winter School on Physiological Modelling, Pune, Cheminfluence: Anna University, Georgia Institute of Technology.

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 the IChemE
President of IChemE 2014–15
Fellow of the Royal Society of Chemistry
Salters' Scholar 1969-72
ICI Fellowship 1972-74
Hutchison Medal of the IChemE, 1999
IChemE 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

My research is built around three main themes:
more efficient recovery of existing hydrocarbons
exploitation of non-conventional sources of hydrocarbons
mitigating the environmental impact of fossil fuels, and managing the transition to alternative energies.

My own expertise centres on thermophysical property measurement and prediction for fluids at extreme conditions, the rheology and flow of complex mixtures in complex flow geometries, carbon capture and storage, smart responsive reservoir treatment processes, reactor engineering, small-scale laboratory studies of new hydrocarbon production, separation and chemical conversion processes and the integration of new sub-surface processes with well engineering requirements.

I am the Director of the Qatar Carbonates and Carbon Storage Research Centre. Existing research projects include:
Measurement of the thermophysical properties of CO2 - hydrocarbon-brine fluids under HTHP reservoir conditions in the context of CO2 storage in carbonate reservoirs: interfacial tension, viscosity, diffusion, phase behaviour.
Using thermophysical property data to develop, calibrate and validate molecular based models applicable over a wide range of reservoir conditions to real crude oils and reservoir brines; this involves close collaboration with the Molecular Systems Engineering team.
The formation, dissociation and gas/salt exchange characteristics of methane gas hydrates in the context of the safe production of gas from natural gas hydrates,
their stabilisation against climate change and potential for CO2 storage.
Renewable production of hydrogen from water using green algae and cyanobacteria photocatalysis.
The rheology and systematic design of colloidal fluids and gelling soft solids for industrial (especially oilfield) applications.

Other Activities

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
President IChemE 2014–15
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
J Chem Eng Data
Journal of Materials Chemistry
Journal of Non-Newtonian Fluid Mechanics Journal of Rheology
Langmuir Molecular Physics Nature
Physical Chemistry Chemical Physics Soft Matter

Industrial Collaborations

Qatar Petroleum, Shell, Schlumberger, Tracesa, Aker Solutions, Tullow Oil.

Journal Articles

1. Photobiological hydrogen production: Design of a novel flat-plate photobioreactor system for green algal hydrogen production. B. Tamburic, F.W. Zemichael, G.C. Maitland and K. Hellgardt Proc. 18th World Hydrogen Energy Conference, Essen Germany, 16th-21st May 2010, Paper HP.1a
2. Maitland G, 2013, Towards a low-carbon fossil fuels future, *TCE*, ISSN:0302-0797, Pages:32-37
3. Peng C, Crawshaw JP, Maitland GC, Trusler JPM,, 2013, The pH of CO2-saturated water at temperatures between 308 K and 423 K at pressures up to 15 MPa, *Journal of Supercritical Fluids*, Vol:82, ISSN:0896-8446, Pages:129-137
4. Georgiadis A, Berg S, Makurat A,, Maitland GC, 2013, Pore-scale micro-computed-tomography imaging: Nonwetting-phase cluster-size distribution during drainage and imbibition, *Physical Review E*, Vol:88, ISSN:1539-3755
5. Georgiadis A, Berg S, Makurat A., Maitland GC,, 2013, Pore-scale micro-computed-tomography imaging: nonwetting-phase cluster-size distribution during drainage and imbibition., *Phys Rev E Stat Nonlin Soft Matter Phys*, Vol:88
6. Tong D, Maitland GC, Trusler JPM, Fennell PS, 2013, Solubility of carbon dioxide in aqueous blends of 2-amino-2-methyl-1-propanol and piperazine, *Chemical Engineering Science*, Vol:101, ISSN:0009-2509, Pages:851-864
7. Hou S-X, Maitland GC, Trusler JPM, 2013, Phase equilibria of (CO2 + H2O + NaCl) and (CO2 + H2O + KCl): Measurements and modeling, *Journal of Supercritical Fluids*, Vol:78, ISSN:0896-8446, Pages:78-88
8. Tamburic B, Dechatiwongse P, Zemichael FW, Hellgardt K, Maitland GC, 2013, Process and reactor design for biophotolytic hydrogen production, *Physical Chemistry Chemical Physics*, Vol:15, ISSN:1463-9076, Pages:10783-10794
9. Li X, Ross DA, Trusler JPM, Boek ES, Maitland GC, 2013, Molecular Dynamics Simulations of CO2 and Brine Interfacial Tension at High Temperatures and Pressures, *Journal of Physical Chemistry B*, Vol:117, ISSN:1520-6106, Pages:5647-5652
10. Al Ghafri SZ, Maitland GC, Trusler JPM, 2013, Densities of SrCl2(aq), Na2SO4(aq), NaHCO3(aq), and Two Synthetic Reservoir Brines at Temperatures between (298 and 473) K, Pressures up to 68.5 MPa, and Molalities up to 3 mol. kg(-1), *Journal of Chemical and Engineering Data*, Vol:58, ISSN:0021-9568, Pages:402-412
11. Hou S-X, Maitland GC, Trusler JPM, 2013, Measurement and modeling of the phase behavior of the (carbon dioxide plus water) mixture at temperatures from 298.15 K to 448.15 K, *Journal of Supercritical Fluids*, Vol:73, ISSN:0896-8446, Pages:87-96
12. Tong D, Trusler JPM, Maitland GC, J. Gibbins, P.S. Fennell, 2012, Solubility of carbon dioxide in aqueous solution of monoethanolamine or 2-amino-2-methyl-1-propanol: Experimental measurements and modelling, International *Journal of Greenhouse Gas Control*, Vol:6, ISSN:1750-5836, Pages:37-47
13. Maitland G, 2012, Cold wars, *Chemistry & Industry*, Vol:76, ISSN:0009-3068, Pages:16-17

14. Tamburic B, Zemichael FW, Maitland GC, Hellgardt K, 2012, A novel nutrient control method to deprive green algae of sulphur and initiate spontaneous hydrogen production, *International Journal of Hydrogen Energy*, Vol:37, ISSN:0360-3199, Pages:8988-9001
15. Li X, Boek ES, Maitland GC, Trusler JPM. 2012, Interfacial Tension of (Brines+CO2): CaCl2(aq), MgCl2(aq), and Na2SO4(aq) at Temperatures between (343 and 423) K, Pressures between (2 and 50) MPa, and Molalities of (0.5 to 5) mol.kg-1, *Journal of Chemical and Engineering Data*, Vol:57, ISSN:0021-9568, Pages:1369-1375
16. Al Ghafri S, Maitland GC, Trusler JPM, 2012, Densities of Aqueous MgCl2(aq), CaCl2(aq), KI(aq), NaCl(aq), KCl(aq), AlCl3(aq), and (0.964 NaCl+00136 KCl)(aq) at Temperatures Between (283 and 472) K, Pressures up to 68.5 MPa, and Molalities up to 6 mol.kg(-1), *Journal of Chemical and Engineering Data*, Vol:57, ISSN:0021-9568, Pages:1288-1304
17. Li X, Boek E, Maitland GC, Trusler JPM, 2012, Interfacial Tension of (Brines + CO2): (0.864 NaCl+0.136 KCl) at Temperatures between (298 and 448) K, Pressures between (2 and 50) MPa, and Total Molalities of (1 to 5) mol.kg(-1), *Journal of Chemical and Engineering Data*, Vol:57, ISSN:0021-9568, Pages:1078-1088

Athanasios (Sakis) Mantalaris

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

Qualifications

MSc in Chemical Engineering (University of Rochester)
PhD 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, 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, Biomaterials, Stem Cells & Development, Biochemical Engineering Journal, Biotechnology & Bioengineering

Academic Collaborations

University of Thessaloniki, ETH, Temple University, NTU

Industrial Collaborations

Novalung

Publications

Book Chapters

"Stem Cells as Building Blocks", A. Samadikuchaksaraei, S. Lecht, P.I. Lelkes, A. Mantalaris, J.M. Polak in Principles of Tissue Engineering, 4th Edition, R. Lanza, R. Langer, J. Vacanti (eds), Academic Press, 2013.

Journal Articles

1. Anti-inflammatory role and immunomodulation of mesenchymal stem cells in systemic joint diseases: Potential for treatment, 2013, MacFarlane, R.J., Graham, S.M., Davies, P.S.E., Korres, N., Tsouchnica, H., Heliotis, M., Mantalaris, A., Tsiridis, E., Expert Opinion on Therapeutic Targets, Volume 17, Issue 3, March 2013, Pages 243-254
2. 2013 Improving embryonic stem cell expansion through the combination of perfusion and bioprocess model design Yeo D., Kiparissides A., Cha J.M., Aguilar-Gallardo C., Polak J.M., Tsiridis E., Pistikopoulos E.N., Mantalaris A. 19326203 PLoS ONE 8 12
3. 2013 Molecular and thermodynamic basis for EGCG-Keratin interaction-part II: Experimental investigation Zhao Y., Chen L., Han L., Marzinek J.K., Mantalaris A., Pistikopoulos E.N., Marzinek J.K., Lian G., Bond P.J., Noro M.G. 11541 AIChE Journal 59 12
4. 2013 Molecular and thermodynamic basis for EGCG-Keratin interaction-part I: Molecular dynamics simulations Marzinek J.K., Lian G., Marzinek J.K., Mantalaris A., Pistikopoulos E.N., Zhao Y., Han L., Chen L., Bond P.J., Noro M.G. 11541 AIChE Journal 59 12
5. 2013 Developing a cyclin blueprint as a tool for mapping the cell cycle in GS-NS0 Garcia Munzer D.G., Kostoglou M., Georgiadis M.C., Pistikopoulos E.N., Mantalaris A. 1369703X Biochemical Engineering Journal 81
6. 2013 An in silico erythropoiesis model rationalizing synergism between stem cell factor and erythropoietin Phan T.H.H., Saraf P., Kiparissides A., Mantalaris A., Song H., Lim M. 16157591 Bioprocess and Biosystems Engineering 36 11
7. 2013 Design of optimal patient-specific chemotherapy protocols for the treatment of acute myeloid leukemia (AML) Pefani E., Panoskaltsis N., Mantalaris A., Georgiadis M.C., Pistikopoulos E.N. 981354 Computers and Chemical Engineering 57
8. 2013 Disease-modifying osteoarthritis drugs: In vitro and in vivo data on the development of DMOADs under investigation Davies P.S.E., Graham S.M., MacFarlane R.J., Leonidou A., Mantalaris A., Tsiridis E. 13543784 Expert Opinion on Investigational Drugs 22 4

Invited Lectures and Seminars

Plenary Lecture at the 8th International Meeting of the Portugese Society for Stem Cells and Cell Therapies, "Development of a perfusion bioreactor for the physiological culture and targeted differentiation of embryonic stem cells", Faro, Portugal, April 2013.

Ruth Misener

Royal Academy of Engineering Research Fellow, Department of Chemical Engineering, Imperial College London

Qualifications

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

Awards and Distinctions

Royal Academy of Engineering Research Fellowship, 2012–2017
Imperial College Junior Research Fellowship (declined), 2012–2015
USA National Science Foundation Graduate Research Fellowship, 2007–2012
Princeton University Gordon Y. S. Wu Fellowship, 2007–2012
Robert C. Byrd Honors Scholarship, 2003–2007
Top Reviewer; Computers & Chemical Engineering, 2013
Best Poster; 2nd Belgian Symposium on Tissue Engineering (BSTE), 2013
Excellence in Teaching; Princeton School of Engineering & Applied Sciences, 2010
Member, MIT Tau Beta Pi-Engineering Honor Society, 2007

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

Computers and Chemical Engineering (Top Reviewer, 2013), European Journal of Operational Research, Industrial and Engineering Chemistry Research, Journal of Global Optimization, Journal of Optimization Theory and Applications, Optimization Letters

Academic Collaborations
Princeton University

Industrial Collaborations
GAMS Development Corp.

Publications
Book Chapters
- Misener R., Chin J., Lai M., Fuentes Garí M., Velliou E., Panoskaltsis N., Pistikopoulos E. N., Mantalaris A. Robust Superstructure Optimisation of a Bioreactor that Produces Red Blood Cells. 24th European Symposium on Computer Aided Process Engineering. Budapest, Hungary; 2014. Accepted
- Skjäl A., Westerlund T., Misener R., Floudas C. A. A Generalization of Classical αBB Underestimation to Include Bilinear Terms. In I. D. L. Bogle and M. Fairweather (Ed.), 22nd European Symposium on Computer Aided Process Engineering. Vol. 30 of Computer-Aided Chemical Engineering. London, England; 2012; pp 1202-1206.

Journal Articles
1. Misener R., Floudas C. A. ANTIGONE: Algorithms for continuous / Integer Global Optimization of Nonlinear Equations, Journal of Global Optimization; In Press, 2014 (DOI: 10.1007/s10898-014-0166-2).
2. Misener R., Floudas C. A. A framework for globally optimizing mixed-integer signomial programs. Journal of Optimization Theory & Applications; In Press, 2013 (DOI: 10.1007/s10957-013-0396-3).
3. Misener R., Floudas C. A. GloMIQO: Global Mixed-Integer Quadratic Optimizer. Journal of Global Optimization; 57: 3 - 50, 2013.
4. Misener R., Floudas C. A. Global Optimization of Mixed-Integer Models with Quadratic and Signomial Functions: A Review. Applied Computational Math.; 11: 317 - 336, 2012.
5. Skjäl A., Westerlund T., Misener R., Floudas C. A. A Generalization of the Classical BB Convex Underestimation via Diagonal and Non-Diagonal Quadratic Terms. Journal of Optimization Theory & Applications; 154: 462 - 490, 2012.
6. Misener R., Floudas C. A. Global Optimization of Mixed-Integer Quadratically Constrained Quadratic Programs (MIQCQP) through Piecewise-Linear and Edge-Concave Relaxations. Mathematical Programming, Series B; 136: 155 - 182, 2012.
7. Li J., Misener R., Floudas C. A. Scheduling of Crude Oil Operations under Demand Uncertainty: A Robust Optimization Framework with Global Optimization. AIChE Journal; 58: 2373 - 2396, 2012.
8. Baliban R. C., Elia J. A., Misener R., Floudas C. A. Global optimization of a MINLP process synthesis model for thermochemical based conversion of hybrid coal, biomass, and natural gas to liquid fuels. Computers & Chemical Engineering; 42: 64 - 86; 2012.
9. Li J., Misener R., Floudas C. A. Continuous-Time Modeling and Global Optimization Approach for Scheduling of Crude Oil Operations. AIChE Journal 58: 205-226; 2012.

Best Poster Award
Misener R., Chin J., Lai M., Fuentes Garí M., Rende M., Velliou E., Panoskaltsis N., Pistikopoulos E. N., Mantalaris A. Optimising a Bioreactor that Produces Red Blood Cells under Uncertainty. 2nd Belgian Symposium on Tissue Engineering, Leuven, BE; 2013.

Conference Contributions
1. Misener R., Floudas C. A. ANTIGONE: Algorithms for continuous / Integer Global Optimization of Nonlinear Equations. AIChE Annual Meeting, San Francisco, CA; 2013.

2. Fuentes- Garí M., Velliou E., Misener R., Britos dos Santos S., Panoskaltsis N., Mantalaris A., Pistikopoulos E. N. Towards a Personalised Treatment of Acute Myeloid Leukaemia: The Impact of Considering the Cell Cycle. AIChE Annual Meeting, San Francisco, CA; 2013.

3. Li J., Xiao X., Misener R., Floudas C. A. Effective Global Optimization Methods for Total Refinery Planning Operations. AIChE Annual Meeting, San Francisco, CA; 2013.

4. Velliou E., Fuentes- Garí M., Britos dos Santos S., Misener R., Panoskaltsis N., Mantalaris A., Pistikopoulos E. N. The effect of oxygen and glucose stress on the evolution of a leukaemia model system in an in vitro bone marrow biomimicry. AIChE Annual Meeting, San Francisco, CA; 2013.

5. Misener R. Towards Rational Chemotherapy Strategies: A Hybrid Computational / Experimental Approach. Royal Academy of Engineering Annual Research Forum, London, UK; 2013.

Invited Lectures and Seminars
1. Misener R., Floudas C. A. Special Mathematical Structure Detection and Exploitation with ANTIGONE. Global Optimisation Workshop, London, England; Invited by Dr. P. Parpas; Dec 2013.

2. Misener R. Architecting ANTIGONE: Design Choices and Tradeoffs. MODAL Workshop on MINLP Solver Technology, Zuse-Institut Berlin, Germany; Invited by Mr. A. Gleixner; Nov 2013.

3. Misener R., Floudas C. A. Globally Optimising Process Networks with ANTIGONE: Automatic Recognition and Adaptation Strategies. COST Workshop on Mixed Integer Nonlinear Programming, Paris, France; Invited by Prof. L. Liberti; Oct 2013.

4. Misener R. Making and Healing Blood: An Engineer's Approach, Royal Academy of Engineering Research Forum, London, England; Invited by Mr. R. Barrett; Sept 2013.

5. Misener R., Floudas C. A. ANTIGONE: A general mixed-integer nonlinear global optimisation framework. 4th International Conference on Continuous Optimization, Lisbon, Portugal; Invited by Prof. A. Mitsos; July 2013.

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

Membership of Professional Bodies

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 Techniske Højskole
Visiting Researcher, Universidad de Sevilla
Visiting Professor, Universidad Pablo de Olavide

Industrial Connections

BP, Modelling of polymer membranes for purification of sea water
Coarse grained molecular simulations of asphaltene containing crude oils
Conoco-Phillips, Molecular modelling of shale gas
P&G, Coarse grained modelling of surfactant solutions

Editorial Boards

Open Chemical Physics Journal, Editorial Board Member
Molecular Simulation, Editorial Board Member
Adsorption Science & Technology, Editor in Chief

Publications

Journal Articles

1. Wu L, Mueller EA, Jackson G, 2014, Understanding and Describing the Liquid-Crystalline States of Polypeptide Solutions: A Coarse-Grained Model of PBLG in DMF, *Macromolecules*, Vol:47, ISSN:0024-9297, Pages:1482-1493
2. Papaioannou V, Lafitte T, Avendano C, et al., 2014, Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments, *Journal of Chemical Physics*, Vol:140, ISSN:0021-9606
3. Lafitte T, Apostolakou A, Avendano C, et al., 2013, Accurate statistical associating fluid theory for chain molecules formed from Mie segments, *Journal of Chemical Physics*, Vol:139, ISSN:0021-9606, Pages:-
4. Long Y, Palmer JC, Coasne B, et al., 2013, On the molecular origin of high-pressure effects in nanoconfinement: The role of surface chemistry and roughness, *Journal of Chemical Physics*, Vol:139, ISSN:0021-9606, Pages:-
5. Santiso EE, Herdes C, Mueller EA, 2013, On the Calculation of Solid-Fluid Contact Angles from Molecular Dynamics, *Entropy*, Vol:15, ISSN:1099-4300, Pages:3734-3745
6. Dominguez H, Haslam AJ, Jackson G, et al., 2013, Modelling and understanding of the vapour-liquid and liquid-liquid interfacial properties for the binary mixture of n-heptane and perfluoro-n-hexane, *Journal of Molecular Liquids*, Vol:185, ISSN:0167-7322, Pages:36-43
7. Herdes C, Prosenjak C, Roman S, et al., 2013, Fundamental Studies of Methyl Iodide Adsorption in DABCO Impregnated Activated Carbons, *Langmuir*, Vol:29, ISSN:0743-7463, Pages:6849-6855
8. Müller EA, 2013, Purification of water through nanoporous carbon membranes: A molecular simulation viewpoint, *Current Opinion in Chemical Engineering*, Vol:2, 2211-3398, Pages:223-228
9. Avendano C, Lafitte T, Adjiman CS, et al., 2013, SAFT-gamma Force Field for the Simulation of Molecular Fluids: 2. Coarse-Grained Models of Greenhouse Gases, Refrigerants, and Long Alkanes, *Journal of Physical Chemistry B*, Vol:117, ISSN:1520-6106, Pages:2717-2733
10. Lu L, Wang S, Mueller EA, et al., 2014, Adsorption and separation of CO2/CH4 mixtures using nanoporous adsorbents by molecular simulation, *Fluid Phase Equilibria*, Vol:362, ISSN:0378-3812, Pages:227-234
11. Wu L, Jackson G, Mueller EA, 2013, Liquid Crystal Phase Behaviour of Attractive Disc-Like Particles, *INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES*, Vol:14, ISSN:1422-0067, Pages:16414-16442
12. Jover J, Haslam AJ, Galindo A, et al., 2012, Pseudo hard-sphere potential for use in continuous molecular-dynamics simulation of spherical and chain molecules, *Journal of Chemical Physics*, Vol:137, ISSN:0021-9606, Pages:-
13. Wu L, Wensink HH, Jackson G, et al., 2012, A generic equation of state for liquid crystalline phases of hard-oblate particles, *Molecular Physics*, Vol:110, ISSN:0026-8976, Pages:1269-1288

14. Lafitte T, Avendano C, Papaioannou V, et al., 2012, SAFT-gamma force field for the simulation of molecular fluids: 3. Coarse-grained models of benzene and hetero-group models of n-decylbenzene, *Molecular Physics*, Vol:110, ISSN:0026-8976, Pages:1189-1203
15. Müller EA, 2012, What carnot's father taught his son about thermodynamics, *Chemical Engineering Education*, Vol:46, ISSN:0009-2479, Pages:165-170
16. Kumar KV, Mueller EA, Rodriguez-Reinoso F, 2012, Effect of Pore Morphology on the Adsorption of Methane/Hydrogen Mixtures on Carbon Micropores, *Journal of Physical Chemistry C*, Vol:116, ISSN:1932-7447, Pages:11820-11829
17. Horsch M, Hasse H, Shchekin AK, et al., 2012, Excess equimolar radius of liquid drops, *Physical Review E*, Vol:85, ISSN:1539-3755
18. Frentrup H, Müller EA, Avendaño C, et al., 2012, Modelling fluid flow in nanoporous membrane materials via non-equilibrium molecular dynamics, *Procedia Engineering*, Vol:44, ISSN:1877-7058, Pages:383-385
19. Frentrup H, Avendano C, Horsch M, et al., 2012, Transport diffusivities of fluids in nanopores by non-equilibrium molecular dynamics simulation, *Molecular Simulation*, Vol:38, ISSN:0892-7022, Pages:540-553

Costas C Pantelides FREng

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

Qualifications

MS in Chemical Engineering (MIT)
PhD, DIC in Chemical Engineering (Imperial College London)

Awards and Distinctions

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 Pharmaceutics
Computational chemistry for prediction of the solid state

Other Activities

Managing Director, Process Systems Enterprise Ltd.
Member of Evaluation Committee of Private Universities, Republic of Cyprus

Publications

Journal

1. Pantelides CC, Renfro JG, 2013, The online use of first-principles models in process operations: Review, current status and future needs, *Computers & Chemical Engineering*, Vol:51, ISSN:0098-1354, Pages:136-148
2. Vasileiadis M, Kazantsev AV, Karamertzanis PG, et al., 2012, The polymorphs of ROY: application of a systematic crystal structure prediction technique, *Acta Crystallographica Section B – Structural Science*, Vol:68, ISSN:0108-7681, Pages:677-685

Lazaros G. Papageorgiou

Professor in Chemical Engineering, Department of Chemical Engineering, UCL.

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

Industrial & Engineering Chemistry Research, Computers and Chemical Engineering, AIChE Journal, Chemical Engineering Research and Design, International Journal of Production Economics, European Journal of Operational Research, Computers and Industrial Engineering, Biotechnology Progress.

Academic Collaborations

Imperial College London, King's College London, University College London, Technical University of Crete, University of Western Macedonia, National Technical University of Athens, University of Wisconsin.

Industrial Collaborations

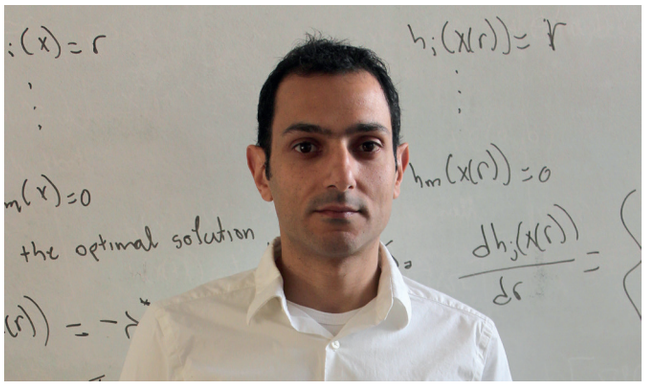
Bayer, Syngenta

Publications

Journal Articles

1. Zhang, D., Samsatli, N. J., Hawkes, A. D., Brett, D. J. L., Shah, N., & Papageorgiou, L. G. (2013). Fair electricity transfer price and unit capacity selection in microgrids. *Energy Economics*. doi:10.1016/j.eneco.2012.11.005
2. Yang, L., Fraga, E. S., & Papageorgiou, L. G. (2013). Mathematical programming formulations for non-smooth and non-convex electricity dispatch problems. *Electric Power Systems Research*, 95, 302-308.
3. Liu, S., & Papageorgiou, L. G. (2013). Multiobjective optimisation of production, distribution and capacity planning of global supply chains in the process industry. OMEGA *International Journal of Management Science*, 41, 369-382.
4. Mehleri, E. D., Sarimveis, H., Markatos, N. C., & Papageorgiou, L. G. (2013). Optimal design and operation of distributed energy systems: application to greek residential sector. *Renewable Energy*, 51, 331-342.
5. Agnolucci, P., McDowall, W., Akgul, O., & Papageorgiou, L. G. (2013). The importance of economies of scale, transport costs and demand patterns in optimising hydrogen fuelling infrastructure: An exploration with SHIPMod (Spatial hydrogen infrastructure planning model). *International Journal of Hydrogen Energy*. doi:10.1016/j.ijhydene.2013.06.071
6. Mehleri, E. D., Sarimveis, H., Markatos, N. C., & Papageorgiou, L. G. (2012). A mathematical programming approach for optimal design of distributed energy systems at the neighbourhood level. *Energy*, 42, 96-104.
7. Bennett, L., Liu, S., Papageorgiou, L. G., & Tsoka, S. (2012). *A Mathematical Programming Approach to Community Structure Detection in Complex Networks.*
8. Liu, S., Simaria, A. S., Farid, S. S., & Papageorgiou, L. G. (2012). A Mixed-integer Nonlinear Programming Model for Antibody Purification Processes.
9. Liu, S., Shah, N., & Papageorgiou, L. G. (2012). A model predictive control approach for multi-echelon supply chain management with price elasticity of demand. *AIChE Journal*, 58, 369-382.
10. Mehleri, E. D., Papageorgiou, L. G., Markatos, N. C., & Sarimveis, H. (2012). *A Model Predictive Framework for Residential Microgrids*.
11. Zhang, D., Samsatli, N. J., Hawkes, A. D., Brett, D. J. L., Shah, N., & Papageorgiou, L. G. (2013). Fair electricity transfer price and unit capacity selection in microgrids. *Energy Economics*. doi:10.1016/j.eneco.2012.11.005
12. Yang, L., Fraga, E. S., & Papageorgiou, L. G. (2013). Mathematical programming formulations for non-smooth and non-convex electricity dispatch problems. *Electric Power Systems Research*, 95, 302-308.
13. Liu, S., & Papageorgiou, L. G. (2013). Multiobjective optimisation of production, distribution and capacity planning of global supply chains in the process industry. OMEGA *International Journal of Management Science*, 41, 369-382.
14. Mehleri, E. D., Sarimveis, H., Markatos, N. C., & Papageorgiou, L. G. (2013). Optimal design and operation of distributed energy systems: application to greek residential sector. *Renewable Energy*, 51, 331-342.
15. Agnolucci, P., McDowall, W., Akgul, O., & Papageorgiou, L. G. (2013). The importance of economies of scale, transport costs and demand patterns in optimising hydrogen fuelling infrastructure: An exploration with SHIPMod (Spatial hydrogen infrastructure planning model). *International Journal of Hydrogen Energy*. doi:10.1016/j.ijhydene.2013.06.071

16. Mehleri, E. D., Sarimveis, H., Markatos, N. C., & Papageorgiou, L. G. (2012). A mathematical programming approach for optimal design of distributed energy systems at the neighbourhood level. *Energy,* 42, 96-104.
17. Bennett, L., Liu, S., Papageorgiou, L. G., & Tsoka, S. (2012). *A Mathematical Programming Approach to Community Structure Detection in Complex Networks*.
18. Liu, S., Simaria, A. S., Farid, S. S., & Papageorgiou, L. G. (2012). *A Mixed-integer Nonlinear Programming Model for Antibody Purification Processes*.
19. Liu, S., Shah, N., & Papageorgiou, L. G. (2012). A model predictive control approach for multi-echelon supply chain management with price elasticity of demand. *AIChE Journal*, 58, 369-382.
20. Mehleri, E. D., Papageorgiou, L. G., Markatos, N. C., & Sarimveis, H. (2012). *A Model Predictive Framework for Residential Microgrids*.
21. Polykarpou, E. M., Dalby, P. A., & Papageorgiou, L. G. (2012). A novel efficient optimisation system for purification process synthesis. *Biochemical Engineering Journal*, 67, 186-193.
22. Akgul, O., Shah, N., & Papageorgiou, L. G. (2012). *A Spatially-Explicit, Multi-Period MILP Modelling Framework for the Optimal Design of a Hybrid Biofuel Supply Chain*.
23. Liu, S., Papageorgiou, L. G., & Gikas, P. (2012). A two-step optimisation approach for integrated water resources management. *Computer Aided Chemical Engineering*, 30, 96-100. doi:10.1016/B978-0-444-59519-5.50020-4
24. Liu, S., Gikas, P., & Papageorgiou, L. G. (2012). A *two-step optimisation approach for integrated water resources management*.
25. Polykarpou, E. M., Dalby, P. A., & Papageorgiou, L. G. (2012). An MILP formulation for the synthesis of protein purification processes. *Chemical Engineering Research and Design*, 90 (9), 1262-1270.
26. Akgul, O., Shah, N., & Papageorgiou, L. G. (2012). An Optimisation Framework for a Hybrid First/Second Generation Bioethanol Supply Chain. *Computers and Chemical Engineering*, 42, 101-114. doi:10.1016/j.compchemeng.2012.01.012
27. Bennett, L., Liu, S., Papageorgiou, L. G., & Tsoka, S. (2012). Detection of disjoint and overlapping modules in weighted complex networks. *Advances in Complex Systems*, 15 (5), 1150023 (20 pages)-?.
28. Bennett, L., Lysenko, A., Papageorgiou, L. G., Urban, M., Hammond-Kosack, K., Rawlings, C., . . . Tsoka, S. (2012). Detection of multi-clustered genes and community structure for the plant pathogenic fungus Fusarium graminearum. In D. Gilbert, M. Heiner (Eds.), Lecture Notes in Computer Science (pp. 69-86).
29. Bennett, L., Lysenko, A., Papageorgiou, L. G., Urban, M., Hammond-Kosack, K., Rawlings, C., . . . Tsoka, S. (2012). *Detection of multi-clustered genes and community structure for the plant pathogenic fungus Fusarium graminearum*.
30. Akgul, O., Shah, N., & Papageorgiou, L. G. (2012). Economic optimisation of a UK advanced biofuel supply chain. *Biomass and Bioenergy*, 41, 57-72. doi:10.1016/j.biombioe.2012.01.040
31. Liu, S., Papageorgiou, L. G., & Gikas, P. (2012). Integrated Management of Non-conventional Water Resources in Anhydrous Islands. *Water Resources Management*, 26 (2), 359-375. doi:10.1007/s11269-011-9921-z
32. Al-Salem, S. M., Papageorgiou, L. G., & Lettieri, P. (2012). Life cycle assessment and optimization on the production of petrochemicals and energy from polymers for the Greater London Area. *Computer Aided Chemical Engineering*, 30 (1), 101-106.
33. Al Salem, S. M., Mehleri, E., Papageorgiou, L. G., & Lettieri, P. (2012). *Life cycle assessment and optimization on the production of petrochemicals and energy from polymers for the Greater London Area*.
34. Mehleri, E. D., Sarimveis, H., Papageorgiou, L. G., & Markatos, N. C. (2012). *Model Predictive Control of Distributed Energy Resources*.
35. Liu, S., Shah, N., & Papageorgiou, L. G. (2012). Multiechelon supply chain planning with sequence-dependent changeovers and price elasticity of demand under uncertainty. AIChE Journal.
36. Liu, S., & Papageorgiou, L. G. (2012). Multiobjective optimisation of production, distribution and capacity planning of global supply chains in the process industry. *Omega*.
37. Fraga, E. S., Yang, L., & Papageorgiou, L. G. (2012). On the modelling of valve point loadings for power electricity dispatch. *Applied Energy*, 91 (1), 301-303. doi:10.1016/j.apenergy.2011.10.001
38. Zhang, D., Papageorgiou, L. G., & Fraga, E. S. (2012). *Optimisation based analysis of a dwelling with an air source heat pump*.
39. Akgul, O., Mac Dowell, N., Shah, N., & Papageorgiou, L. G. (2012). *Optimisation of Bioelectricity Supply Chains*.
40. Akgul, O., Shah, N., & Papageorgiou, L. G. (2012). *Optimisation of Integrated First/Second Generation Biofuel Supply Chains*.
41. Siganporia, C., Ghosh, S., Daszkowski, T., Papageorgiou, L. G., & Farid, S. S. (n.d.). *Production planning of batch and semi-continuous bioprocesses across multiple biopharmaceutical facilities*.
42. Konstantopoulou, F., Liu, S., Papageorgiou, L. G., & Gikas, P. (2012). *The utilization of non conventional water resources to subsidize insufficient water balances: Case study for Santorini Island, Greece*.



Panos Parpas

Lecturer, Department of Computing, Imperial College London

Qualifications
PhD in Computer Science (2006), Imperial College London,
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
Automatica, Computational and Applied Mathematics, Computational Management Science, Computational Optimization and Applications, Computational Statistics and Data Analysis, Computers and Operations Research, European Journal of Operational Research, IMA Journal of Management Mathematics, Information Processing Letters, INFORMS Journal on Computing, International Review of Economics and Finance, Journal of Computational Finance, Journal of Global Optimization, Journal of the Operational Research Society, Kybernetika, Management Science, Mathematics of Operations Research, Mathematical Programming, Operations Research, Optimization Methods and Software, Quantitative Finance, SIAM Journal on Control and Optimization,

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

1. P. Parpas, and M. Webster. A stochastic multiscale model for electricity generation capacity expansion, European Journal of Operational Research, Volume 232, Issue 2, Pages 359-374, January 2014.
2. P. Parpas, and G. Tavares. On the information-based complexity of stochastic programming, Operations Research Letters, Volume 41, Issue 6, Pages 622-626, November 2013.
3. P. Parpas and M. Webster. A Stochastic Minimum Principle and a mesh-free method for Stochastic Optimal Control , Automatica, Volume 49, Issue 6, Pages 1663-1671, June 2013.
4. F.W Kong, P. Parpas, and B. Rustem. Sum of Non-Concave Utilities Maximization for MIMO Interference Systems, IEEE Transactions on Wireless Communications, Volume 12, No 4, Pages 1744-1751, April 2013.
5. M. Webster and Nidhi Santen and P. Parpas. An approximate dynamic programming framework for modeling global climate policy under decision-dependent uncertainty Computational Management Science,Volume 9, Issue 3, pp 339-362. August 2012.
6. Kai Ye, P. Parpas, B. Rustem. Robust portfolio optimization: a conic programming approach, Computational Optimization and Applications, Volume 52, Issue 2, pp 463-481, June 2012.

Conference Contributions
D. V.N. Luong, P. Parpas, D. Rueckert, and B. Rustem Solving MRF Minimization by Mirror Descent. Advances in Visual Computing Lecture Notes in Computer Science Volume 7431, 2012, pp 587-598

Invited Lectures and Seminars
1. Optimal Control of Weakly Connected Markov Decision Processes, Applied Mathematics and Mathematical Physics Seminar, Department of Mathematics, Imperial College London.
2. Multiscale Stochastic Volatility, Algorithmic Trading Conference, Imperial College London.
3. Dimensionality Reduction and Multiscale Stochastic Processes, 21st International Symposium on Mathematical Programming, Berlin.
4. Computational Optimization of Multiscale Stochastic Processes in Energy Systems LANCS Energy Workshop, UK.
5. Hierarchical Algorithms for Simulation and Optimization, University of California, Berkeley, USA.
6. Multiresolution Parameter Estimation of Markov Processes, University of Nottingham, UK.

Efstratios N Pistikopoulos FREng

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

Qualifications

FREng
Dipl Eng in Chemical Engineering (Aristotle University, Greece)
PhD in Chemical Engineering (Carnegie Mellon University, USA)

Awards and Distinctions

Fellow of the Royal Academy of Engineering, 2013
Computing in Chemical Engineering Award, 2012
Imperial College, Rector's Research Excellence Award, 2009 (part of MSE's 6-member team)
European Research Council (ERC) Advanced Grant, 2008
Royal Academy of Engineering, Mac Robert Award, 2007 (part of PSE Ltd's 5-member team)
Fellow, Institution of Chemical Engineers, 2005
Imperial College, Rector's Award for Research Excellence, 2005
ICI/Royal Academy of Engineering Fellowship, 1991-1996

Research Interests

Theory, algorithms and computational tools for continuous and integer multi-parametric programming, and multi-parametric control. Advanced model based control and its biomedical, industrial and energy systems applications. Energy and the environment – sustainable process, product and network systems development

Other activities

Co-Chair, Computational Management Science CMS 2012, Imperial College London
Co-Editor, Book Series in Process Systems Engineering, Wiley-VCH
Co-Editor, Series on Computer-Aided Chemical Engineering, Elsevier
Editor, Computers and Chemical Engineering, Elsevier
Editorial Board, Industrial & Engineering Chemistry Research
Editorial Board, Journal of Global Optimization, Kluwer
Editorial Board, Computational Management Science, Springer
Editorial Board, Frontiers of Energy and Power Engineering in China, Springer
Editorial Board, Energy Systems, Springer
Co-Founder and Senior/ Consultant, PSE Ltd
Founder and Director, PAROS Ltd
Plenary Lectures FOCAPO 2012
International Programme Committee member – ESCAPE22, FOCAPO 2012, PSE 2012
Member, Computer Aided Process Engineering (CAPE) Working Party, European Federation of Chemical Engineers
Member of the Advisory Scientific Committee, European Enterprise Institute (EPPED Association)
Author or co-author of 1 book, 2 patents, 7 edited books, 250 journal publications, over 150 refereed conference publications, over 60 Chapters in books & chapter contributions to encyclopaedias

Academic Collaborations

Tsinghua University (China), Cranfield University, DTU (Denmark), UPC (Spain), University of Coimbra (Portugal), University of Thessaloniki & CPERI (Greece), University of Western Macedonia (Greece), University of Pannonia (Hungary), Princeton University (USA)

Industrial Collaborations

BASF, Air Products, BMS, GSK, BP, Unilever

Publications

Journals

1. Muenzer DGG, Kostoglou M, Georgiadis MC, et al., 2013, Developing a cyclin blueprint as a tool for mapping the cell cycle in GS-NSO, *Biochemical Engineering Journal*, Vol:81, ISSN:1369-703X, Pages:97-107
2. Yeo D, Kiparissides A, Cha JM, et al., 2013, Improving Embryonic Stem Cell Expansion through the Combination of Perfusion and Bioprocess Model Design, *PLOS One*, Vol:8, ISSN:1932-6203, Pages:-
3. Marzinek JK, Lian G, Marzinek JK, et al., 2013, Molecular and Thermodynamic Basis for EGCG-Keratin Interaction-Part I: Molecular Dynamics Simulations, *AICHE Journal*, Vol:59, ISSN:0001-1541, Pages:4816-4823
4. Zhao Y, Chen L, Han L, et al., 2013, Molecular and Thermodynamic Basis for EGCG-Keratin Interaction-Part II: Experimental Investigation, *AICHE Journal*, Vol:59, ISSN:0001-1541, Pages:4824-4827
5. Wittmann-Hohlbein M, Pistikopoulos EN, 2013, Proactive Scheduling of Batch Processes by a Combined Robust Optimization and Multiparametric Programming Approach, *AICHE Journal*, Vol:59, ISSN:0001-1541, Pages:4184-4211
6. Pefani E, Panoskaltsis N, Mantalaris A, et al., 2013, Design of optimal patient-specific chemotherapy protocols for the treatment of acute myeloid leukemia (AML), *Computers & Chemical Engineering*, Vol:57, ISSN:0098-1354, Pages:187-195
7. Liu P, Georgiadis MC, Pistikopoulos EN, 2013, An energy systems engineering approach for the design and operation of microgrids in residential applications, *Chemical Engineering Research & Design*, Vol:91, ISSN:0263-8762, Pages:2054-2069

8. Wittmann-Hohlbein M, Pistikopoulos EN, 2013, On the global solution of multi-parametric mixed integer linear programming problems, *Journal of Global Optimization*, Vol:57, ISSN:0925-5001, Pages:51-73
9. Mansoornejad B, Pistikopoulos EN, Stuart PR, 2013, Scenario-based strategic supply chain design and analysis for the forest biorefinery using an operational supply chain model, *International Journal of Production Economics*, Vol:144, ISSN:0925-5273, Pages:618-634
10. Voelker A, Kouramas K, Pistikopoulos EN, 2013, Simultaneous design of explicit/multi-parametric constrained moving horizon estimation and robust model predictive control, *Computers & Chemical Engineering*, Vol:54, ISSN:0098-1354, Pages:24-33
11. Lambert RSC, Rivotti P, Pistikopoulos EN, 2013, A Monte-Carlo based model approximation technique for linear model predictive control of nonlinear systems, *Computers & Chemical Engineering*, Vol:54, ISSN:0098-1354, Pages:60-67
12. Mansoornejad B, Pistikopoulos EN, Stuart P, 2013, Metrics for evaluating the forest biorefinery supply chain performance, *Computers & Chemical Engineering*, Vol:54, ISSN:0098-1354, Pages:125-139
13. Zhao Y: Pistikopoulos EN,2013, Dynamic modelling and parametric control for the polymer electrolyte membrane fuel cell system, *Journal of Power Sources*, Vol:232, pages 270-278
14. Ziogou C, Pistikopoulos EN, Georgiadis MC, et al., 2013, Empowering the Performance of Advanced NMPC by Multiparametric Programming-An Application to a PEM Fuel Cell System, I*ndustrial & Engineering Chemistry Research*, Vol:52, ISSN:0888-5885, Pages:4863-4873
15. Voelker A, Kouramas K, Pistikopoulos EN, 2013, Moving horizon estimation: Error dynamics and bounding error sets for robust control, *Automatica*, Vol:49, ISSN:0005-1098, Pages:943-948
16. Zhou Z, Zhang J, Liu P, et al., 2013, A two-stage stochastic programming model for the optimal design of distributed energy systems, *Applied Energy*, Vol:103, ISSN:0306-2619, Pages:135-144
17. Dominguez LF, Pistikopoulos EN, 2013, A Quadratic Approximation-Based Algorithm for the Solution of Multiparametric Mixed-Integer Nonlinear Programming Problems, *AICHE Journal*, Vol:59, ISSN:0001-1541, Pages:483-495
18. Kouramas KI, Panos C, Faisca NP, et al., 2013, An algorithm for robust explicit/multi-parametric model predictive control, *Automatica*, Vol:49, ISSN:0005-1098, Pages:381-389
19. Kopanos GM, Georgiadis MC, Pistikopoulos EN, 2013, Energy production planning of a network of micro combined heat and power generators, *Applied Energy*, Vol:102, ISSN:0306-2619, Pages:1522-1534
20. Zhou Z, Liu P, Li Z, et al., 2012, Impacts of equipment off-design characteristics on the optimal design and operation of combined cooling, heating and power systems, *Computer Aided Chemical Engineering*, Vol:31, ISSN:1570-7946, Pages:990-994
21. Kopanos GM, Pistikopoulos EN, 2013, Reactive Scheduling of micro Combined Heat and Power Systems via Multiparametric Programming, *23 EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING*, Vol:32, ISSN:1570-7946, Pages:277-282
22. Chang H, Pistikopoulos EN, Astolfi A, 2013, Robust Multi-parametric Model Predictive Control for Discrete-time LPV Systems, 2013 *AMERICAN CONTROL CONFERENCE (ACC)*, ISSN:0743-1619, Pages:431-436
23. Kopanos GM, Georgiadis MC, Pistikopoulos EN, 2013, Operational Planning in Energy Networks based on Microgeneration, *2013 AMERICAN CONTROL CONFERENCE (ACC)*, ISSN:0743-1619, Pages:2940-2945
24. Khajuria H, Pistikopoulos EN, 2013, Optimization and Control of Pressure Swing Adsorption Processes Under Uncertainty, *AICHE Journal*, Vol:59, ISSN:0001-1541, Pages:120-131
25. Pistikopoulos EN, 2012, From multi-parametric programming theory to MPC-on-a-chip multi-scale systems applications, *Computers & Chemical Engineering*, Vol:47, ISSN:0098-1354, Pages:57-66
26. Klemes JJ, Pistikopoulos EN, Georgiadis MC, et al., 2012, Energy systems engineering, *Energy*, Vol:44, ISSN:0360-5442, Pages:2-5
27. Pistikopoulos EN, Georgiadis MC, Kokossis A, 2012, CACE Special Issue of ESCAPE-21 Preface, *Computers & Chemical Engineering*, Vol:42, ISSN:0098-1354, Pages:1-1
28. Rivotti P, Lambert RSC, Pistikopoulos EN 2012, *Combined model approximation techniques and multiparametric programming for explicit nonlinear model predictive control*, 21st European Symposium on Computer-Aided Process Engineering (ESCAPE), PERGAMON-ELSEVIER SCIENCE LTD, Pages:277-287, ISSN:0098-1354
29. Wittmann-Hohlbein M, Pistikopoulos EN, 2012, A Two-Stage Method for the Approximate Solution of General Multiparametric Mixed-Integer Linear Programming Problems, *Industrial & Engineering Chemistry Research*, Vol:51, ISSN:0888-5885, Pages:8095-8107
30. Zhou Z, Liu P, Li Z, et al., 2013, Impacts of equipment off-design characteristics on the optimal design and operation of combined cooling, heating and power systems, *Computers & Chemical Engineering*, Vol:48, ISSN:0098-1354, Pages:40-47
31. Pefani E, Panoskaltsis N, Mantalaris A, et al. 2012, *A DECISION TOOL FOR THE DESIGN OF OPTIMAL PERSONALISED CHEMOTHERAPY PROTOCOLS FOR THE TREATMENT OF ACUTE MYELOID LEUKAEMIA (AML)*, 4th WIN Symposium on Efficacy of Biomarkers and Personalized Cancer Therapeutics, OXFORD UNIV PRESS, Pages:33-33, ISSN:0923-7534
32. Zhou Z, Liu P, Li Z, et al., 2012, Impacts of equipment off-design characteristics on the optimal design and operation of combined cooling, heating and power systems, *Computer Aided Chemical Engineering*, Vol:31, ISSN:1570-7946, Pages:990-994
33. Ziogou C, Pistikopoulos EN, Voutetakis S, et al., 2012, A Multivariable Nonlinear Model Predictive Control Framework for a PEM Fuel Cell System, *Computer Aided Chemical Engineering*, Vol:31, ISSN:1570-7946, Pages:1617-1621
34. Pefani E, Panoskaltsis N, Mantalaris A, et al. 2012, *Design of optimal disease and patient-specific chemotherapy protocols for the treatment of Acute Myeloid Leukaemia (AML)*, 11th

International Symposium on Process Systems Engineering (PSE), ELSEVIER SCIENCE BV, Pages:1717-1721, ISSN:1570-7946

35. Zondervan E, de Haan AB, Nikacevic N, Khajuria, H, et al., 2012, Integrated Operation and Design of a Simulated Moving Bed Reactor, *Computer Aided Chemical Engineering*, Vol:30, ISSN:1570-7946, Pages:642-646
36. Kopanos GM, Georgadis MC, Pistikopoulos EN 2012, *Efficient Scheduling of Complex Multipurpose Chemical Batch Processes*, 22nd European Symposium on Computer Aided Process Engineering (ESCAPE), ELSEVIER SCIENCE BV, Pages:862-866, ISSN:1570-7946
37. Pefani E, Panoskaltsis N, Mantalaris A, et al. 2012, *Modelling and Simulation of Drug Delivery Systems for the Treatment of Acute Myeloid Leukemia*, 5th European Conference of the International Federation for Medical and Biological Engineering, SPRINGER, Pages:259-262, ISSN:1680-0737
38. Panos, C; Kouramas, K.I; Georgiadis, M.C; et al. 2012, *Chemical Engineering Science* Vol:67, Issue 1, Special Issue: SI Pages: 15-25
39. He F, Li Z, Liu P, et al. 2012, *Operation window and part-load performance study of a syngas fired gas turbine*, ELSEVIER SCI LTD, Pages:133-141, ISSN:0306-2619

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, May 2006)

Research Interests
Optimisation Algorithms, Decision and Design under uncertainty, worst-case design, stochastic optimisation

Other Activities
Past Managing Editor: Journal of Economic Dynamics & Control: 1987-2002

Academic Collaborations
Brunel University; University of Warwick; University of Frankfurt; University of Florida; MIT; Technion

Industrial Collaborations
JP Morgan; Credit Suisse; Orange; BAe Systems

Competence Areas
Optimisation and minimax algorithms
Global optimisation
Stochastic optimisation
Risk management
Robust decisions/design under uncertainty, engineering, finance, energy, defence

Editor
Automatica
Computational Management Science

Editorial Advisory Board
Journal of Economic Dynamics & Control

Associate Editor
Royal Society Proceedings (Series A)
Computational Economics
J of Global Optimization
Optimization Letters
Computational Science & Engineering

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

Organiser and Programme Committee Co-Chair
Computational Management Science,Imperial College London, April 2012 http://cms2012.doc.ic.ac.uk/

Activities
Associate Director – Research – Centre for Process Systems Engineering, Imperial College
Systems Engineering Initiative, Research Director, Faculty of Engineering, Imperial College

Publications
Journal Articles

1. Kong FW, Rustem B, 2013, Welfare-maximizing correlated equilibria using Kantorovich polynomials with sparsity, *Journal of Global Optimization*, Vol:57, ISSN:0925-5001, Pages:251-277
2. Kong FW, Parpas P, Rustem B, 2013, Sum of Non-Concave Utilities Maximization for MIMO Interference Systems, *IEEE Transactions on Wireless Communications*, Vol:12, ISSN:1536-1276, Pages:1744-1751
3. Wiesemann W, Tsoukalas A, Kleniati P-M, et al., 2013, PESSIMISTIC BILEVEL OPTIMIZATION, *SIAM Journal on Optimization*, Vol:23, ISSN:1052-6234, Pages:353-380
4. Wiesemann W, Kuhn D, Rustem B, 2013, Robust Markov Decision Processes, *Mathematics of Operations Research*, Vol:38, ISSN:0364-765X, Pages:153-183
5. Fonseca RJ, Rustem B, 2012, International portfolio management with affine policies, *European Journal of Operational Research*, Vol:223, ISSN:0377-2217, Pages:177-187
6. Fonseca RJ, Rustem B, 2012, Robust hedging strategies, *Computers & Operations Research*, Vol:39, ISSN:0305-0548, Pages:2528-2536
7. Wiesemann W, Kuhn D, Rustem B, 2012, Robust resource allocations in temporal networks, *Mathematical Programming*, Vol:135, ISSN:0025-5610, Pages:437-471
8. Zymler S, Kuhn D, Rustem B, 2013, Distributionally robust joint chance constraints with second-order moment information, *Mathematical Programming*, Vol:137, ISSN:0025-5610, Pages:167-198
9. Zymler S, Kuhn D, Rustem B, 2013, Worst-Case Value at Risk of Nonlinear Portfolios, *Management Science*, Vol:59, ISSN:0025-1909, Pages:172-188
10. Ye K, Parpas P, Rustem B, 2012, Robust portfolio optimization: a conic programming approach, *Computational Optimization and Applications*, Vol:52, ISSN:0926-6003, Pages:463-481
11. Vayanos P, Kuhn D, Rustem B, 2012, A constraint sampling approach for multi-stage robust optimization, *Automatica*, Vol:48, ISSN:0005-1098, Pages:459-471
12. Kong FW, Kleniati P-M, Rustem B, 2012, Computation of Correlated Equilibrium with Global-Optimal Expected Social Welfare, *Journal of Optimization Theory and Applications*, Vol:153, ISSN:0022-3239, Pages:237-261
13. Wiesemann W, Kuhn D, Rustem B, 2012, Multi-resource allocation in stochastic project scheduling, *Annals of Operations Research*, Vol:193, ISSN:0254-5330, Pages:193-220

Nilay Shah

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

Qualifications
MEng in Chemical Engineering (Imperial College)
PhD in Process Systems Engineering (Imperial College)

Awards and Distinctions
Fellow of the IChemE
RAEng MacRobert Award and Prize (2007)
RSC/SCI/IOM Beilby Medal (2005)
ICI/RAEng Fellowship (1997-2002)
Imperial College Faculty of Engineering Teaching Award (2009)
Hutchison Medal (2013)

Research Interests
Design and analysis of energy systems:
Bioenergy systems and technologies
Urban Energy Systems
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 & Chemical Engineering
Chemical Engineering Science
A-Star research council (Singapore)

Academic Collaborations

University College London, Department of Chemical Engineering
Newcastle and Strathclyde Universities, CPACT
Georgia Institute of Technology
Tsinghua University, Clean Energy Centre
National University of Singapore
Delft University of Technology
Rothamsted Research
IBERS – University of Aberystwyth
University of York
Aston University

Industrial Collaborations

BP (Urban Energy Systems Project)
Syngenta (Supply Chain Network Design)
Sainsbury's (Store of the Future)
Unilever (Sustainable Supply Chains Design)
Energy Technologies Institute (Bioenergy Value Chain)
Biosep (Biomass Fractionation)

Publications

Journal Publications

1. Giarola S, Bezzo F, Shah N, 2013, A risk management approach to the economic and environmental strategic design of ethanol supply chains, *Biomass & Bioenergy*, Vol:58, ISSN:0961-9534, Pages:31-51
2. Pantaleo AM, Camporeale SM, Shah N, 2013, Thermo-economic assessment of externally fired micro-gas turbine fired by natural gas and biomass: Applications in Italy, *Energy Conversion and Management*, Vol:75, ISSN:0196-8904, Pages:202-213
3. Kontoravdi C, Samsatli NJ, Shah N, 2013, Development and design of bio-pharmaceutical processes, *Current Opinion in Chemical Engineering*, ISSN:2211-3398
4. Zhang D, Shah N, Papageorgiou LG, 2013, Efficient energy consumption and operation management in a smart building with microgrid, *Energy Conversion and Management*, Vol:74, ISSN:0196-8904, Pages:209-222
5. Mavromatidis G, Acha S, Shah N, 2013, Diagnostic tools of energy performance for supermarkets using Artificial Neural Network algorithms, *Energy and Buildings*, Vol:62, ISSN:0378-7788, Pages:304-314
6. Zuniga MM, Kucherenko S, Shah N, 2013, Metamodelling with independent and dependent inputs, *Computer Physics Communications*, Vol:184, ISSN:0010-4655, Pages:1570-1580
7. Pantaleo A, De Gennaro B, Shah N, 2013, Assessment of optimal size of anaerobic co-digestion plants: An application to cattle farms in the province of Bari (Italy), *Renewable & Sustainable Energy Reviews*, Vol:20, ISSN:1364-0321, Pages:57-70
8. Mac Dowell N, Shah N, 2013, Identification of the cost-optimal degree of CO2 capture: An optimisation study using dynamic process models, *International Journal of Greenhouse Gas Control*, Vol:13, ISSN:1750-5836, Pages:44-58
9. Hayes-Labruto L, Schillebeeckx SJD, Workman M, et al., 2013, Contrasting perspectives on China's rare earths policies: Reframing the debate through a stakeholder lens, *Energy Policy*, Vol:63, ISSN:0301-4215, Pages:55-68
10. Mac Dowell N, Samsatli NJ, Shah N, 2013, Dynamic modelling and analysis of an amine-based post-combustion CO2 capture absorption column, *International Journal of Greenhouse Gas Control*, Vol:12, ISSN:1750-5836, Pages:247-258
11. Caritte V, Acha S, Shah N, 2013, Enhancing Corporate Environmental Performance Through Reporting and Roadmaps, *Business Strategy and the Environment*, ISSN:0964-4733, Pages:-
12. Pantaleo AM, Shah N, Camporeale S, 2013, Natural gas-biomass dual fuelled microturbines: Comparison of operating strategies in the Italian residential sector, *Applied Thermal Engineering*, ISSN:1359-4311
13. Zhang D, Samsatli NJ, Hawkes AD, et al., 2013, Fair electricity transfer price and unit capacity selection for microgrids, *Energy Economics*, Vol:36, ISSN:0140-9883, Pages:581-593
14. Arce A, Mac Dowell N, Shah N, et al., 2012, Flexible operation of solvent regeneration systems for CO2 capture processes using advanced control techniques: Towards operational cost minimisation, *International Journal of Greenhouse Gas Control*, Vol:11, ISSN:1750-5836, Pages:236-250
15. Liu S, Shah N, Papageorgiou LG, 2012, Multiechelon supply chain planning with sequence-dependent changeovers and price elasticity of demand under uncertainty, *AIChE Journal*, Vol:58, ISSN:0001-1541, Pages:3390-3403
16. Konda NVSNM, Shah N, Brandon NP, 2012, Dutch hydrogen economy: evolution of optimal supply infrastructure and evaluation of key influencing elements, *Asia-Pacific Journal of Chemical Engineering*, Vol:7, ISSN:1932-2135, Pages:534-546

17. Akgul O, Shah N, Papageorgiou LG, 2012, Economic optimisation of a UK advanced biofuel supply chain, *Biomass & Bioenergy*, Vol:41, ISSN:0961-9534, Pages:57-72
18. Keirstead J, Samsatli N, Shah N, et al., 2012, The impact of CHP (combined heat and power) planning restrictions on the efficiency of urban energy systems, *Energy*, Vol:41, ISSN:0360-5442, Pages:93-103
19. Mokhtar M, Ali MT, Khalilpour R, et al., 2012, Solar-assisted Post-combustion Carbon Capture feasibility study, *Applied Energy*, Vol:92, ISSN:0306-2619, Pages:668-676
20. Almansoori A, Shah N, 2012, Design and operation of a stochastic hydrogen supply chain network under demand uncertainty, *International Journal of Hydrogen Energy*, Vol:37, ISSN:0360-3199, Pages:3965-3977
21. Khor CS, Shah N, Mahadzir S, et al., 2012, Optimisation of petroleum refinery water network systems retrofit incorporating reuse, regeneration and recycle strategies, *Canadian Journal of Chemical Engineering*, Vol:90, ISSN:0008-4034, Pages:137-143
22. Alhajaj A, Shah N, 2012, Design and analysis of CO2 capture, transport, and storage networks, Society of Petroleum Engineers - Carbon Management Technology Conference 2012, Vol:2, Pages:813-817
23. McGlashan N, Shah N, Caldecott B, et al., 2012, High-level techno-economic assessment of negative emissions technologies, *Process Safety and Environmental Protection*, Vol:90, ISSN:0957-5820, Pages:501-510
24. Seong Khor C, Chachuat B, Shah N, 2012, Optimal water network synthesis with membrane separation-based regenerators, *Computer Aided Chemical Engineering*, Vol:30, ISSN:1570-7946, Pages:37-40
25. Akgul O, Dowell NM, Shah N, et al., 2012, Optimisation of bioelectricity supply chains, AIChE 2012 - 2012 *AIChE Annual Meeting*, Conference Proceedings
26. Liang H, Long W, Keirstead J, et al., 2012, Urban energy system planning and Chinese low-carbon eco-city case study, *Advanced Materials Research*, Vol:433-440, ISSN:1022-6680, Pages:1338-1345
27. Giarola S, Shah N, Bezzo F, 2012, A comprehensive approach to the design of ethanol supply chains including carbon trading effects, *Bioresource Technology*, Vol:107, ISSN:0960-8524, Pages:175-185

Refereed Conference Proceedings

1. Khor CS, Chachuat B, Shah N 2012, *A superstructure optimization approach for water network synthesis with membrane separation-based regenerators*, 21st European Symposium on Computer-Aided Process Engineering (ESCAPE), PERGAMON-ELSEVIER SCIENCE LTD, Pages:48-63, ISSN:0098-1354
2. Akgul O, Shah N, Papageorgiou LG 2012, *An optimisation framework for a hybrid first/second generation bioethanol supply chain*, 21st European Symposium on Computer-Aided Process Engineering (ESCAPE), PERGAMON-ELSEVIER SCIENCE LTD, Pages:101-114, ISSN:0098-1354
3. Keirstead J, Samsatli N, Pantaleo AM, et al. 2012, *Evaluating biomass energy strategies for a UK eco-town with an MILP optimization model*, Conference and Exhibition on Biomass for Energy (WORLD BIOENERGY), PERGAMON-ELSEVIER SCIENCE LTD, Pages:306-316, ISSN:0961-9534
4. Mehdizadeh A, Shah N, Raikar N, et al. 2012, *An optimization of the food quality products throughout the supply chain, 11th International Symposium on Process Systems Engineering (PSE)*, ELSEVIER SCIENCE BV, Pages:1025-1029, ISSN:1570-7946
5. Mehdizadeh A, Shah N, Raikar N, et al. 2012, *Food supply chain planning and quality optimization approach, 22nd European Symposium on Computer Aided Process Engineering (ESCAPE)*, ELSEVIER SCIENCE BV, Pages:1172-1176, ISSN:1570-7946
6. Acha S, van Dam KH, Shah N 2012, *Modelling Spatial and Temporal Agent Travel Patterns for Optimal Charging of Electric Vehicles in Low Carbon Networks*, General Meeting of the IEEE-Power-and-Energy-Society, IEEE, 1944-9925
7. Khor CS, Chachuat B, Shah N 2012, *Optimal water network synthesis with detailed membrane-based regenerator models*, 11th International Symposium on Process Systems Engineering (PSE), ELSEVIER SCIENCE BV, Pages:1457-1461, ISSN:1570-7946
8. Khor CS, Chachuat B, Shah N 2012, *Optimal water network synthesis with membrane separation-based regenerators*, 22nd European Symposium on Computer Aided Process Engineering (ESCAPE), ELSEVIER SCIENCE BV, Pages:36-40, ISSN:1570-7946

Invited/Keynote Lectures

"Process design challenges in biomass conversion"; RSC Symposium on High-value Chemicals from Biomass, London, 2013.

Eva Sørensen

Reader in Chemical Engineering, Department of Chemical Engineering, UCL. 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)
Exxon Mobil Award for Excellence in Teaching, Royal Academy of Engineering (2013)
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

Other Activities
Editor-in-Chief of Chemical Engineering Research & Design
Member of the European Federation of Chemical Engineers (EFCE) Executive Board
Chair of EFCE's Working Party on Fluid Separations (2007–2013)
Treasurer 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)
Member of European Society for Engineering Education (SEFI)
Member of EFSRC Peer Review College
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
Greek Ministry for Education, Life Long Learning and Religious Affairs
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
Novasep, Pfizer, Yorkshire Water

Publications
Journal Articles
1. Close, E. Salm, J., Bracewell, D. G., Sorensen, E. (2013). Modelling of industrial biopharmaceutical multicomponent chromatography. Chemical Engineering Research and Design. doi: 10.1016/j.cherd.2013.10.022.
2. Lam, K.F., Sorensen, E., Gavriilidis, A. (2013). Review on gas-liquid separations in microchannel devices. Chemical Engineering Research and Design 91, 1941-1953. doi: 10.1016/j.cherd.2013.07.031.
3. Ng, C. K., Rousset, F., Valery, E., Bracewell, D. G., Sorensen, E. (2013). Design of high productivity sequential multi-column chromatography for antibody capture. Food and Bioproducts Processing. doi: 10.1016/j.fbp.2013.10.003.
4. Foerster, M., Lam, K. F., Sorensen, E., Gavriilidis, A. (2013). In situ monitoring of microfluidic distillation. Chemical Engineering Journal 227, 13-21. doi:10.1016/j.cej.2012.11.125.
5. Close, E. J., Salm, J.R., Iskra, T., Sorensen, E., Bracewell, D. G. (2013). Fouling of an anion exchange chromatography operation in a monoclonal antibody process: Visualization and kinetic studies. Biotechnology and Bioengineering 110, 2425-2435. doi: 10.1002/bit.24898.

6. Sorensen, E. (2013). Implementation and student perceptions of e-assessment in a Chemical Engineering module. European Journal of Engineering Education 38 (2), 172-185. doi: 10.1080/03043797.2012.760533.
7. Ng, C. K., Osuna-Sanchez, H., Valéry, E., Sorensen, E., Bracewell, D. G. (2012). Design of high productivity antibody capture by protein A chromatography using an integrated experimental and modeling approach. Journal of Chromatography B 899(15), 116-126. doi:10.1016/j.jchromb.2012.05.010.

Conference Contributions

1. Sorensen, E., Fraga, E. S., Triana, C. F. (2013). Optimal energy consumption in the production of bioethanol from lignocellulosic biomass. AIChE 2013 Annual Meeting. paper 608a.
2. Sorensen, E. (2013). Using advanced modelling and computation tools in an undergraduate programme. AIChE 2013 Annual Meeting. paper 76g.
3. Sorensen, E., Thornhill, N. F., Akinmolayan, F. (2013). Predictive modelling of a conventional clean water treatment work. AIChE 2013 Annual Meeting. paper 86c.
4. Sorensen, E., Bracewell, D. G., Close, E. J. (2013). A methodology based on advanced process modelling for the assessment of risk within a quality by design (QbD) framework. AIChE 2013 Annual Meeting. paper 203b.
5. Sorensen, E., Bracewell, D. G., Patel, N. (2013). High-throughput bioprocess development for polymer-polymer aqueous two-phase systems. AIChE 2013 Annual Meeting. paper 9h.
6. Close, E., Bracewell, D. G., Sorensen, E. (2013). A model based approach to an adaptive design space in chromatography. 23rd European Symposium on Computer Aided Process Engineering (ESCAPE). (Vol. 32 pp.115-120).
7. Sorensen, E., Close, E., Bracewell, D. G. (2013). A model based approach to constructing probabilistic design spaces in the face of chromatography process variability. 9th European Congress on Chemical Engineering (ECCE).
8. Sorensen, E, Manage, M., Brett, D. J. L., Simons, S. J. R. (2013). A feasibility study on the integration of power stations with intermediate-temperature steam electrolysers. 9th European Congress on Chemical Engineering (ECCE).
9. Sorensen, E, Triana, C., Fraga, E. S. (2013). Optimal operation and heat integration of bioethanol production. 9th European Congress on Chemical Engineering (ECCE).
10. Sorensen, E., Thivyathasan, V., Akinmolayan, F., Papageorgiou, L.G. (2013). Synthesis of clean water treatment processes using optimisation techniques. 9th European Congress on Chemical Engineering (ECCE).
11. Sorensen, E., Law, L. M., Elson, T. P. (2013), “Simulating dividing wall columns in commercial software. 9th European Congress on Chemical Engineering (ECCE).
12. Anssari-Benham, A., Thornhill, N. F., Sorensen, E. (2013), A real-time operational risk management system for water treatment processes. 9th European Congress on Chemical Engineering (ECCE).
13. Close, E., Jin, J., Salm, J., Sorensen, E., Bracewell, D. G. (2012). Understanding chromatography fouling in therapeutic protein manufacture. 8th Annual Protein Engineering Summit (PEGS).
14. Ng, C., Osuna-Sanchez, H., Valery, E., Bracewell, D., Sorensen, E. (2012). Optimization of protein A chromatography for antibody capture. 22nd European Symposium on Computer Aided Process Engineering (ESCAPE). (Vol. 30 pp.1367-1371).
15. Close E., Jin, J., Salm, J., Sorensen, E., Bracewell, D.G. (2012). Understanding chromatography fouling in vaccine and therapeutic protein manufacture. American Society of Chemistry National Meeting (ACS).
16. Close, E., Salm, J., Sorensen, E., Bracewell, D. G. (2012). Model-based experimental design and parameter estimation for the mechanistic modelling of an industrial hydrophobic interaction chromatography step. 22nd European Symposium on Computer Aided Process Engineering (ESCAPE).
17. Förster, M., Lam, K. F., Sorensen, E., Gavriilidis, A. (2012). In-situ measurements and analysis of on-chip microdistillation. International Conference on Microreaction Technology (IMRET’12). Paper T3.O.03.
18. Close, E. J., Iskra, T., J. Salm, J., Sorensen, E., Bracewell, D. G. (2011). Characterising the fouling of an industrial anion exchange polishing step during the manufacturing process of a commercial therapeutic protein. AIChE 2011 Annual Meeting. paper 444fe.
19. Close, E. J., Salm, J., Lyons, J., Bracewell, D. G., Sorensen, E. (2011). Model based experimental design and parameter estimation for an industrial hydrophobic interaction chromatography step from a Quality by Design (QbD) perspective. AIChE 2011 Annual Meeting. paper 700e.
20. Ng, C., Osuna-Sanchez, H., Valery, E., Sorensen, E., Bracewell, D. G. (2011). Optimisation of antibody capture by protein A chromatography, International Chemical and Biological Engineering Conference (ChemPor).
21. Förster, M., Lam, K. F., Sorensen, E., Gavriilidis, A. (2011). Separation of toluene and benzaldehyde by microchannel distillation. 8th European Congress on Chemical Engineering (ECCE).

Michail Stamatakis

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

Qualifications

PhD in Chemical and Biomolecular Engineering
(Rice University, USA)
Diploma in Chemical Engineering (National Technical University of Athens, Greece)

Awards and Distinctions

2013 Chartered Scientist
2007 Kobayashi Fellowship, Rice University
2004 Silver medal, National Technical University of Athens

Research Interests

Michail Stamatakis's research focuses on developing stochastic multiscale methods for understanding complex systems, and applying these methods for solving practical problems in Chemistry, Biology and Engineering. He is the creator of Zacros, a software package for simulating reaction kinetics on heterogeneous catalysts (http://www.e-lucid.com/i/software/material_modelling/Zacros.html).

Other Activities

Member of the Institution of Chemical Engineers (IChemE)
Member of the Royal Society of Chemistry (RSC)
Member of the American Institute of Chemical Engineers (AIChE)
Member of the organising committee of the Recent Appointees in Materials Modelling 2014 Conference

Reviewer for

AIChE Journal
Chemical Engineering Journal
Computers & Chemical Engineering
ACS Nano
Journal of Chemical Physics
Physical Review E
Physical Review Letters
Biofabrication
Biophysical Journal
BMC Bioinformatics

Academic Collaborations

Dr Giannis Mpourmpakis. Computational studies of CO oxidation on Au nanoclusters. Chemical & Petroleum Engineering, Swanson School of Engineering, University of Pittsburgh, USA.
Dr Simone Piccinin. Detailed kinetic Monte Carlo simulations of CO oxidation on Pd. Istituto Officina dei Materiali (CNR-IOM), Scuola Internazionale Superiore di Studi Avanzati, Italy
Prof. E. Charles H. Sykes. Investigations of molecular phenomena on a bimetallic hydrogenation catalyst. Department of Chemistry, Tufts University, USA

Publications

Journal Articles

1. Herrmann, S., Stamatakis, M., Andriotis, A. N. and G. Mpourmpakis (2014). "Adsorption Behavior of Noble Metal Clusters and Their Alloys". Journal of Computational and Theoretical Nanoscience 11(2): 511-520.
2. Nielsen, J., d'Avezac, M., Hetherington, J. and M. Stamatakis (2013). "Parallel Kinetic Monte Carlo Simulation Framework Incorporating Accurate Models of Adsorbate Lateral Interactions". Journal of Chemical Physics 139(22): 224706.
3. Guo, W., Stamatakis, M. and D. G. Vlachos (2013). "Design Principles of Heteroepitaxial Bimetallic Catalysts". ACS Catalysis 3: 2248-2255.
4. Marcinkowski, M. D., Jewell, A. D., Stamatakis, M., Boucher, M. B., Lewis, E. A., Murphy, C. J., Kyriakou, G. and E. C. H. Sykes (2013). "Controlling a Spillover Pathway with the Molecular Cork Effect". Nature Materials 12(6): 523-528.
5. M. Stamatakis. (2013). "Cell Population Balance and Hybrid Modeling of Population Dynamics for a Single Gene with Feedback". Computers and Chemical Engineering 53: 25-34.
6. Stamatakis, M., Christiansen, M., Vlachos, D. G. and G. Mpourmpakis (2012). "Multiscale Modeling Reveals Poisoning Mechanisms on MgO-supported Au Catalysts in CO Oxidation". Nano Letters 12(7): 3621-3626.
7. Stamatakis, M., Chen, Y. and D. G. Vlachos (2011). "First Principles-Based Kinetic Monte Carlo Simulation of the Structure-Sensitivity of the Water-Gas Shift Reaction on Platinum Surfaces". Journal of Physical Chemistry C 115(50): 24750-24762.
8. Mpourmpakis, G., Stamatakis, M., Herrmann, S., Vlachos, D. G. and A. N. Andriotis (2011). "Predicting the Adsorption Behavior in Bulk from Metal Clusters". Chemical Physics Letters 518: 99-103.
9. Stamatakis, M. and D. G. Vlachos (2011). "Equivalence of on-Lattice Stochastic Chemical Kinetics with the Well-Mixed Chemical Master Equation in the Limit of Fast Diffusion". Computers and Chemical Engineering 35(12): 2602-2610.
10. Salciccioli, M., Stamatakis, M., Caratzoulas, S. and D. G. Vlachos (2011). "A Review of Multiscale Modeling of Metal-Catalyzed Reactions: Mechanism Development for Complexity and Emergent Behavior". Chemical Engineering Science 66(19): 4319-4355.
11. Stamatakis, M. and K. Zygourakis (2011). "Deterministic and Stochastic Population-Level Simulations of an Artificial *lac* Operon Genetic Network". BMC Bioinformatics 12: 301.

12. Stamatakis, M. and D. G. Vlachos (2011). “A Graph-Theoretical Kinetic Monte Carlo Framework for on-Lattice Chemical Kinetics”. Journal of Chemical Physics 134(21): 214115.
13. Wang, H., Stamatakis, M., Hansgen, D., Caratzoulas, S. and D. Vlachos (2010). “Understanding Mixing of Ni and Pt in the Ni/Pt(111) Bimetallic Catalyst via Molecular Simulation and Experiments”. Journal of Chemical Physics 133(22): 224503.
14. Stamatakis, M. and N. V. Mantzaris (2010). “Intrinsic Noise and Division Cycle Effects on an Abstract Biological Oscillator”. Chaos 20: 033118. *[Among the top 20 Chaos articles with the most full-text downloads during October 2010. Selected for the October 1, 2010 issue of the Virtual Journal of Biological Physics Research]*.
15. Stamatakis, M. and K. Zygourakis (2010). “A Mathematical and Computational Approach for Integrating the Major Sources of Cell Population Heterogeneity”. Journal of Theoretical Biology 266(1): 41-61.
16. Collins, S., Stamatakis, M. and D. G. Vlachos (2010). “Adaptive Coarse-Grained Monte Carlo Simulation of Reaction and Diffusion Dynamics in Heterogeneous Plasma Membranes”. BMC Bioinformatics 11: 218.
17. M. Stamatakis. (2010). “Cell Population Balance, Ensemble and Continuum Modeling Frameworks: Conditional Equivalence and Hybrid Approaches”. Chemical Engineering Science 65(2): 1008-1015.
18. Stamatakis, M. and N. V. Mantzaris (2009). “Comparison of Deterministic and Stochastic Models of the lac Operon Genetic Network”. Biophysical Journal 96(3): 887-906.
19. Stamatakis, M. and N. V. Mantzaris (2007). “Astrocyte Signaling in the Presence of Spatial Inhomogeneities”. Chaos 17: 033123.
20. Stamatakis, M. and N. V. Mantzaris (2006). “Modeling of ATP-Mediated Signal Transduction and Wave Propagation in Astrocytic Cellular Networks”. Journal of Theoretical Biology 241(3): 649-668.

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-Sept 2005.
Royal Academy of Engineering Foresight Award with University of Alberta, Canada, January-Sept 2001.
Royal Society Industry Fellowship with BP International, 1992–5

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

Journal Articles

1. Cecilio, I., Ottewill, J., Pretlove, J., and Thornhill, N.F., 2014, Nearest neighbors method for detecting transient disturbances in process and electromechanical systems, submitted to Journal of Process Control.
2. Ikram, W., Petersen, S., Orten, P., and Thornhill, N.F., 2013, Adaptive multi-channel transmission power control for industrial wireless instrumentation, IEEE Transactions on Industrial Informatics, accepted for publication.
3. Schleburg, M., Christiansen, L., Fay, A., and Thornhill, N.F., 2013, A combined analysis of plant connectivity and alarm logs to reduce the number of alerts in an automation system, Journal of Process Control, 23, 839-851.
4. Stonier, A., Pain, D., Westlake, A., Hutchinson, N., Thornhill, N.F., and Farid, S.S., 2013, Integration of stochastic simulation with multivariate analysis: short term facility fit prediction, Biotechnology Progress, 29, 368-377.
5. Sharifzadeh, M., and Thornhill, N.F., 2013, A novel optimization framework for integrated design and control, using dynamic inversely controlled process models, Computers & Chemical Engineering, 48, 121-134.
6. Shukla, V., Naim, M., and Thornhill, N.F., 2012, Rogue seasonality detection in supply chains, International Journal of Production Economics, 138, 254-272.
7. Meland, E., Thornhill, N.F., Lunde, E., and Rasmussen, M., 2012, Quantification of valve leakage rates, AIChE Journal. 58, 1181–1193.

Conference Presentations

1. Ikram, W., and Thornhill, N.F., 2013. Towards the development of a wireless network node lifetime calculation tool, a work in-progress paper, IEEE EFTA Conference, Cagliari, Italy, September 10th-13th 2013.
2. Cicciotti, M., Martinez-Botas, R., Romagnoli, A., Thornhill, N.F., Geist, S., and Schild, A., 2013, Systematic one zone meanline modelling of centrifugal compressors for industrial online monitoring applications, Proceedings of ASME Turbo Expo 2013, San Antonio, Texas, June 3-7 2013, paper GT2013/95821.
3. Linash P. Kunjumuhammed, L.P, Pal, B.C., Anaparthi, K., Thornhill, N.F., 2013, Effect of wind penetration on power system stability, IEEE Power & Energy Society General Meeting, 21-25 July, 2013, Vancouver, Canada.
4. Barocio, E., Pal, B.C., Fabozzi, D., Thornhill, N.F., 2013 Detection and visualization of power system disturbances using principal component analysis, 2013 IEEE IREP Symposium - Bulk Power System Dynamics and Control - IX Optimization, Security and Control of the Emerging Power Grid, August 25-30, 2013, Rethymnon, Greece.
5. Cecılio, I.M., Ersdal, A.M., Fabozzi, D., and Thornhill, N.F., 2013, An open-source educational toolbox for power system frequency control tuning and optimization, accepted for the 4th European Innovative Smart Grid Technologies Conference IEEE PES ISGT Europe 2013.
6. Ersdal, A.M., Cecılio, I.M., Fabozzi, D., Imsland, L, and Thornhill, N.F., 2013, MPC for power system frequency control taking into account imbalance uncertainty, accepted for the 4th European Innovative Smart Grid Technologies Conference IEEE PES ISGT Europe 2013.
7. Cecilio, I., and Thornhill, N.F, 2013, Nearest neighbors methods for detecting and removing interfering disturbances from oscillating signals, submitted to DYCOPS 2013. (withdrawn)
8. Fabozzi, D., Thornhill, N.F., and Pal, B.C., 2013, Frequency restoration reserve control scheme with participation of industrial loads, IEEE PowerTech 2013.
9. Kunjumuhammed, L.P., Pal, B.C., and Thornhill, N.F., 2013, A test system model for stability studies of the UK power grid, IEEE PowerTech 2013.
10. Thornhill, N.F, Fabozzi, D., and Pal, B.C., 2013, Monitoring and management of power transmission dynamics in an Industrial Smart Grid, IEEE PowerTech 2013.
11. Yang, Y., Farid, S.S., and Thornhill, N.F., 2013, Prediction of biopharmaceutical facility fit issues using decision tree analysis, 23rd European Conference on Computer Aided Process Engineering (ESCAPE 23), Lappeenranta, Finland, June 9-12, 2013.
12. Cicciotti, M., Geist, S., Schild, A., Martinez-Botas, R., Romagnoli, A., and Thornhill, N.F., 2013, Systematic one zone meanline modelling of centrifugal compressors for industrial on-line applications, Paper GT2013-95821, ASME Turbo Expo 2013.
13. Cicciotti, M., Martinez-Botas, R., Gozalbo, R., Geist, S., Thornhill, N.F., and Kahrs, O., 2012, Assessment of meanline models for centrifugal compressors in the process plant industry, 5th International Symposium on Fluid Machinery and Fluids Engineering (ISFMFE 2012), Jeju, Korea, Oct. 24-27, 2012.

14. Thornhill, N.F., Discovering how process operation and control technology really works, 22nd European Conference on Computer Aided Process Engineering (ESCAPE 22), London, June 18-20, Invited keynote talk.
15. Schleburg, M., Christiansen, L., Fay, A., and Thornhill, N.F., 2012, Reduction of alerts in automated systems based on a combined analysis of process connectivity and alarm logs, 22nd European Conference on Computer Aided Process Engineering (ESCAPE 22), London, June 18-20.
16. Cecilio, I.M., Rapp, K., and Thornhill, N.F., 2012, Process performance analysis in large-scale systems integrating different sources of information, ADCHEM 2012, Singapore, July 10-13.

Wolfram Wiesemann

Assistant Professor, Management Science and Operations, Fellow, KPMG Centre for Advanced Business Analytics, Business School, Imperial College London

Research Interests

Optimisation under uncertainty with applications in operations management, energy and finance.

Reviewer for

Annals of Operations Research, Applied Mathematical Modelling, Asia-Pacific Journal of Operational Research, Automatica, Computational Management Science, The Computer Journal, Computers & Chemical Engineering, Energy Systems, European Journal of Operational Research, IIE Transactions, Journal of Global Optimization, Journal of Network and Systems Management, Management Science, Mathematical Programming, Mathematics of Operations Research, Operations Research, Operations Research Letters, Optimization and Engineering, Optimization Letters, SIAM Journal on Optimization, Transportation Science, as well as the IFAC Conference on Manufacturing, Modelling, Management and Control
Academic Collaborations: Carnegie Mellon University, Columbia University, National University of Singapore, Princeton University
Picture: please take the one from my homepage or the CPSE website.

Publications

Books

W. Wiesemann. Optimization of Temporal Networks under Uncertainty. Springer, 2012.
(A review of this book appeared in INFORMS Journal on Computing.)

Book Chapters

1. C. E. Gounaris, P. P. Repoussis, C. D. Tarantilis, W. Wiesemann and C. A. Floudas. An Adaptive Memory Programming Framework for the Robust Capacitated Vehicle Routing Problem. Under 2nd-Round Review for Transportation Science.
2. W. Wiesemann, A. Tsoukalas, P.-M. Kleniati and B. Rustem. Pessimistic Bi-Level Optimisation. SIAM Journal on Optimization 23(1):353–380, 2013.
3. C. E. Gounaris, W. Wiesemann and C. A. Floudas. The Robust Capacitated Vehicle Routing Problem under Demand Uncertainty. Operations Research, Articles in Advance.
4. W. Wiesemann, D. Kuhn and B. Rustem. Robust Markov Decision Processes. Mathematics of Operations Research, Articles in Advance.
5. W. Wiesemann, D. Kuhn and B. Rustem. Robust Resource Allocations in Temporal Networks. Mathematical Programming 135(1–2):437–471, 2012.

Conference Papers

1. C. E. Gounaris, W. Wiesemann and C. A. Floudas. *The Robust Rounded Capacity Inequalities*. Proceedings of the 5th International Workshop on Freight Transportation and Logistics, Mykonos (Greece), 2012.

Invited Lectures and Seminars

Workshop on Controlled Stochastic Processes: Theory and Applications, University of Liverpool (UK), March 2013. Invited plenary lecture on Distributionally Robust Markov Decision Processes.
Management Science and Operations Group, London Business School (UK), February 2013. Invited seminar on Scenario-Free Stochastic Programming and its Applications in Operations Management.
IMS Workshop on Optimization under Uncertainty, National University of Singapore (Singapore), December 2012. Invited plenary lecture on Distributionally Robust Convex Optimization.
Singapore University of Technology and Design (Singapore), December 2012. Invited seminar on Scenario-Free Stochastic Programming and its Applications in Operations Management.
Centre for Discrete Mathematics and its Applications, University of Warwick, November 2012. Invited seminar on Distributionally Robust Convex Optimization.
IBM T. J. Watson Research Center, Hawthorne NY (USA), October 2012. Invited seminar on Scenario-Free Stochastic Programming and its Applications in Operations Management.
Centre for Operational Research, Management Sciences and Information Systems, University of Southampton, February 2012. Invited seminar on Scenario-Free Stochastic Programming and its Applications in Operations Management.

CPSE Academics and Staff Directory
2012–2013 CPSE Annual Report

Imperial College London

Department of Chemical Engineering
Professor Claire S. Adjiman, Professor of Chemical Engineering
Dr Edo Boek, Senior Lecturer
Dr Benoit Chachuat, Senior Lecturer
Dr Peter DiMaggio, Lecturer
Professor Amparo Galindo, Professor of Physical Chemistry
Professor George Jackson, Professor of Chemical Physics
Dr Cleo Kontoravdi, Lecturer (Lonza/RCUK Academic Fellowship)
Dr J Krishnan, Lecturer
Professor Geoffrey C. Maitland, Professor of Energy Engineering
Professor Athanasios (Sakis) Mantalaris,
Professor of BioSystems Engineering
Dr Ruth Misener, Royal Academy of Engineering Research Fellow
Professor Erich Müller, Professor of Thermodynamics
Professor Costas C. Pantelides, Professor of Chemical Engineering
Professor Efstratios (Stratos) Pistikopoulos,
Professor of Chemical Engineering
Professor Nilay Shah, Professor of Process
Systems Engineering, Director CPSE
Professor Nina F. Thornhill, Professor of Process Automation

Business School
Dr Wolfram Wiesemann, Assistant Professor

Department of Civil and Environmental Engineering
Dr James Keirstead, Lecturer

Department of Computing
Dr Panos Parpas, Lecturer
Professor Berc Rustem, Professor of Computing

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

Emeritus and Honorary Academics
Professor Roger Benson
Graham Elkes
Professor John Perkins
Professor Paul Rutter
Professor Roger W. H. Sargent

University College London

Department of Chemical Engineering
Professor I. David Bogle, Professor of Chemical
Engineering and Head of UCL Graduate School
Dr Vivek Dua, Senior Lecturer
Professor Eric S. Fraga, Professor of Process Systems Engineering
Professor Lazaros Papageorgiou, Professor of Chemical Engineering
Dr Eva Sørensen, Reader in Chemical Engineering
Dr Michail Stamatakis, Lecturer

Academic Staff

Prof Claire S Adjiman	c.adjiman@imperial.ac.uk
Dr Edo Boek	boek@imperial.ac.uk
Prof I David L Bogle	d.bogle@ucl.ac.uk
Prof Nigel Brandon	n.brandon@imperial.ac.uk
Dr Benoit Chachuat	b.chachuat@imperial.ac.uk
Dr Peter DiMaggio	p.dimaggio@imperial.ac.uk
Dr Vivek Dua	v.dua@ucl.ac.uk
Prof Eric S Fraga	e.fraga@ucl.ac.uk
Prof Amparo Galindo	a.galindo@imperial.ac.uk
Prof George Jackson	g.jackson@imperial.ac.uk
Dr James Keirstead	j.keirstead@imperial.ac.uk
Dr Cleo Kontoravdi	cleo.kontoravdi98@imperial.ac.uk
Dr J Krishnan	j.krishnan@imperial.ac.uk
Prof Geoffrey C Maitland	g.maitland@imperial.ac.uk
Prof Athanasios Mantalaris	a.mantalaris@imperial.ac.uk
Dr Ruth Misener	r.misener@imperial.ac.uk
Prof Erich Müller	e.muller@imperial.ac.uk
Prof Costas C Pantelides	c.pantelides@imperial.ac.uk
Prof Lazaros Papageorgiou	l.papageorgiou@ucl.ac.uk
Dr Panos Parpas	p.parpas@imperial.ac.uk
Prof Efstratios N Pistikopoulos	e.pistikopoulos@imperial.ac.uk
Prof Berc Rustem	b.rustem@imperial.ac.uk
Prof Nilay Shah (CPSE Director)	n.shah@imperial.ac.uk
Dr Eva Sørensen	e.sorensen@ucl.ac.uk
Dr Michail Stamatakis	m.stamatakis@ucl.ac.uk
Prof Nina F Thornhill	n.thornhill@imperial.ac.uk
Dr Wolfram Wiesemann	ww@imperial.ac.uk

Emeritus and Honorary Academics

Prof Roger Benson	roger.s.benson@btinternet.com
Graham Elkes	graham.elkes@imperial.ac.uk
Prof John Perkins	john.perkins@imperial.ac.uk
Prof Paul Rutter	p.rutter@imperial.ac.uk
Prof Roger W.H. Sargent	r.w.h.sargent@imperial.ac.uk

Research Associates

Dr Salvador Acha Izquierdo	salvador.acha06@imperial.ac.uk
Dr Afshin Anssari-Benham	a.anssari-benam@ucl.ac.uk
Dr Laura Bennett	laura.bennett@ucl.ac.uk
Dr John Blamey	j.blamey07@imperial.ac.uk
Dr Alexandros Chremos	a.chremos@imperial.ac.uk
Dr Carlos Henrique Correia Braga	c.correia-braga@imperial.ac.uk
Dr Simon Dufal	simon.dufal07@imperial.ac.uk
Dr Iliana Fauzi	iliana.fauzi05@imperial.ac.uk
Dr Esther Forte	e.forte-serrano07@imperial.ac.uk
Dr Federico Galvanin	f.galvanin@ucl.ac.uk
Dr Apostolos Georgiadis	a.georgiadis07@imperial.ac.uk
Dr Sara Giarola	s.giarola10@imperial.ac.uk
Dr Miao Guo	
Dr Andrew Haslam	a.haslam@imperial.ac.uk
Dr Carmelo Herdes Moreno	c.herdes@imperial.ac.uk
Dr Ioscani Jimenez Del Val	ioscani.jimenez-del-val06@imperial.ac.uk
Dr Maria G. Serratos Jimenez	m.jimenez-serratos@imperial.ac.uk
Dr Oleksiy Klymenko	o.klymenko@imperial.ac.uk
Dr Sergei Kucherenko	s.kucherenko@imperial.ac.uk
Dr Kamal Kuriyan	kkuriyan@ic.ac.uk
Dr Romain Lambert	romain.lambert 08@imperial.ac.uk
Dr Songsong Liu	s.liu@ucl.ac.uk
Dr Xiaomei Lu	xiaomei.lu@imperial.ac.uk
Dr Evgenia Mechleri	e.mehleri@imperial.ac.uk
Prof Richard John Murphy	r.murphy@imperial.ac.uk
Dr Jordan Muscatello	jordan.muscatello05@imperial.ac.uk
Dr HongXing Niu	h.niu@imperial.ac.uk
Dr Vasileios Papaioannou	v.papaioannou08@imperial.ac.uk
Dr Remigijus Paulavicius	remigijus.paulavicius@imperial.ac.uk
Dr Varma Penumathsa	b.penumathsa@imperial.ac.uk
Dr Thomas Pogiatzis	t.pogiatzis@imperial.ac.uk
Dr Vassilios Raptis	v.raptis@imperial.ac.uk
Dr Maria Rende	m.rende@imperial.ac.uk
Dr Pedro Rivotti	p.rivotti@imperial.ac.uk
Dr Kate Elizabeth Royle	kate.royle05@imperial.ac.uk
Dr Majid Sadeqzadeh	m.sadeqzadeh@imperial.ac.uk
Dr Nouri Samsatli	n.samsatli@imperial.ac.uk
Dr Sheila Samsatli	s.samsatli@imperial.ac.uk
Dr Mahdi Sharifzadeh	mahdi.sharifzadeh08@imperial.ac.uk
Dr Paul Shearing	p.shearing@imperial.ac.uk
Dr Eirini Siougkrou	e.siougkrou09@imperial.ac.uk
Dr Shufang Song	shufang.song@imperial.ac.uk
Dr Panagiotis Theodorakis	p.theodorakis@imperial.ac.uk
Dr Koen Van Dam	k.van-dam@imperial.ac.uk
Dr Manolis Vasileiadis	m.vasileiadis09@imperial.ac.uk
Dr Eirini Velliou	e.velliou@imperial.ac.uk
Dr Spiros Vernardis	s.vernardis@imperial.ac.uk
Dr Yang Yang	yang.yang@imperial.ac.uk
Dr Ioannis Zacharoudiou	i.zacharoudiou@imperial.ac.uk
Dr Di Zhang	di.zhang.09@ucl.ac.uk
Dr Fessehaye Zemichael	f.zemichael@imperial.ac.uk
Dr Yunbo Zhao	yunbo.zhao@imperial.ac.uk

Support Staff

CPSE Administration and Research Officer
Miss Cristina Romano,
c.romano@imperial.ac.uk

External Relations Manager
Miss Senait Selassie,
s.selassie@imperial.ac.uk

Head of Computing Services
Mr Graham Stuart
g.stuart@imperial.ac.uk

CPSE Research Project List
Professor Berc Rustem

"The assets of Imperial College and University College London are their students and their collegiate environment."

Research Project List
2012–2013 CPSE Annual Report

Adam Alexandros
Integrated Heating and Power Systems for Dwellings
Supervisor: Prof Eric Fraga
Start date: October 2011
Finish date: September 2014

Jorge Aguerrevere
Network Analysis of DNA Damage Response and Cellular Signalling in Different KRAS Mutated Colorectal Cancer Cell Lines
Supervisor: Prof David Bogle
Start date: September 2012
Finish date: October 2016

Folashade Akinmolayan
Real-time Operational Risk Management Through Advanced Multi-scale Modelling
Supervisors: Dr Eva Sørensen and Prof Nina Thornhill
Start date: August 2011
Finish date: July 2014

Ali Salim Al Qahtani
Technical, Economic and Environmental Impact of Future Fuel Formulations
Supervisor: Prof Nilay Shah
Start date: October 2010
Finish date: October 2014

Aiman Alam Nazki
Mathematical Modelling and Systems Approaches for Investigating Dynamic Behaviour of Signalling in Systems and Synthetic Biology
Supervisor: Dr Jawahar Krishnan
Start date: January 2010
Finish date: May 2014

Yasmeen Aldawsari
Techno-economic Analysis of Strategies and Technologies to Decarbonise the Transport Sector
Supervisor: Prof Nilay Shah
Start date: September 2013
Finish date: September 2016

Amos Aleji
Viscosity of Reservoir Fluids
Supervisor: Prof Geoffrey Maitland
Start date: February 2011
Finish date: May 2014

Mark Allenby
Development of a Bio-inspired in Silico-in Vitro Platform: Towards Personalised Healthcare through Optimisation of Leukaemia Chemotherapy
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: September 2013
Finish date: September 2016

Nihal Almuraikhi
Stem Cell Bioprocessing
Supervisor: Prof Athanasios Mantalaris
Start date: October 2010
Finish date: August 2015

Diego Alonso Martinez
Profiling Substrate Specificity of Histone Lysine Methyltransferases
Supervisor: Dr Peter DiMaggio
Start date: September 2013
Finish date: September 2016

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

Tareg AlSoudani
Multiscale Modelling for Operation and Control of PSA Units
Supervisor: Prof David Bogle
Start date: October 2005
Finish date: May 2014

Daniel Aluma
Network Optimisation for Gas Production
Supervisor: Prof Nilay Shah and Prof Costas Pantelides
Start date: November 2012
Finish date: November 2018

Oluwamayowa Amusat
Storage Systems for Solar Thermal use in Continuous Processing
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

Christos Argyropoulos
Numerical Simulation of Turbulent Two-Phase Pipe Flows
Supervisor: Dr Edo Boek
Start date: February 2010
Finish date: October 2014

William Ashworth
Systems Biology of the Liver
Supervisor: Prof David Bogle
Start date: October 2013
Finish date: May 2017

Joakim Beck
Surrogate Modelling for Optimal Design of Carbon Capture
Supervisor: Prof Eric Fraga
Start date: March 2010
Finish date: May 2014

Asif Bhatti
Synthesis and Design of Biological Systems Under Uncertainty
Supervisor: Dr Vivek Dua
Start date: October 2010
Finish date: September 2014

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

Aaron Borg
Characterizing the Function of Chromatin-Modifying Protein Complexes
Supervisor: Dr Peter DiMaggio
Start date: August 2012
Finish date: July 2015

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

Sara Budinis
Process Systems Engineering
Supervisor: Prof Nina Thornhill
Start date: September 2011
Finish date: September 2014

Gizem Buldum
Bacterial Cellulose Production
Supervisor: Prof Athanasios Mantalaris
Start date: October 2011
Finish date: September 2014

Gonzalo Bustos Turu
Modelling and Optimisation Strategies for Urban Energy Systems
Supervisor: Prof Nilay Shah
Start date: March 2014
Finish date: March 2017

Shane Cadogan
Diffusion and Diffusion Processes in Fractured Media
Supervisor: Prof Geoffrey Maitland
Start date: October 2011
Finish date: September 2014

Claudio Calabrese
Viscosity and Density of Reservoir Fluids Under CO2 Injection
Supervisor: Prof Geoffrey Maitland
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

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

Emily Chapman
Micro-Model Pore-Scale Flow Studies of Fluid Displacement in Carbonate Rock with Application to CO2 Storage
Supervisor: Dr Edo Boek
Start date: October 2010
Finish date: March 2014

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

Edward Close
Process Modelling Approaches to Biological Complexity in the Production of Therapeutic Proteins
Supervisor: Dr Eva Sørensen
Start date: September 2009
Finish date: September 2014

Ibrahim Asaad I M Daher
Reactive Transport in Micromodels of Porous Media
Supervisors: Dr Edo Boek and Prof Geoffrey Maitland
Start date: January 2013
Finish date: January 2016

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

Pongsathorn Dechatiwongse
Solar Hydrogen
Supervisor: Prof Geoffrey Maitland
Start date: October 201
Finish date: September 2014

Aikaterini Diamanti
Predicting the Effect of Temperature and Solvents on the Rate of Organic Reactions
Supervisors: Prof Claire Adjiman and Prof Amparo Galindo
Start date: October 2012
Finish date: September 2015

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

Nasim Elahi
Multiscale Modelling of Carbon Capture and Storage
Supervisor: Prof Nilay Shah
Start date: October 2010
Finish date: January 2014

Daniel Kunisch Eriksen
Molecular Modelling and Thermodynamics of Oil Systems in the Presence of Brine and CO2
Supervisor: Prof Amparo Galindo and
Prof George Jackson
Start date: October 2012
Finish date: September 2015

Koca Esma
Global Launch Decisions and Product Rollover Strategies for Substitutable Products
Supervisor: Dr Wieseman Wolfram
Start date: October 2013
Finish date: March 2017

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

Maria Fuentes Gari
Bioprocess Design for Production of Biopolymers
Supervisor: Prof Athanasios Mantalaris
Start date: September 2011
Finish date: December 2015

David Garcia Munzer
Modelling of Mammalian Cell Culture Systems
Supervisors: Prof Athanasios Mantalaris and
Prof Efstratios Pistikopoulos
Start date: October 2010
Finish date: February 2014

Christina Gatsiou
Crystal Structure Prediction
Supervisors: Prof Claire Adjiman and Prof Constantinos Pantelides
Start date: March 2012
Finish date: February 2015

Anastasia Georgiou
Cartilage Tissue Engineering: The Role of Statins and Mechanical Stimulation in Generating 3D Cellular Constructs
Supervisor: Prof Athanasios Mantalaris
Start date: October 2009
Finish date: July 2014

Cher Goey
Towards Advanced Modelling of Whole Bioprocesses
Supervisor: Dr Cleo Kontoravdi
Start date: February 2013
Finish date: January 2016

Smitha Gopinath
Molecular Design Based on Advanced Thermodynamic Models
Supervisors: Prof Claire Adjiman and Prof Amparo Galindo
Start date: September 2013
Finish date: September 2016

Farrel Gray
Pore-scale Multiphase Flow
Supervisor: Dr Edo Boek
Start date: October 2012
Finish date: September 2015

Boram Gu
Modelling of RO Membrane Process Performance and Transport Phenomena for Performance Aanalysis and Optimisation
Supervisor: Prof Claire Adjiman
Start date: April 2013
Finish date: April 2016

Grani Hanasusanto
Decision Making Under Uncertainty: Robust and Data-Driven Approaches
Supervisors: Dr Daniel Kuhn, Prof Berc Rustem and Wolfram Wieseman
Start date: October 2011
Finish date: September 2015

Abdihakim Hassan
Modelling Solvent Mixtures and their Effects on Reactions
Supervisors: Prof Claire Adjiman and Prof Amparo Galindo
Start date: November 2010
Finish date: January 2015

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

Rayane Hoballah
Effect of Impurities in the CO2 Stream on Phase Behaviour
Supervisor: Prof Geoffrey Maitland
Start date: December 2012
Finish date: December 2015

Ruien Hu
The Viscosity and Flow Behaviour of CO2 Interacting with Reservoir Fluids
Supervisor: Dr Edo Boek
Start date: October 2012
Finish date: September 2015

Panatpong Hutacharoen
Molecular Systems Engineering for Pharmaceuticals
Supervisors: Prof Claire Adjiman, Prof Amparo Galindo, Prof George Jackson and Prof Erich Müller
Start date: May 2013
Finish date: May 2016

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

Philip Jedrzejewski
A Platform for the Optimisation of Metabolic Pathways for Glycosylation to Achieve a Narrow and Targeted Glycoform Distribution
Supervisor: Dr Cleo Kontoravdi
Start date: October 2011
Finish date: September 2014

Suela Jonuzaj
Optimisation Approaches to Mixture Design
Supervisor: Prof Claire Adjiman
Start date: August 2013
Finish date: July 2016

Nikolaos Kazazakis
Deterministic Global Optimization Techniques
Supervisor: Prof Claire Adjiman
Start date: September 2012
Finish date: August 2015

Mariya Koleva
Optimisation of Wastewater Systems
Supervisor: Prof Lazaros Papageorgiou
Start date: March 2013
Finish date: September 2015

Gabriel Lau
Droplets: From Molecular Nanoclusters to the Atmospheric Aerosols
Supervisor: *Prof George Jackson*
Start date: March 2013
Finish date: September 2015

Georgia Lazarou
Molecular Systems Engineering for Pharmaceuticals
Supervisors: Prof Claire Adjiman, Prof Amparo Galindo, Prof George Jackson and Prof Erich Müller
Start date: October 2013
Finish date: September 2016

David Leng
Fault Propagation, Detection and Analysis in Process Systems
Supervisor: Prof Nina Thornhill
Start date: September 2013
Finish date: September 2019

Olga Lobanova
Coarse Grained Molecular Simulations of Amphiphiles and Biosystems
Supervisors: Prof George Jackson and Erich Müller
Start date: June 2010
Finish date: June 2014

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 2014

Mithila Manage
An Investigation into the Feasibility of Integrating Intermediate-Temperature Solid Oxide Electrolysers with Power Plants
Supervisor: Dr Eva Sørensen
Start date: September 2009
Finish date: September 2014

Nikiforos Maragkos
Novel Design Methods with Composites
Supervisor: Prof Efstratios Pistikopoulos
Start date: October 2009
Finish date: June 2014

Jan Marzinek
Molecular Dynamics and Dissipative Particle Dynamics Modelling of Surfactant/Polymer Self Assembly
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: October 2010
Finish date: April 2014

Kristian Mc Caul
A Multiscale and Multiphysics Modelling Framework for Processes Involved in Production of Fuels from Lignocelluloses
Supervisors: Prof Nilay Shah and Dr Cleo Kontoravdi
Start date: September 2013
Finish date: August 2016

Ali Mehdizadeh
Supply Chain Optimisation
Supervisor: Prof Nilay Shah
Start date: October 2009
Finish date: December 2013

Hadjiyiannis Michael
Robust Control and Optimisation
Supervisor: Dr Daniel Kuhn
Start date: October 2009
Finish date: March 2014

Nur Amirah Izzati Mohd Noor
Industrial Smart Grid
Supervisor: Prof Nina Thornhill
Start date: September 2013
Finish date: September 2016

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: December 2013

Dimitrios Nerantzis
Deterministic Global Optimisation Techniques
Supervisor: Prof Claire Adjiman
Start date: September 2012
Finish date: September 2015

Candy Ng
Optimum Design, Operation and Control of Sequential Multi-column Chromatography for Separation of Biomolecules
Supervisor: Dr Eva Sørensen
Start date: September 2008
Finish date: September 2014

Andreas Nikolaou
Optimal Design and Operation of Biological Processes to Deliver Multiple Energy Vectors
Supervisor: Dr Benoit Chachuat
Start date: November 2011
Finish date: November 2014

Richard Oberdieck
Development and Application of New Algorithms for the Solution of Multiparametric Mixed Integer Quadratic Programming Problems
Supervisor: Prof Efstratios Pistikopoulos
Start date: September 2013
Finish date: January 2015

Donald O'Donoghue
Mathematical Modelling of Ion Transport in Healthy and Cystic Fibrosis Human Airway Epithelia
Supervisor: Dr Vivek Dua
Start date: September 2010
Finish date: October 2014

Hui Lin Bernice Oh
Bioengineering
Supervisor: Prof Athanasios Mantalaris
Start date: November 2009
Finish date: May 2014

Funmilayo Olabode
Parameter Estimation Using Neural Networks
Supervisor: Dr Vivek Dua
Start date: January 2014
Finish date: January 2021

Silvia Padula
Capacity Planning for Water Supply Networks
Supervisor: Prof Lazaros Papageorgiou
Start date: September 2009
Finish date: August 2013

Antonio Marco Pantaleo
Process Systems Engineering, Chemical Engineering
Supervisor: Prof Nilay Shah
Start date: May 2008
Finish date: May 2014

Maria Papathanasiou
Mammalian Cells Bioprocessing
Supervisors: Prof Efstratios Pistikopoulos and Prof Athanasios Mantalaris
Start date: November 2012
Finish date: November 2014

Olga Parkes
A Quantitative Methodology to Enhance the Sustainability Performance of Major International Events
Supervisor: Prof David Bogle
Start date: October 2010
Finish date: May 2014

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

Cheng Peng
Physical and Chemical Properties of Brine-CO2-Mineral Systems
Supervisor: Prof Geoffrey Maitland
Start date: October 2011
Finish date: September 2014

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 Benoit 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

Ana Luz Quiroga Campano
Mammalian Cell Bioprocessing
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: October 2012
Finish date: October 2015

Sadia Rahman
Molecular Simulation of Ionic Surfactants
Supervisors: Prof Erich Müller, Prof Amparo Galindo and Prof George Jackson
Start date: September 2012
Finish date: August 2015

Jai Rajyaguru
Global Optimization of Transient Chemical and Biochemical Processes
Supervisor: Dr Benoit Chachuat
Start date: October 2011
Finish date: September 2014

Tom Ravalde
Highly-Integrated Urban Resource Systems
Supervisor: Dr James Keirstead
Start date: October 2012
Finish date: September 2015

Krisztian Ronaszegi
Water Splitting for Hydrogen Production for Use in Dwellings
Supervisor: Prof Eric Fraga
Start date: May 2011
Finish date: September 2014

Daniel Ross
Multi-Scale Simulation of the Transport of Hydrocarbons in Porous Engine Deposits
Supervisor: Dr Edo Boek
Start date: October 2012
Finish date: September 2015

Luong Ryan
Optimisation Algorithms for Image Processing
Supervisors: Prof Berc Rustem and Dr Panos Parpas
Start date: October 2009
Finish date: March 2014

Howe Sei
Asymptotically Optimal Aggregation of Large-Scale Dynamic Networks
Supervisor: Dr Panos Parpas
Start date: October 2012
Finish date: September 2016

Christine Seifried
Reactive Transport of CO2 and Hydrocarbon Reservoir Fluids in Micro-Fluidic and Rheology Experiments for Enhanced Oil Recovery and Carbon Storage
Supervisor: Dr Edo Boek
Start date: May 2012
Finish date: April 2015

Saurabh Mahesh Kumar Shah
Multi-Scale Pore Imaging of Multiphase Flow in Porous Media
Supervisor: Dr Edo Boek
Start date: January 2011
Finish date: February 2015

Cyrus Siganporia
Production Planning for Biopharmacicals
Supervisor: Prof Lazaros Papageorgiou
Start date: September 2010
Finish date: February 2015

Roochi Solanki
Novel Thermally-Powered Pumping Devices for Low Grade Heat Integration
Supervisor: Prof Amparo Galindo
Start date: October 2009
Finish date: February 2015

Si Nga Sou
Development of a Computational Tool for Predicting the Impact of Bioprocess Conditions on Protein Glycosylation
Supervisor: Dr Cleo Kontoravdi
Start date: October 2011
Finish date: February 2015

Ioanna Chrysoula Stefani
A Framework for Understanding the Link between ER Stress and Alzheimer's Disease
Supervisor: Dr Cleo Kontoravdi
Start date: October 2010
Finish date: February 2015

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: February 2015

Thapanar Suwanmajo
Mathematical Modelling for Biotechnology
Supervisor: Dr Jawahar Krishnan
Start date: October 2010
Finish date: February 2015

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: February 2015

Naveed Tariq
Dynamic Modelling of Power Plants and CCS
Supervisor: Prof Nilay Shah
Start date: October 2012
Finish date: February 2015

Ailing Teo
Chemical and Biomolecular Engineering
Supervisor: Prof Athanasios Mantalaris
Start date: November 2009
Finish date: February 2015

Quang Tran
Sampling Algorithms for Stochastic Programming Using Importance Sampling and Markov Chain Monte Carlo
Supervisors: Prof Berc Rustem and Panos Parpas
Start date: October 2011
Finish date: February 2015

Cristian Triana
Heat Integration for Bioethanol Processes
Supervisors: Prof Eric Fraga and Dr Eva Sørensen
Start date: October 2011
Finish date: September 2014

Argyro Tsipa
Closing the Loop, From in Silico to in Vivo; Modeling and Optimisation of Bacterial Cell Culture Systems
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: September 2011
Finish date: December 2014

Chonlatep Usaku
Modelling of Mammalian Cell Bioprocesses
Supervisors: Prof Athanasios Mantalaris and Prof Efstratios Pistikopoulos
Start date: October 2010
Finish date: June 2014

Hovhannisyan Vahan
Multilevel Algorithms for Big Data
Supervisor: Dr Panos Parpas
Start date: October 2013
Finish date: September 2017

Rallia-Iliana Velliou
Computer Simulation of Thermodynamic Properties of Solids from ab initio Potentials
Supervisors: Prof Claire Adjiman and Prof Amparo Galindo
Start date: October 2012
Finish date: September 2015

Mario Villanueva
Global Optimization Methodology for Uncertain Dynamic Processes
Supervisor: Dr Benoit Chachuat
Start date: October 2011
Finish date: September 2014

Avagyan Vitali
Optimisation and Energy Systems Engineering
Supervisors: Prof Berc Rustem and Dr Panos Parpas
Start date: October 2012
Finish date: March 2016

Roitch Vladimir
Optimisation Applied to Cloud Computing
Supervisor: Dr Daniel Kuhn
Start date: October 2010
Finish date: September 2014

Carmen Wouters
Micro-grid Integration with Regulatory Constraints
Supervisor: Prof Eric Fraga
Start date: February 2013
Finish date: January 2016

Dionysios Xenos
ENERGY-SMARTOPS
Supervisor: Prof Nina Thornhill
Start date: September 2011
Finish date: September 2014

Lingjian Yang
Data Analysis Using Optimisation Techniques
Supervisor: Prof Lazaros Papageorgiou
Start date: September 2011
Finish date: March 2015

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 Zamorano Mosnaim
Bone Tissue Engineering
Supervisor: Prof Athanasios Mantalaris
Start date: January 2012
Finish date: January /2015

Stamatina Zavitsanou
Modeling and Multi Parametric Control Drug Delivery Systems for Diabetes Type 1
Supervisor: Prof Efstratios Pistikopoulos
Start date: December 2009
Finish date: December 2014

PhD Graduates
Professor I. David L. Bogle

"We aim to give our PhD students the best possible research training experience through supervision by our team of international Process Systems research leaders, collaboration with industry, training in all the skills needed for a research career, exposure to the full range of topics in Process Systems Engineering, and building networks within the Centre and our collaborators that will last them for their whole career."

PhD Graduates
2012–2013 CPSE Annual Report

Dr Ozlem Akgul
Supervisors: Dr L.G Papageorgiou and Prof N Shah
Title of Thesis: *Optimisation of bioenergy supply chains*
Employer: Baringa

Dr Hala Al Fulaij
Supervisor: Prof D Bogle
Title of Thesis: *Dynamic modelling and control of multi stage flash (MSF) desalination plant*
Employer: University of Kuwait

Dr Tareg Al Soudani
Supervisor: Prof D Bogle
Title of Thesis: *Multiscale modelling for operation and control of PSA units*
Employer: Honeywell (Saudi Arabia)

Dr Sheila MC Ang (Samsatli)
Supervisors: Prof E Fraga and Dr D Brett (UCL Chemical Engineering)
Title of Thesis: *Optimal design of fuel cell systems*
Employer: Imperial College London

Dr Charles Brand
Supervisors: Prof. C.S Adjiman, Prof A Galindo and Prof G Jackson
Title of Thesis: *CO2 capture using monoethanolamine solutions: Development and validation of a process model based on the SAFT-VR equation of state*
Employer: Process Systems Enterprise

Dr Ning Chen
Supervisors: Dr C Kontoravdi and Dr C Jaques (Lonza Biologics)
Title of Thesis: *Modelling of protein-producing Chinese hamster ovaries cells*
Employer: Assistant Research Fellow at Beijing Genomics Institute, Shenzhen

Dr Edward Close
Supervisors: Dr E Sorensen and Dr D Bracewell (UCL)
Title of Thesis: *Process modelling approaches to biological complexity in the production of therapeutic proteins*
Employer: Process Systems Enterprise

Dr Simon Dufal
Supervisors: Dr A Galindo and Prof G Jackson
Title of Thesis: *Development and application of advanced thermodynamic molecular description for complex reservoir fluids containing carbon dioxide and brines*
Employer: Imperial College London

Dr Iliana Fauzi
Supervisor: Prof A Mantalaris
Title of Thesis: *Differentiation of murine embryonic cells towards the haematopoietic cell lineage using the HepG2 conditioned medium and encapsulation in a rotating wall vessel bioreactor*
Employer: Imperial College London

Dr Ioscani Jimenez del Val
Supervisor: Dr C Kontoravdi
Title of Thesis: *Assessment of the interactions between bioprocess conditions and protein glycosylation in antibody-producing mammalian cell cultures*
Employer: Imperial College London

Dr Waqas Ikram
Supervisor: Prof N.F Thornhill
Thesis of Thesis: *Plant-wide and wireless process control and automation*
Employer: ABB Process Automation, Oil, Gas, and Petrochemicals, Oslo, Norway

Dr Oluwatope Ebenezer Iyun
Supervisor: Prof N.F Thornhill
Title of Thesis: *Plant-wide diagnosis: cause-and-effect analysis using process connectivity and directionality Information*
Employer: ExxonMobil Corporation in the USA

Dr Cheng Seong Khor
Supervisors: Prof N Shah and Dr B Chachuat
Title of thesis: *Optimization of water network systems synthesis and design*
Employer: Petronas

Dr Alexandros Kiparissides
Supervisors: Prof E.N Pistikopolus and Dr S Mantalaris
Title of Thesis: *Development of a combined mathematical and experimental framework for the control and optimisation of mammolian cell cultures*
Employer: EPFL

Dr Xuesong Li
Supervisors: Professors M Trusler and G Maitland
Title of Thesis: *Interfacial properties of reservoir fluids and rocks*
Employer: Shell, Rijswijk, Netherlands

Dr Cong Liu
Supervisor: Dr Krishnan
Title of Thesis: *A systems-based bottom-up mathematical modelling framework for investigating the effect of drugs on solid tumours*
Employer: Imperial College London

Dr Songsong Liu
Supervisor: Dr L.G Papageorgiou
Title of Thesis: *Optimisation for the process industry*
Employer: University College London

Dr Mark McBride-Wright
Supervisors: Professors M Trusler and G Maitland
Title of Thesis: *Viscosity and density of aqueous fluids with carbon dioxide*
Employer: Granherne-KBR, UK

Dr Candy Ng
Supervisors: Dr E Sorensen and Dr D Bracewell (UCL)
Title of Thesis: *Optimal design, operation and control of continuous separation of biomolecules*
Employer: Novasep, France

Dr Christos Panos
Supervisor: Prof E.N Pistikopoulos
Title of Thesis: *Modelling and explicit/multi-parametric model predictive control (mp-MPC) of PEM fuel cell systems*
Employer: INVISTA

Dr Idtisak Paopo
Supervisors: Dr S Mantalaris and Dr Xu
Title of Thesis: *Design and modelling of the airlift bioreactor for stem cell bioprocessing*
Employer: Moved to Thailand

Dr Vasileios Papaioannou
Supervisors: Prof. C.S Adjiman, Prof A Galindo and Prof G Jackson
Title of Thesis: *A molecular-based group contribution equation of state for the description of fluid phase behaviour and thermodynamic derivative properties of mixtures (SAFT-γ Mie)*
Employer: Imperial College London

Dr Nina Soraya Ramrattan
Supervisors: Dr A Galindo and Dr E Muller
Title of Thesis: *Molecular models for the description of solid-fluid behaviour of chain-like molecules*
Employer: Det Norske Veritas (DNV)

Dr Kate Elisabeth Royle
Supervisors: Dr D Leak (Department of Life Sciences) and Dr C Kontoravdi
Title of Thesis: *Modelling as a guide to improving Pichia pastoris protein production*
Employer: Imperial College London

Dr Daniel Seaton
Supervisor: Dr Krishnan
Title of Thesis: *Mathematical modelling and systems analysis of signalling networks and the budding yeast cell cycle*
Employer: University of Edinburgh

Dr Mahdi Sharifzadeh
Supervisor: Prof N.F Thornhill
Title of Thesis: *Integrated design and control with a focus on control structures*
Employer: Imperial College London

Dr Danlu Tong
Supervisors: Professors M Trusler, G Maitland and Dr P Fennell
Title of Thesis: *Development of Advanced Amine Systems with Accurate Vapour-Liquid Equilibrium Measurements*
Employer: BP, Pangbourne, UK

Dr Manolis Vasileiadis
Supervisors: Prof C.S Adjiman and Prof C.C Pantelides
Title of Thesis: *Calculation of the free energy of crystalline solids*
Employer: Imperial College London

Dr Liang Wu
Supervisors: Prof G Jackson and Dr E Muller
Title of Thesis: *Modelling ordering in fluid mixtures*
Employer: Nanjing University of Technology, Nanjing 210009, PR China

Dr Di Zhang
Supervisor: Dr L.G Papageorgiou
Title of Thesis: *Optimal design and planning of energy microgrids*
Employer: University College London

Notes

Notes

Centre for
Process
Systems
Engineering

Centre for Process Systems Engineering (CPSE), Imperial College London, Roderic Hill Building, South Kensington Campus, London SW7 2AZ, Email: cpse@imperial.ac.uk, Phone: +44 (0)207 594 6605/11,
http://www3.imperial.ac.uk/centreforprocesssystemsengineering