Centre for
Process
Systems
Engineering

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Centre for Process Systems Engineering | Annual Report 2010 – 2011

Imperial College London | UCL

CPSE | Contents

Profile

The Centre for Process Systems Engineering (CPSE) is a multi-institutional research centre inaugurated in August 1989. It involves Imperial College London and University College London, and is based at Imperial College London.

The Centre is an international research leader in Process Systems Engineering. It is a subject that encompasses the management of complexity in uncertain systems, modelled across many time and scale lengths. Process Engineers are concerned with systems involving physical and chemical change and aim to manage complexity in such systems.

Process Systems Engineering is the study of approaches to analysis and design of complex process engineering systems and the development of tools and techniques required for this. These tools enable Process Systems Engineers to systematically develop products and processes across a wide range of systems involving chemical and physical change: from molecular and genetic phenomena, to manufacturing processes and related business processes.

The Centre is dedicated to research and to the development of integrated models, methodologies and tools to exploit complex, multi-scaled physical, engineering and industrial systems through:

- Requirements and functional analysis
- Modelling and design
- Simulation
- Optimisation
- Experimentation
- Visualisation

Our research is relevant to a range of industries including the oil and gas, petrochemicals, pharmaceuticals, fine chemicals, polymers, food and beverage and consumer sectors.

Introduction

The Centre for Process Systems Engineering is a unique multi-institutional research Centre which focuses on the development and application of model-based methods for analysis and optimisation of material and energy conversion processes.

We have 22 academic staff from multi-disciplinary backgrounds, including mathematics, physics, chemistry and engineering. Our academic staff's diverse disciplines, coupled with their renowned international reputations has enabled the Centre to attract grants worth more than £20 million, 98 exceptional PhD students and 17 high calibre research fellows and associates.

CPSE History

CPSE has a distinguished history. It was inaugurated in 1989 by Professor Roger WH Sargent, the founding Director of the Centre from 1989 to his retirement in 1992. Professor Sargent is credited for playing a unique role in shaping the future of systems engineering research. Since Professor Sargent established the Centre over 21 years ago, CPSE has continued his legacy and remains a Centre of Excellence. The Centre's outstanding record has been recognized by many awards. An example is in 2007, Process Systems Enterprise Limited, a spin-out from Centre for Process Systems Engineering received Royal Academy of Engineering MacRobert Award for its cutting-edge mathematical modelling systems developed to help make chemical plants safer and more efficient. The MacRobert Award is the UK's highest award for innovation in engineering and it recognized PSE's highly innovative modelling software gPROMS, which to date remains "the leading modelling product within the chemical industry". Previous winners of this prestigious Award, include IBM, Rolls Royce and BP International.

Professor Nilay Shah, CPSE Director

Recent examples of research include the optimal **selection of reaction media** using quantum mechanical calculation, the dynamic modelling and control of **multi-stage flash desalination plant**, the design and operational optimisation of **carbon capture technology**, the development of an advanced system for **sequential multicolumn chromatography**, the development of models for **complex glycolysation processes** and multi-scale modelling to optimise the control of pressure **swing adsorption processes**.

Explicit /multiparametric modelling has recently been applied to manage the performance of items as diverse as **unmanned air vehicles** and **fuel cell systems** and CPSE's wide area measurement system has grown into a major **process automation** activity.

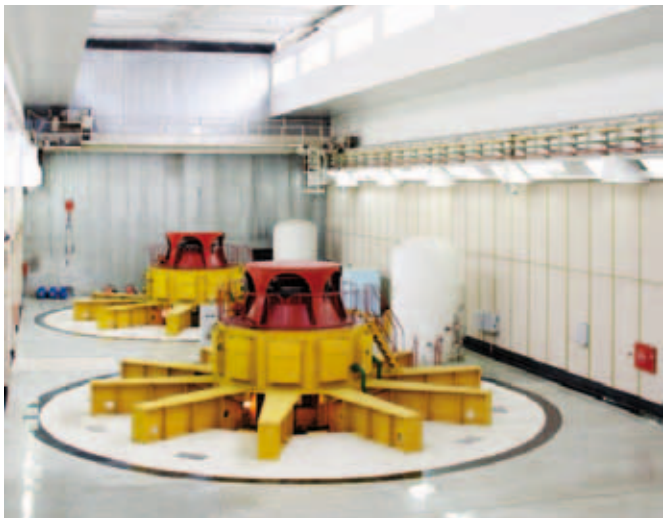
CPSE has a successful biological systems engineering programme which focuses on the application of model based tools for the analysis and optimisation of **bacterial and mammalian cell culture** systems. This has led to significant advances in **synthetic biology and biomedical engineering**.

At the macro end of the size scale CPSE has made significant advances in modelling **healthcare systems, biomass and bioethanol supply chains and vehicle emissions**. Growing interest in energy systems has enabled CPSE to create a leading research programme in modelling and optimising **urban energy systems, polygeneration, energy systems for buildings and bioenenergy conversion processes and distribution**.

The Research programme 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

The diverse research projects undertaken in the Centre has lead to numerous collaborations with UK Research Councils, UK and International industry, the European Commission and other funding bodies. The Centre fosters the collaboration further, through the Industrial Consortium which 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. The CPSE Consortium has continued to grow, and this year Praxair became our newest member. Praxair is a global Fortune 300 company that supplies atmospheric, process and specialty gases, high-performance coatings, and related services and technologies. You can find out more about our Industrial Consortium later in this report. Companies and organisations wishing to learn more about the membership benefits can contact me, Professor Nilay Shah at: **n.shah@imperial.ac.uk.**



Research Income

The Centre's cutting-edge research requires significant funding. With the current world financial turmoil, funding for research has decreased considerably and this has resulted in increased competition. Despite this, the Centre's academic staff managed to secure major grants and the Centre's income has increased significantly. Research income has risen to over £5 million each year with substantial funding being provided by the UK Research Councils, the European Union, industry and overseas governments. We now have a portfolio of grants worth more than £20 million. This higher level of funding indicates the growing importance attached to PSE issues and the outstanding work that is carried out in the Centre.

Highlights of 2010–2011

It is with great pleasure that I highlight some of the CPSE staff's activities during 2010–2011.

New Academic Members

The Centre has two new academic staff. Dr Benoit Chachuat, Senior Lecturer in Chemical Engineering joined us from McMaster University, ON, Canada. Dr Edo Boek, Senior Lecturer was at Schlumberger Cambridge Research before he joined Imperial.

Academic Promotions

Four CPSE academics received promotions: Sakis Mantalaris, Claire Adjiman and Amparo Galindo were promoted to Professor. Professor Stratos Pistikopoulos is now Director of Research for the Department.

High Profile Conferences and Events

Our academic staff have been busy organising high profile conferences: Professor Stratos Pistikopoulos co-organised the 21st European Symposium on Computer-Aided Process Engineering (ESCAPE-21) conference which was held in Greece in June 2011. In addition, Professor David Bogle is co-organising the ESCAPE-22 due to take place at University College London in June 2012. The conference will explore how computer aided process engineering (CAPE) plays a key design and operations role in the process industries.

Each year, the Centre hosts the Annual Professor Roger W.H. Sargent Lecture as a tribute to Professor Roger Sargent's vision, leadership, significant technical contributions and to his legacy in the field of Process Systems Engineering. The distinguished speakers who delivered the Lectures in 2010, were Professor Michael F. Doherty University of California, Santa Barbara and in 2011, Professor Lorenz T. Biegler, Carnegie Mellon University.

Honours and Awards

The Centre's staff and students received several awards. The Centre's Molecular Systems Engineering group were awarded the Research Excellence Award along with £150k. The group were given this award at the post-graduate graduation ceremony on 5 May 2010. Team leader: Professor George Jackson, Dr Claire Adjiman, Dr Amparo Galindo, Dr Erich A Muller, Professor Costas Pantelides, Prof Stratos Pistikopoulos, Dr Carlos Avendano, Dr Andrew J Haslam, Dr Panagiotis Karamertzanis, Dr Thomas Lafitte,

Dr Felix Llovell, Dr Alexandr Malijevsky, Dr Henricus H Wensink.The Research Excellence Awards Scheme rewards research teams that have demonstrated high academic achievement and have significant future potential.

Professor Geoff Maitland was awarded the 2010 Chemical Engineering Envoy of the Year by iChemE at their annual gala dinner on 4th November 2010, in recognition of his excellent work representing Chemical Engineers during the recent BP/Gulf of Mexico affair.

Professor Claire Adjiman was awarded a Leadership Fellowship from the EPSRC. She was one of 7 people at Imperial to receive this prestigious award, totalling more than £6 million. The Fellowships run for up to five years and aims to help academics develop into international research leaders who can set and drive new research agendas. Professor Adjiman was also awarded the Henry E. Armstrong Memorial Lecture by the Society of Chemical Industry.

PhD student Ioscani Jimenez del Val won the best poster award at the 2010 Annual bioProcessUK Conference for his work on the development of a mathematical model for monoclonal antibody glycosylation in maturing golgi cisternae.

Professor Sakis Mantalaris was elected to the College of Fellows of the American Institute for Medical and Biological Engineering (AIMBE). The College of Fellows has 1,000 individuals who are outstanding bioengineers in academia, industry and government. These leaders in the field have distinguished themselves through their contributions in research, industrial practice and/or education. Fellows are nominated each year by their peers and represent the top 2% of the medical and biological engineering community.

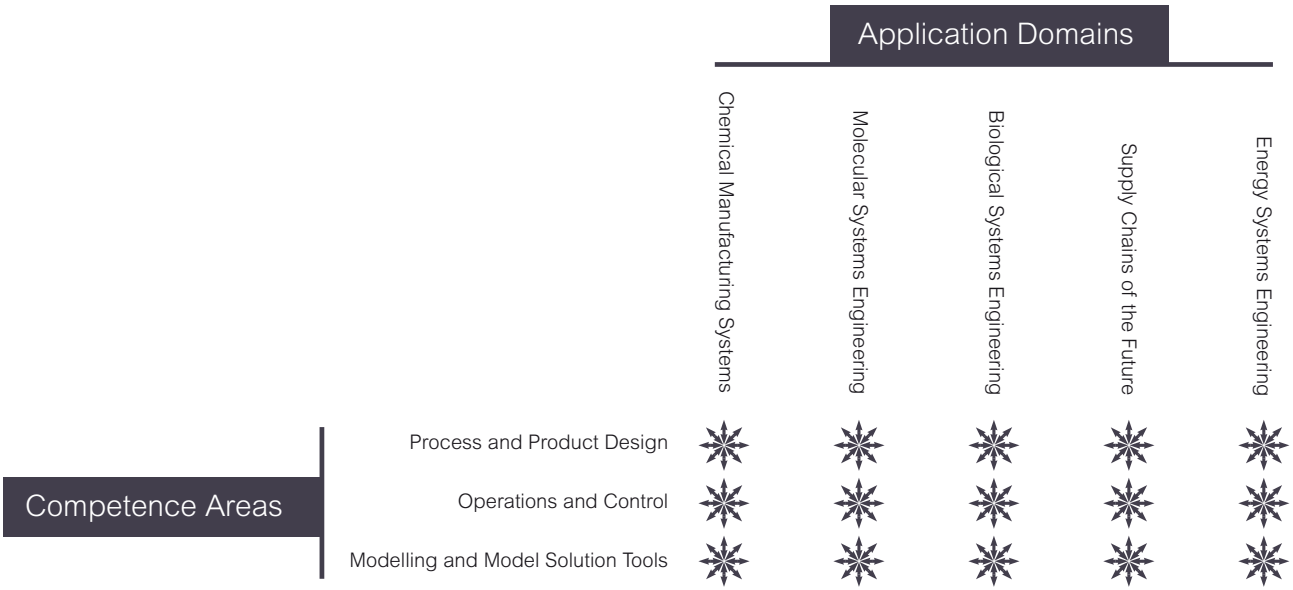
Professor Costas Pantelides was elected a Fellow of the Royal Academy of Engineering. Royal Academy of Engineering is Britain's national academy for engineering and brings together the country's most eminent engineers from all disciplines to promote excellence in the science, art and practice of engineering.

It is with pleasure that I conclude my introduction of the CPSE 2010–2011 Annual Report. I am confident that you will find much of interest in our report. You can also find out more about the Centre from our website:

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

Professor Nilay Shah
Director, Centre for Process Systems Engineering

Research Programme



CPSE Industrial Consortium

Since its inauguration, the Centre has given high priority to fostering interaction between academics and industry and this was the basis for setting up the Industrial Consortium.

The Consortium 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. It also assists the Centre in keeping fully up to date with business issues and priorities in Process Systems Engineering.

Benefits for Members

Members have privileged access to CPSE academic and research staff and students and 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
- There is also a Spring workshop devoted to a specific topic of interest to members.
- 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 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 material, 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:

ABB Corporate Research Professor Nina F Thornhill
Bristol-Myers Squibb Professor Amparo Galindo
BP Professor Nilay Shah
Petrobras Professor David Bogle
Praxair Professor Claire Adjiman
PSE Professor Costas C Pantelides
Proctor and Gamble Professor George Jackson
Shell Research and Technology Professor Geoffrey C Maitland
Syngenta Professor Claire Adjiman

In addition to the member companies, CPSE has strong links and research collaborations with a number of other companies and research organisations. Research income has risen to about £5 million each year with substantial funding being provided by the UK Research Councils, the European Union, industry and overseas governments. This higher level of funding indicates the growing importance attached to PSE issues. Member companies have access to and benefit from the research work performed in the Centre. Companies and organisations wishing to join the CPSE Consortium should contact the CPSE Director, Professor Nilay Shah at **n.shah@imperial.ac.uk**

Competence Areas

Competence Area | Product and Process Design

The central objective of our research within the Product and Process Design competence area is to develop systematic model-based methodologies for the rational design of processes and products. It 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

Systematic methodologies for modeling and optimization of chromatographic processes

In collaboration with different industrial partners and the Department of Biochemical Engineering at UCL, we are considering strategies for efficient modeling of chromatographic bio-separations for advanced process development and manufacturing support. Our focus is on model development from an industrial perspective. Therefore, it is important to consider the limited material available and tight time constraints associated with simultaneously developing the purification processes of multiple candidate molecules.

As an example, we have developed a detailed model of a key purification step in the production of a commercial therapeutic protein with annual revenue of over $700 million.

We have minimized the experimental and computational effort required to develop the model by utilizing high throughput micro-well experimentation on a robotic platform. Using this technique we can rapidly generate targeted experimental data required for parameter estimation within our industrial constraints. We have also considered resin fouling and ageing over a column's lifecycle using confocal laser scanning microscopy, substantiated with column and batch binding experimentation to enable us to predict mass transfer as fouling progresses. One of our main objectives is to consider potential applications of the models in a Quality by Design (QbD) paradigm, and we are able to determine the multidimensional combination and interaction of input variables and process parameters that provide assurance of product quality.

We have also considered integrated experimental and modeling approaches for the efficient design and control of chromatographic processes, such as antibody capture by protein A chromatography. Advanced control strategies for continuous multi-column operation have also been developed and verified.

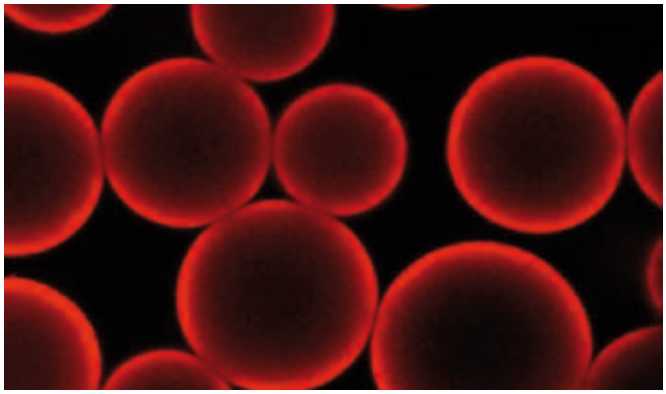


Figure 1. Confocal image of resin particles

Operation and control of bioethanol production

A new initiative is within ethanol production from lignocellulosic biomass. Bioethanol has been widely investigated, but with limited commercial application to date, as a potential substitute for fossil fuels in order to reduce the "green house" effect caused by their toxic emissions following combustion. The objective of this project is to develop a dynamic modelling framework for bioethanol production from lignocellulosic material, and with this, to evaluate optimal process operation with particular emphasis on pre-treatment alternatives, separation method alternatives and heat integration options. The analysis will be extended to other metabolites for both fuel and biochemicals production.

Development and validation of models of CO_2 capture processes – from molecules to processes

Carbon dioxide (CO_2) emissions are largely considered to play a major role in climate change and particularly in global warming. Fossil fuel power plants are the major fixed point-source emitters of CO_2. In order to abate global warming, the UK Committee on Climate Change suggested reducing the emission from 500 gCO_2/kWh to 100 gCO_2/kWh in the electricity sector by 2050. In this context, the development of carbon capture systems is a necessity that must be addressed in the short term and amine-based post-combustion capture processes are seen as the most promising technology in terms of development and applicability. The major advantage of this technology is that it can be retrofitted to existing power plants.

There are, however, several concerns with this technology, including large energy requirements, solvent degradation, and the environmental and health impact that may result from solvent leaks and solvent degradation products. Modelling studies can play an invaluable role in addressing some of these issues, including the choice of solvent and operating conditions that yield optimal performance.

A key challenge is to develop models that can accurately predict the behaviour of the process under different conditions, including for different solvents. We address this challenge by developing a model of the CO_2 absorber that incorporates an advanced thermodynamic model of the physical properties and reactions into a rate-based process model. We use a version of the statistical associating fluid theory (SAFT), SAFT-VR, to model the complex physico-chemical interactions between CO_2 and the solvent. Based on the assumption that the process is mass-transfer limited, and that the reactions can therefore be considered to reach equilibrium, we model an absorber. We obtain a diffusion coefficient for the carbamate complex from one pilot plant run, and validate the absorber model using a number of other runs.

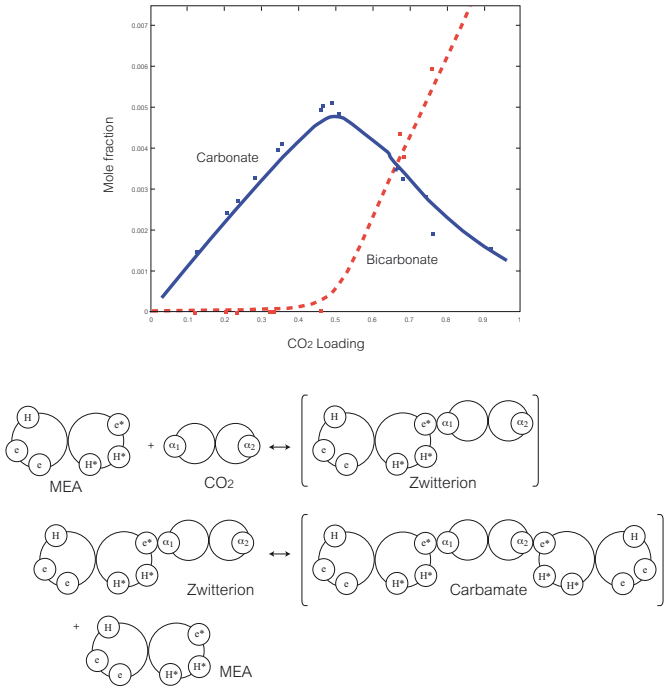


Figure 2. Schematic of the reaction mechanism captured within the SAFT thermodynamic framework for CO_2 and monoethanolamine (MEA). This results in the prediction of the speciation shown in the top figure, in excellent agreement with experimental data from Jou et al (1995) and Böttinger et al (2008).

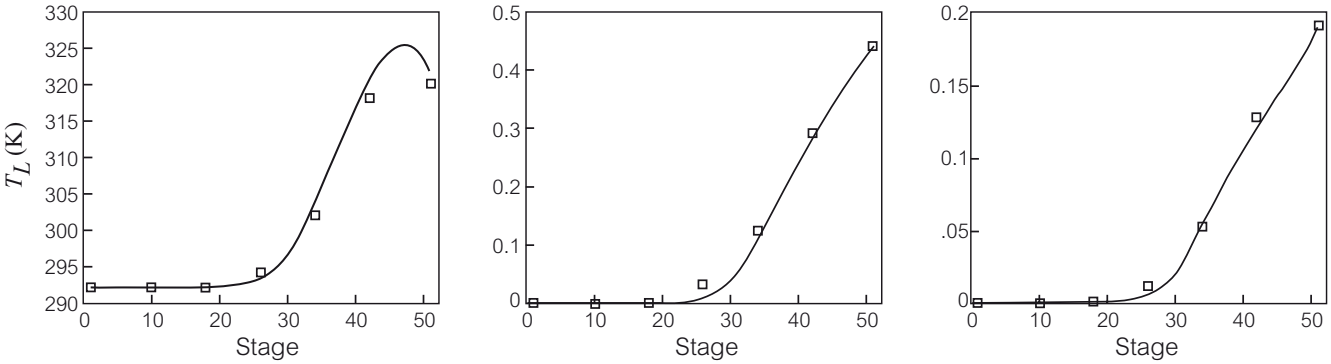


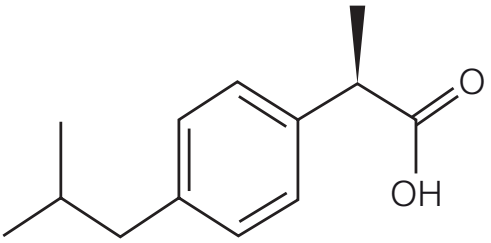
Figure 3. Model predictions (lines) and pilot plant data from Tontiwachwuthikul et al (1992), for liquid temperature, CO_2 loading in the liquid phase and gas phase CO_2 mole fraction as a function of column stage

The design of optimal solvent mixtures

The design of mixtures is an important and challenging problem with numerous industrial applications. Of particular interest are applications in separation processes, such as liquid-liquid extraction, which require suitable solvents to meet given specifications. Solvents are also used in chemical reactions to enhance the reaction rate and in product design as constituents of the final product formulations. However, the choice of solvents can have a significant impact on the performance of most processes as seen in crystallisation, where undesired crystal morphology can arise in some solvents, resulting in difficulties in the downstream processing and even in decreases in product performance for the case of drug manufacturing. Furthermore, solvent mixtures are particularly desirable as they are known to achieve higher performance over pure solvents. Hence, there is a need for a systematic approach to find optimal solvent mixtures.

Computer Aided Mixture Design (CAM^{b}D, where b stands for "blend") has been used in various forms to determine the optimal solvent mixture. CAM^{b}D methods generally use Mixed Integer Non-Linear Programming (MINLP) techniques to model the discrete decisions inherent in the solvent design problem. However, in most existing formulations, the number of components in the mixture is predetermined and the identities of all but one of the mixture constituents are known a priori. Furthermore, modelling processes directly as MINLP problems can lead to severe numerical singularities for cases involving complex property models and a large combinatorial space.

In this project, we formulate the optimal mixture design problem using Generalised Disjunctive Programming (GDP) as proposed by Grossmann and coworkers. GDP is a logic-based method, thus offering a natural way to formulate the discrete choices in an optimisation problem. It has proved very successful in the design of complex processing networks but has not yet been applied to molecular design. We follow a systematic approach to developing GDP formulations for CAMbD, considering increasingly complex problems: we start with mixtures with a fixed number of components and progress to optimise both the number of components in the mixture as well as the components themselves. In particular, in solid-liquid and liquid-liquid equilibrium applications we select N solvents from a list, where N is either fixed or it can vary. In the former case, disjunctions are required for each solvent molecule in the mixture, while in the latter case, disjunctions are required for the number of solvents and for the choice of solvents. The relevant solubility model equations are integrated within the disjunctions. Thus, numerical difficulties arising from the presence/absence of specific components can be avoided. The application of this approach to the identification of optimal solvent blends for solid-liquid and liquid-liquid equilibrium has clearly demonstrated the benefits of such an approach and the performance enhancements that can be achieved.



	X_{ibu}	S1	X_{s1}	S2	X_{s2}	S3	X_{s3}
N=1	0.3180	$CHCl_3$	0.6820				
N=2	0.3338	$CHCl_3$	0.5229	CH_3OH	0.1432		
N=3	0.3331	$CHCl_3$	0.5200	CH_3OH	0.1369	C_2H_5OH	0.01
N≤4	0.3338	$CHCl_3$	0.5229	CH_3OH	0.1432		

Figure 4. Identification of optimal solvent blends for ibuprofen

Synthesis of biorefinery treatment plants for energy and nutrient recovery

Processing organic wastes and wastewater together in a single biorefinery treatment plant offers many benefits and might also have a profound impact on the structure and the approach of conventional depollution strategies. Apart from the effective treatment of waste/wastewater, a highly valuable product can be produced such as methane, biofuels, phosphorus, nitrogen and heavy metals. The use of recycled waste streams also presents the additional benefit of reducing the raw material requirement, again reducing costs. Quite clearly, the ultimate goal is a closed-cycle process, where all waste streams are recycled and the only output is saleable/valuable product. This project aims to develop and apply a systematic, model-

based methodology for the synthesis of biorefinery treatment plants that are both economically attractive and sustainable. The main objective is to assess the merits and viability of such integrated concepts using this methodology. A superstructure modelling approach is considered, which can account for a large number of promising treatment and separation technologies (units) along with all feasible interconnections between them. The optimization objective is to determine the process configuration (unit types, interconnections and flows) that maximizes the net present value over the project lifetime (based on capital and operating costs and revenues from energy/product sales). Constraints are also imposed for the treated effluent to comply with local or federal regulations. This approach leads to MINLP models that can be implemented and solved for global optimality, e.g., with the optimization solvers available in GAMS. Pivotal to the success of this methodology is the development/selection of mathematical models for the units that are simple enough, yet provide reliable estimates of their performance and capital/operating costs. This is especially challenging for the biological treatment units since the available models typically carry a significant uncertainty. As a first approximation, commercial wastewater treatment simulators have been used to derive simple response surface models for performance prediction as well as for costing.

The results of a case study are shown in the figure. Here, a biorefinery treatment plant fed with 100 m3/h of tequila vinasse (100 gCOD/L, 8 gTSS/L, 120 mgN/L and 700 mgP/L) is synthesized based on a small superstructure that consists of 3 biological treatment units (UASB, SAMBR, activated sludge), 1 filtration unit (sand filter), and 2 nutrient recovery units (struvite crystallizer, zeolite adsorber). Maximum allowable limits are enforced for these concentrations, in agreement with current Mexican regulations. The model recommends the installation of submerged anaerobic membrane bioreactors (SAMBRs) that enable large COD concentration abatement and biogas production. It then recommends to further process part of the SAMBR outlet in struvite crystallizers (36%) and sand filters (37%), the remaining fraction (26%) being discharged without further treatment. A positive NPV is achieved in this scenario, which is mostly due to the sales of electricity from biogas and, to a lesser extent, the sales of struvite fertilizers. Alternative process configurations have also been obtained in different scenarios (feed flowrate and concentrations, looser discharge regulations).

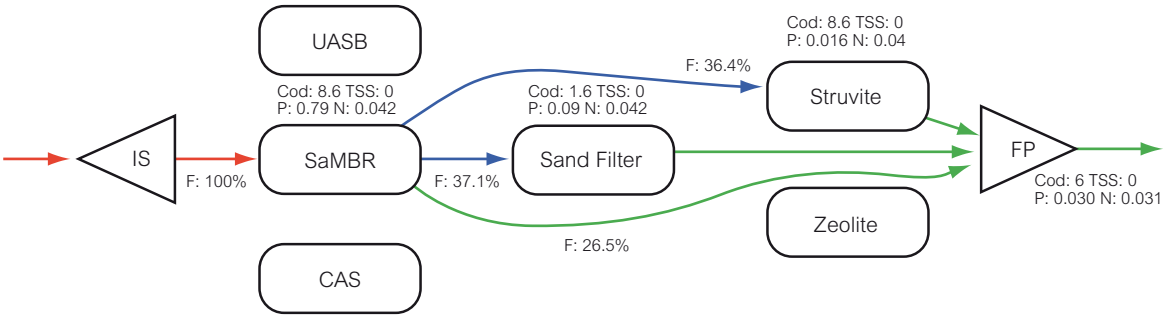
Dynamic modelling and control of multi stage flash (MSF) desalination plant

Multistage flash desalination units have the potential to provide energy efficient and flexible water particularly in hot climates. A dynamic model was developed for use in design, control, startup/shutdown and troubleshooting. Lumped parameter dynamic models were developed for the once through (MSF-OT) and the brine circulation (MSF-BC) processes. The model predictions for both MSF-OT and MSF-BC in steady state and dynamic conditions showed good agreement against data from existing MSF plants with an error less than 1.5%. Dynamic analysis was made to study plant performance upon making step variations in system manipulated variables and identify stable operating regimes. Behaviour is consistent with the actual plant data. The demister section has a major effect on performance so the FLUENT software was used to model the MSF demister using different combinations of Eulerian and Lagrangian approaches to model the vapour and brine droplets. A new demister design was made by varying the wire diameter which led to an efficient design with low pressure drop and high separation efficiency. This design was used in the MSF/gPROMS model to predict its effect on the heat transfer area. The new design provided reductions of 3-39% in the condenser heat transfer area without affecting dynamic performance. Since the tubing system accounts for almost 70% of the capital cost, then this would reduce the plant capital cost and product unit cost. The project is now complete although collaborations are on going.

Multiscale modelling for operation and control of PSA units

This dynamic modeling project aims to investigate the optimal control of Pressure Swing Adsorption (PSA) and Pressure Swing Adsorption Reaction (PSAR) processes. The model crosses several length scales. An approach for investigated optimum design and operation of PSA units is being investigated through formulating the problem as a mixed-integer programming problem. The model has a number of discontinuities which cause difficulties to solvers. We have developed an algorithm that eliminates integrator discontinuities through two steps. First, it determines the optimum switch point between two empirical correlations spanning two or more domains.

Figure 5. (below). Optimal biorefinery treatment plant for tequilla vinasse



The optimum switch point is determined through searching for a "jump point" that minimizes discontinuity between results obtained through calculating a parameter using two or more different methods at an intersection or proximity of their validity domains. Second, it links the two adjacent discontinuous domains with an interpolating function.

Refinery-wide optimisation using MIPANN

The oil refining industry mainly uses linear programming (LP) modelling tools for refinery optimisation and planning purposes, on a daily basis. LPs are attractive from the computational time point of view; however these models have limitations such as the nonlinearity of the refinery processes is not taken into account. The main aim of this work is to develop approximate models to replace the rigorous ones providing a good accuracy without compromising the computational time, for refinery optimisation. The data for deriving approximate models has been generated from rigorous process models from a commercial software, which is extensively used in the refining industry. In this work we present novel model reduction techniques based upon optimal configuration of artificial neural networks to derive approximate models and demonstrate how these models can be used for refinery-wide energy optimisation. The key advantage of the MIPANN approach is having reduced models that are easy to implement and maintain for a complex refinery. The usefulness of the proposed approach was demonstrated by using the topping refinery model for feedstock selection, process optimisation and energy minimisation cases. Also, comparison of the proposed approach with LP techniques used in refinery planning models for CDU modelling, has shown a clear advantage of using the proposed model reduction approach.

Disaggregation-aggregation based model reduction for refinery-wide optimisation

In this work, reduced nonlinear refinery models are developed by generating and using input–output data from a process simulator. In particular, rigorous process models of continuous catalytic reformer (CCR) and naphtha splitter units are used for generating the data. To deal with complexity associated with large amounts of data, that is usually available in the refineries, a disaggregation–aggregation based approach is presented. The data is split (disaggregation) into smaller subsets and reduced artificial neural network (ANN) models are obtained for each of the subset. These ANN models are then combined (aggregation) to obtain an ANN model which represents all the data originally generated. The disaggregation step can be carried out within a parallel computing platform. Refinery optimization studies are carried out to demonstrate the applicability and the usefulness of the proposed model reduction approach.

Sustainable Water Desalination

Poor quality and availability of the dinking water is one of the major causes of illness and death in the developing world. In the developed world, increasing energy prices are challenging the economic feasibility of the traditional desalination technologies. On the other hand, process and other industries routinely emit a large amount of heat into the atmosphere as a waste, further exacerbating the climate change problem. This waste heat is a low-grade heat i.e. the temperature of the emissions is low, making it difficult to be recovered and utilised for the processes within the industry. In this project we aim to model and optimise the utilisation of the low-grade heat for desalination, thus simultaneously addressing the challenges of sustainable potable water production and global warming. A solvent extraction based process is considered for water desalination. The process consists of a heat-transfer contactor (HTC), a wash contactor (WC) and heat exchangers. The solvent recovers the salt from the saline feed stream in the HTC and gives up the salt in the WC. This process relies on the following two properties of the solvent: (i) it is immiscible with water at particular temperatures and miscible at others, and (i) it has low solubility in water, hence when the polymer separates from the water, the aqueous phase contains no solvent. An objective of this work is to use optimisation-based techniques in order to minimise the energy consumption of the existing process, by investigating the effect of varying the specific operating conditions.

Competence Area | Operations and Control

The Operations and Control competence area has a broad range of activity ranging from research in fundamental control theory through to technology transfer. The goal is to move new theory rapidly towards practical realization and help industry and society to take early advantage of developments. Emerging themes include multi-scale control and integrated process operation.

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. The research within the Centre covers optimization of the operations of existing plants, optimal designs for new plants that take account of dynamic operation at the design stage, management of supply chains and of batch processing.

Process Control

Covers the theory and practice of advanced automation and control 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:

Robust Optimization of Nonlinear Processes under Uncertainty: Many important questions and challenges in process systems design, operation and control can be posed as nonlinear optimization problems. To date, most optimal decision making tools for such problems are mainly based on deterministic mathematical models, where all parameter values in the model are assumed to be known precisely. In practice, however, mathematical models are merely approximate descriptions of the real system, and parameters such as future demands, prices, equipment wear-out and process conditions are subject to significant uncertainty. It has been frequently shown that disregarding such uncertainty can lead

to severe performance losses, increased costs, and energy & environmental penalties. The overall aim of our work is to develop robust local and global optimization methods for nonlinear dynamic processes under uncertainty. In particular, the main objective is the theoretical and algorithmic development of robust optimization methods for mixed-integer nonlinear dynamic processes under uncertainty. It is intended to employ, adapt, further develop and implement multi-parametric programming and robust optimization techniques, two prominent approaches to decision making under uncertainty. Over the next couple of years, industrial applications will also be investigated and the developed methods will be applied to the integrated design, optimization and control of specific process systems under uncertainty.

Robust explicit Model Predictive Control and applications to a Fuel Cell system: Fuel cells are a promising technology for electrical power generation, widely regarded as a potential alternative for stationary and mobile applications. The electrical efficiency of the fuel cell is higher than the most conventional devices for power generation, as they avoid intermediate steps of production of mechanical energy. The transport sector is one of the major contributors to global fossil fuel consumption and carbon emissions. The primary type of fuel cells for automotive industry application is Proton Exchange Membrane (PEM) fuel cells, due to their suitable properties for vehicle applications. We have developed a mathematical model for a 1kW PEM fuel cell system, in order to investigate the optimal operation range and to develop an explicit Model Predictive Controller (mp-MPC) under uncertainty. Next, a prototype PEMFC-based power generation system will be designed and implement. Control algorithms will be tested and validated in silico, via

mathematical models and simulations. Finally, the designed model based controllers will be applied and tested in the lab, via suitable hardware and data acquisition system.

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.

Processes 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. A recent highlight in January 2012 was a fact-finding visit hosted by Statnett and Statoil to Alta and Hammerfest in the north of Norway where such interactions are of great importance. 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. Approaches and sub-projects include:

- Advanced dynamic signal analysis of process measurements;
- Capturing and analyzing process connectivity and topology from P&IDs;
- Understanding the dynamics of PCS-MES-ERP integration;
- Integrated design and control with a focus on control structures;
- Creating site-wide approaches taking account of process units, utilities, rotating equipment and electrical systems;
- Analyzing wide-area systems such as a.c. electrical transmission where interactions extend across a region or continent;
- Examining the impact of wireless technology in process automation.

CPSE visitors coming to Imperial cannot fail to see the new CO_2 capture pilot plant and the ABB Control Room. The generous donation from ABB of instrumentation and the flagship industrial 800xA control system has given Imperial College a state of the art process automation system which will have a major impact on student training and process automation research.

More information on Process Automation is available at: **http://www3.imperial.ac.uk/processautomation**

Operations and Control – Highlighted Project

Real-time operational risk management of water treatment processes through advanced multi-scale modelling: Water treatment processes are intended to remove suspended matter from the source water, in order to maintain a desired water quality for urban use. Water treatment works generally include sub-processes such as coagulation, flocculation, settling and filtration, alongside other customised procedures, such as disinfection, depending on the source water particulars (Figure 1). Whilst these are separate processes involving highly specific functions and specialized equipment, the efficiency and outcome of these processes are inter-dependent. As such, sub-optimal settings within each process may result in a significant Opex increase in the overall energy and chemicals consumption used in the water treatment plant, and may further lead to poor water quality. The biggest operational risk to a water treatment company's ability to control its operations thus stems from the day-to-day management and optimisation of its many water treatment works. Our industrial partner has a vision to manage this risk in real time and to move away from reactive ways of working.

Real time optimisation cannot be achieved through separate optimisation of individual sub-processes, but necessitates design and implementation of an integrated system, which ensures the generation and flow of the data relevant to each sub-process, and accommodates the required hardware to adjust the control and manufacturing settings accordingly. In our work, we are developing a multi-scale model representation of a Computer-Integrated Manufacturing (CIM) system involving Enterprise Resource Planning (ERP), Manufacturing Execution System (MES) and Process Control System (PCS), which thus enables integration between the control and manufacturing systems within the water treatment plant. The main issues which need to be addressed are dynamic functional dependencies within the CIM system and the effects of propagation of uncertainty. A multi-level modelling representation structure is being created, spanning time scales from minutes to months, with appropriate detail at each level. An important part of this work is thus detailed mathematical modelling of all the main sub-processes of a standard water treatment work. A systematic modelling methodology including parameter estimation is being developed to allow for quick and accurate model verification from one water treatment work to the next.

At the heart of the interface of the CIM representation lay computers, and prior to the implementation of real-time optimisation procedures, a detailed CIM infrastructure is being established within the water treatment arenas. The lowest level (PCS) will employ first principles and data-driven modelling with short timescales. The highest level (ERP) requires modelling of tasks and information flow over extended time scales. The middle level (MES) will involve causal model structures, i.e. equations whose forms are known but whose parameters are uncertain.

Figure 1. Common sub-processes of a water treatment works

Competence Area | Modelling and Model Solution Tools

Modelling and the solution of models are at the heart of Process Systems Engineering and research in this area is central to our activities. We seek to model and to solve ever more difficult problems as we address larger scale and more complex nonlinear and discrete problems.

For the lifetime of the Centre and beyond solving optimization problems, and developing new methods for their efficient solution, has been a major part of our activities such that now we (and even the undergraduate students) routinely solve multiple cascaded optimization problems without difficulty. Current work is described here in three sections: i) new methods for solving multi-parametric integer programming problems which arise particularly when dealing systematically with uncertainty, ii) methods for global optimization, and iii) advances in model development paradigms.

i) Advances in Multi-Parametric Mixed Integer Programming and its Applications

Multi-parametric programming has received growing attention over the past decades in the field of optimization under uncertainty. The method we have developed is an exact solution method which expresses the optimal solution as a function of the parameters and is a powerful tool to account for the presence of uncertainty in the model.

Despite many advances in this area, the important classes of the general multi-parametric linear and mixed-integer linear problem, respectively, have not yet been fully addressed. The latter has applications in chemical process design, production planning and scheduling under uncertainty, and in explicit model predictive control of hybrid systems.

These projects focus on the development of multi-parametric programming theory and algorithms, and on demonstrating its potential in pro-active scheduling.

The solution of the general multi-parametric mixed integer linear programming (mp-MILP) problem (Wittmann-Hohlbein, Pistikopoulos)

This research is concerned with the development of novel mp-MILP algorithms. The first approach deals with the global solution of the general mp-MILP problem where strategies from deterministic nonlinear optimization are adapted to the multi-parametric framework. The second approach considers two-stage methods for which the computational burden is reduced compared to global optimization at the price of deriving suboptimal parametric solutions of the general mp-MILP problem. The novel two-step procedures favourably combine various techniques, such as robust optimization and suitable relaxation methods to linearize the constraints, with multi-parametric programming. Future effort will also focus on the extension of the proposed approaches to address multi-parametric mixed integer quadratic problems.

Pro-active scheduling via multi-parametric programming (Wittmann-Hohlbein, Pistikopoulos)

In this research, short-term scheduling of batch processes is considered. It is assumed that the scheduling model is contaminated with uncertain data introduced by price, demand, and processing time or conversion rate uncertainty, respectively. In order to deal with all types of parameter variation in the scheduling model, we apply the proposed two-stage methods for its approximate solution providing a guaranteed estimate of the overall profit of the scheduling task. The hybrid pro-active scheduling approach is computationally efficient. Piecewise affine scheduling policies are obtained and once the true values of the parameters are known the optimal policy is determined via simple function evaluation.

Approximate Multi-parametric Programming Based B&B Algorithm for MINLPs (Dua)

In this work an improved branch and bound algorithm for MINLPs is proposed. The basic idea of the proposed algorithm is to treat binary variables as parameters and obtain the solution of the resulting multi-parametric NLP (mp-NLP) as a function of the binary variables, relaxed as continuous variables, at the root node of the search tree. It is recognized that solving the mp-NLP at the root node can be more computationally expensive than exhaustively enumerating all the terminal nodes of the tree. Therefore, only a local approximate parametric solution, and not a complete map of the parametric solution, is obtained. The approximate parametric programming solution at the root node and other fractional nodes of the branch and bound tree is then used to estimate the solution at the terminal nodes in different sections of the tree. These estimates are then used to guide the search in the tree, resulting in fewer nodes being evaluated

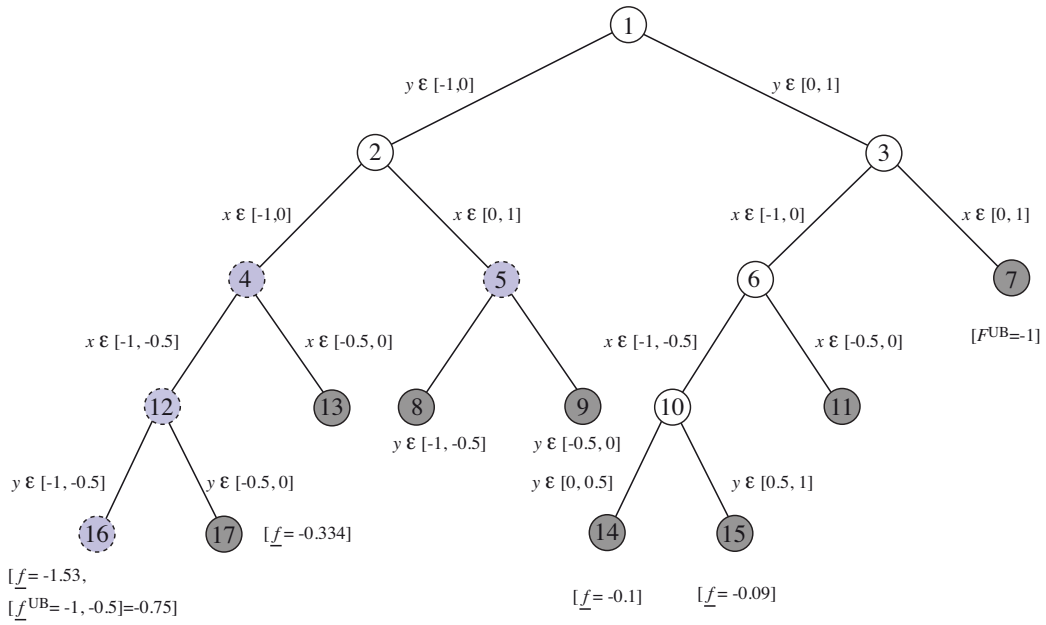


Figure 1. Branch-and-Sandwich branch-and-bound tree for a nonconvex literature example

and a reduction in the computational effort. Preliminary computational results are encouraging and future work will involve testing the proposed algorithm on larger scale problems and comparing with other algorithms reported in the literature.

ii) Methods for Global Optimization

Efficient and reliable global optimization is a key plank of the Centre's work and remains a significant challenge. Work continues on a number of fronts using branching, stochastic and interval based methods. Here we present just one project where important progress has been made.

A Deterministic Global Optimization Algorithm for Optimistic Bi-Level Programming Problems (Kleniati, Adjiman)

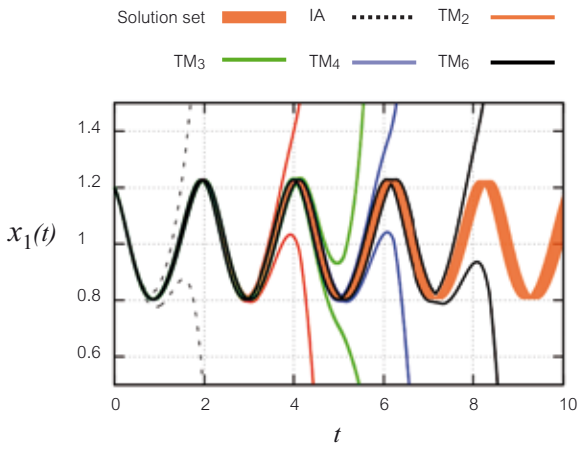
Real-life decisions are often made hierarchically. For instance, the allocation of resources by a multinational company is a multilevel allocation process where one level of management distributes resources to several local levels of management, e.g., processing plants. The overall objective of such a decision process is to achieve the best performance for the company. However, each local management team will react independently according to best serving their own interests; these (rational) reactions may be gainful or detrimental to the overall objective. Hence, decision making within such a framework requires careful analysis in order to ensure the best possible outcome for all the decision makers. The concept of hierarchical decision making, in the presence of two decision makers, namely one leader and one follower, dates back to 1952 when von Stackelberg introduced the basic leader/follower strategy in a duopoly setting. Since then, hierarchical decision making has found application to numerous practical problems across various disciplines, such as economics, management, agriculture, transportation and engineering. Of particular interest are hierarchical systems in parameter estimation, environmental policies in biofuel production and chemical equilibria.

Over the past year, we have been developing a novel algorithm, Branch-and-Sandwich, to solve general nonconvex bi-level programming problem to global optimality. Special cases of this problem have been studied intensively and many algorithms have been proposed in the literature. However, the general nonconvex form, which is most applicable to process systems engineering problems, is a very challenging problem for which only two algorithms exist to the best of our knowledge: the first method for general (nonconvex) bi-level problems developed by Mitsos, Lemonidis and Barton (*J. Global Optim*. 42(4), 475–513, 2008) and the approximation method introduced by Tsoukalas, Rustem and Pistikopoulos (*J. Global Optim*. 44(2), 235–250, 2009). The Branch-and-Sandwich algorithm is based on the exploration of two solution spaces (corresponding to the inner and the outer problems) using a single branch-and-bound tree. To achieve this, the well known features of branch-and-bound algorithms are customised appropriately. To this end, we first introduce a novel branching scheme such that the hierarchy in the decisions is maintained and the requirement for (global) optimality in the inner problem is satisfied. This approach has the distinct advantage that large regions of the inner variable space can often be eliminated from consideration early on in the branch-and-bound tree, leading to improved convergence. The theoretical convergence properties of the algorithm have been demonstrated and the algorithm has been applied to 35 literature examples. We are currently developing a fully automated implementation so that larger examples can be tested.

Bounding Strategies for Global and Robust Dynamic Optimization (Villanueva, Sahlodin, Chachuat)

Dynamic optimization problems encountered in various engineering and scientific fields frequently exhibit multiple suboptimal solutions. A prototypical example is in the fields of model identification, where failure to determine the best

possible fit can lead to false conclusions regarding the validity of a candidate model. Other applications are in the field of robust and scenario-integration optimization. In this project, we are investigating deterministic global optimization methods, such as spatial branch-and-bound, which have the appealing property that a global optimum can be located, at an arbitrary precision, in a finite number of iterations. Pivotal to the success of these procedures is the ability to compute tight estimators for the solutions of the underlying differential equations (ODEs).



Among the approaches currently available for parametric ODEs, the method of differential inequalities proceeds by constructing an auxiliary system of ODEs, the solutions of which provide the desired estimators, either as interval bounds or as convex/concave relaxations. We have developed an approach that combines differential inequalities with Taylor models, namely estimators which consist of a multivariate polynomial part and an interval remainder term. The advantage of propagating Taylor model estimators, as opposed to interval bounds, is that the former enjoy a high-order of convergence, which makes their use particularly attractive in the context of global dynamic optimization. An illustration of the resulting bounds for Taylor models of various orders is shown in the figure opposite for the case study of a Lotka-Volterra (predator-prey) system.

Another class of approaches builds upon interval methods for ODEs to determine a rigorous enclosure of the ODE solution set. Traditional interval methods discretize the integration domain into a finite number of steps, and each step proceeds in two phases. In the first phase, an a priori enclosure of the solutions over the current integration step is computed; in the second phase, a tightened enclosure at the end of the current step is then computed, with special care taken to mitigate the wrapping effect. An extension of this approach was proposed recently, whereby Taylor models are used instead of simple natural interval extensions in order to reduce the dependency problem. In this project, we went one step further and computed convex/concave relaxations based on a new type of Taylor models, called McCormick-Taylor models. For a majority of problems, the methods based on Taylor models and McCormick-Taylor models have proved to be more efficient for global dynamic optimization than the ones based on interval analysis and McCormick relaxations, as a result of their higher order of convergence. Dynamic optimization problems with up to 10-12 decision variables could be solved to global optimality with such bounding techniques.

All these methods are automated in the software library MC++ that is currently developed in the group of Dr. Chachuat.

iii) Advances in Modelling Paradigms and Tools

We continue to seek alternative ways of representing process systems and formulating the resulting models for efficient solution. Here we review five projects, two using Artificial Neural Networks for model reduction and parameter estimation and three exploring particular problem representations in biological systems modelling and for pressure swing adsorption which is a semi-continuous process.

Optimal Configuration of Artificial Neural Networks (MIPANN) for Model Reduction (Dua)

A mathematical programming approach for automatic computation of the optimal configuration of artificial neural networks (ANNs) has been developed. Training of the network is modelled as a mixed-integer program (MIP) where 0–1 binary variables are introduced to represent the existence (binary variable = 1) and non-existence (binary variable = 0) of the nodes and the interconnections between the nodes. The objective is to minimize the number of nodes and/or interconnections to meet a given error criterion. From a modelling point of view, the key advantage of the proposed approach is that the user does not have to try different configurations of the network as a solution of the proposed MIP formulation automatically generates the optimal configuration of the network. For the implementation of an ANN, a simplified representation of the network is obtained where redundant nodes and interconnections have been eliminated. The solution of the proposed MIPANN is more complex than that for training by using the traditional ANN approach, but has several practical advantages. For networks that are updated on-line a simpler structure with fewer parameters is easier to maintain. When the networks are used for a target application they will have faster implementation times. For certain applications where these networks will be implemented through electronic chips, over-design costs can be reduced. Formulation of the ANN problem as a constrained optimization problem also allows incorporating constraints that reflect any available insight or understanding of the system. A number of case studies have been carried out to demonstrate the applicability of the proposed approach.

Parameter Estimation of ODEs using Neural Network Approximations (Dua)

Parameter estimation for system of ordinary differential equations (ODEs) can be formulated as a nonlinear programming (NLP) problem. The objective function of the NLP consists of two terms, which are simultaneously minimized. The first term is the summed square of the difference between the ODE model predictions and experimental data. The solution of the ODE model is postulated as an Artificial Neural Network (ANN)

model given by time points as inputs and the state variables as the outputs. The outputs of the ANN model can be analytically differentiated with respect to the input, providing the differential terms of the ODE model. The summed square of the difference between these differential terms and the right hand side of the ODE model represents the second term in the objective function of the NLP. ANNs have been well known for their ability to approximate highly nonlinear functions but this ability has not been systematically used for parameter estimation of ODEs. An advantage of the ANN based approach that has been presented is that highly nonlinear multi-input multi-output functions can be approximated by ANNs, which is expected to open avenues for parameter estimation of highly nonlinear ODEs.

Interval models for Systems Biology (Bogle)

Given the difficulty in getting complete descriptions of complex physiological systems, if deterministic models are to gain currency in medicine it will be necessary to provide reliable predictions for safe operating limits. We have been exploring the use of interval models in Systems Biology to obtain bounded outputs for physiological systems on the basis of given uncertainties derived from conservatively estimated measurement ranges. It will be important to be able to provide conservative ranges for predictions of key variables as a result of actions arising from environmental and pharmacological interventions in normal and diseased systems. The project is using the glucose homeostasis 'composite' model developed in previous projects at UCL. We have been solving an initial value problem arising from a model of the activation of a hormone (glucagon) receptor in liver cells by increased adrenaline in the bloodstream. Preliminary results show that bound predictions are conservative and useful bounds can be obtained with careful model formulation. However the rapid growth of bounds remains a challenge.

Modelling of biological cellular systems (Krishnan)

Modelling of cellular signal processing focuses on a combination of modelling of specific biological processes, and modelling and systems based approaches to elucidate core aspects of signal transduction. Multiple modelling formalisms and approaches are used. Some specific projects are:

1. The systems-based bottom-up modelling of drug response of tumour cells (with Liu and Xu). Modelling here combines fluid flow transport and cellular response.

2. Elucidating the regulation of the budding yeast cell-cycle by external signals (with Seaton). This project involves modelling of control of non-linear dynamic cell cycle circuits.

3. The coupling of pathways and processes through shared components: (a) through bottom-up modelling and (b) through modelling the influence of allostery on crosstalk in the phosphatidylinositol signalling pathways (with Seaton) which involves modelling of full, as well as simplified, signal transduction pathways.

4. Modelling signal transduction in spatial signalling networks (with Alam-Nazki) using modelling and analysis of spatial signalling in representative signalling circuits.

5. Lattice hopping models to investigate the interplay of feedback regulation on translation (with Nemanja Mikac) using stochastic lattice-hopping models with feedback.

Detection of Disjoint and Overlapping Modules in Weighted Complex Networks (Papageorgiou)

Community structure detection is widely accepted as a means of elucidating the functional properties of complex networks. Complex networks can arise from different real world situations such as social interaction networks, the Internet and biological networks. Complex networks comprise vertices (or nodes) and edges (or links) and exhibit certain properties such as high clustering coefficients, scale-free distribution of nodes, small-world properties and community structure. Community structure is the existence of communities of nodes, also known as clusters or modules, with more interactions within a community than between different communities. Communities can be thought of as groups of nodes that function semi-independently to the rest of the network, resulting in robust and adaptable systems.

In this project, two novel mathematical programming algorithms for module detection are developed. First, disjoint modules in weighted and unweighted networks are detected by formulating modularity maximisation as a mixed integer non-linear (MINLP) programming model. The solution obtained is then used to detect overlapping modules through a further MINLP model. The inclusion of two parameters controlling the extent of overlapping offers flexibility in user requirements. Comparative results show that these methodologies perform competitively to previously proposed methods.

Application Domains

Application Domains | Chemical Manufacturing Systems

Chemical Manufacturing Systems form a key application domain of CPSE: 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.

Most academics involved in CPSE have a foothold in this area. In this section, a few of the ongoing projects are highlighted, including some that address cross-sector issues such as the optimal synthesis of water networks.

Optimal Synthesis of Water Networks with Membrane Regenerators

C.S. Khor (PhD Student), B. Chachuat, N. Shah

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.

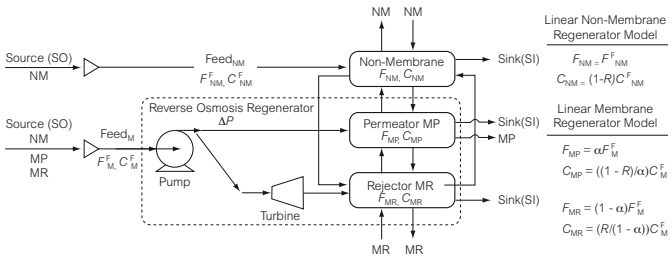


Figure 1. Superstructure for the water regeneration subnetwork

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. Our model formulation relies on a fixed-flowrate representation for water-using units. In particular, the permeator and the rejector in membrane regenerators are considered as two separate entities, both of which are treated as regenerators. Moreover, the main physical parameters for such membrane regenerators are accounted for in the mathematical model, including the types, sizes, number of modules, and orientations. Figure 1 shows the superstructure around the water regeneration subnetwork that is representative of the entire network in general.

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. The nonlinearity is due to contaminant mixing while the integrality pertains to discrete decisions on selection of the interconnections and the regenerators. 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

E.Fraga

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.

PSA offers a broad range of design possibilities. In the last decade much attention has been devoted towards efficient modelling, simulation and optimisation of various PSA cycles.

The PSA beds are modelled with hyperbolic/parabolic partial algebraic differential equations and the process performance should be assessed at cyclic steady state (CSS). Unfortunately, with such detailed mathematical models, the necessity to determine CSS, which commonly takes hundreds or thousands of cycles to reach and the use of multiple adsorption beds with interconnections become too computationally expensive for optimal design. The search for optimal PSA design is therefore precluded for many interesting industrial applications.

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.

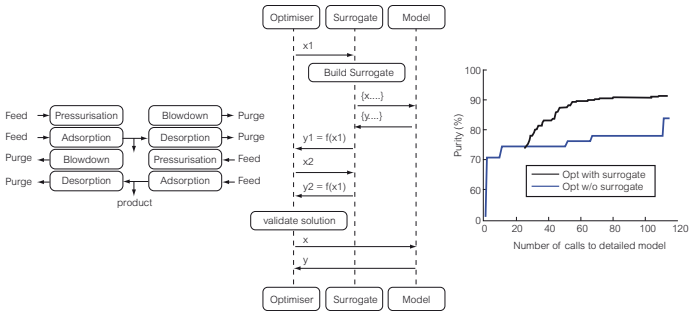


Figure 2. Optimization of pressure swing adsorption process – from process modelling to surrogate-based optimisation

Multiscale modelling of biorefineries

There is a large body of literature regarding the choice and optimization of different processes for converting feedstock to biofules 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, butalso 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.

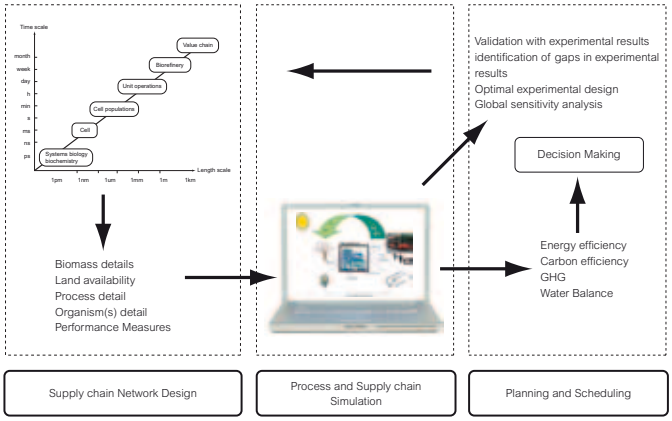


Figure 3. Integration of models for bioenergy/biofuels. A variety of activities have been undertaken under this project. A particular advance has been the development of detailed models of hydrolysis of cellulose by different enzymes; this then enable the optimisation of the enzyme mix and process conditions for hydrolysis, which is one of the performance-limiting elements of the chain

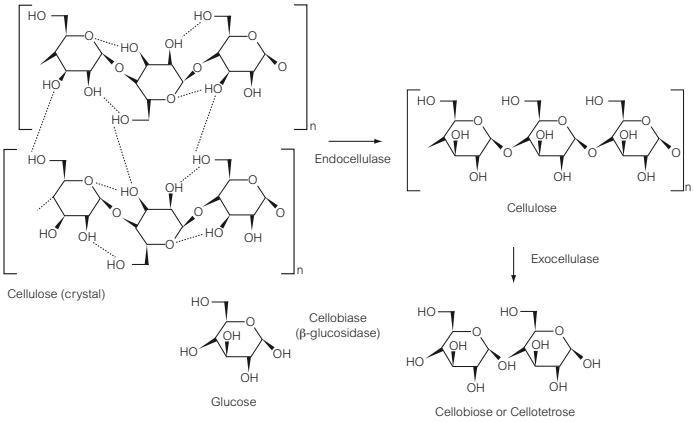


Figure 4. Mechanisms of cellulose hydrolysis

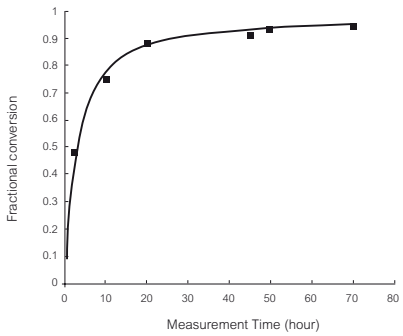


Figure 5. Model fit to experimental data

Application Domains | Molecular Systems Engineering

The next set of challenges. The molecular systems engineering area continues to grow from strength to strength. Currently we are 6 lead investigators, 7 postdocs, 14 PhD students, and a programmer, working in the development of methods and tools for the design of better products and processes in applications where molecular interactions play a central role.

We have recently secured a £1.8M Platform Grant from the Engineering and Physical Sciences Research Council (EPSRC) of the UK Government to build on the expertise of the group and fund the next generation of post-doctoral researches that will allow us to tackle new challenges. We are extremely thankful to BMS, Chemistry Innovation, GSK, P&G and Syngenta, for their support in this bid; we would not have succeeded without it.

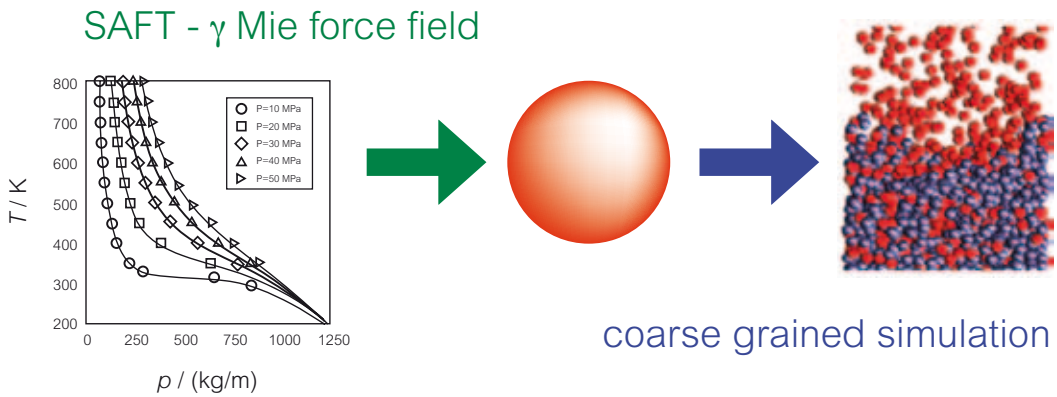
In this grant we will be working under the heading "Molecular Systems Engineering of High-Value Structured and Formulated Products". A strategic objective for the next 5 years is to make a leap to the challenging high-value manufacturing arena, where formulated and structured products are required. The combination of a fundamental physical understanding, mathematical models, and numerical methods is the cornerstone of our approach, allowing us to reduce our dependence on rules-of-thumb, which have traditionally been used to make models tractable, but which have a limited validity. The key is to bridge the length-scales involved in understanding the molecular-structure/assembly-stability-property relations by developing robust force fields and new methods that integrate the evaluation of fluid (unstructured) properties and those of the structured/crystalline phases, and that can be used to address non-equilibrium as well as equilibrium problems. We are in a very good position to start addressing the challenges we have set for ourselves. As an example the strength of a novel approach to determine coarse-grained potentials for use in computer simulation, the latest results in the determination of optimal solvents for reactions, and our state-of-the-art determination of solid forms of flexible molecules are highlighted below.

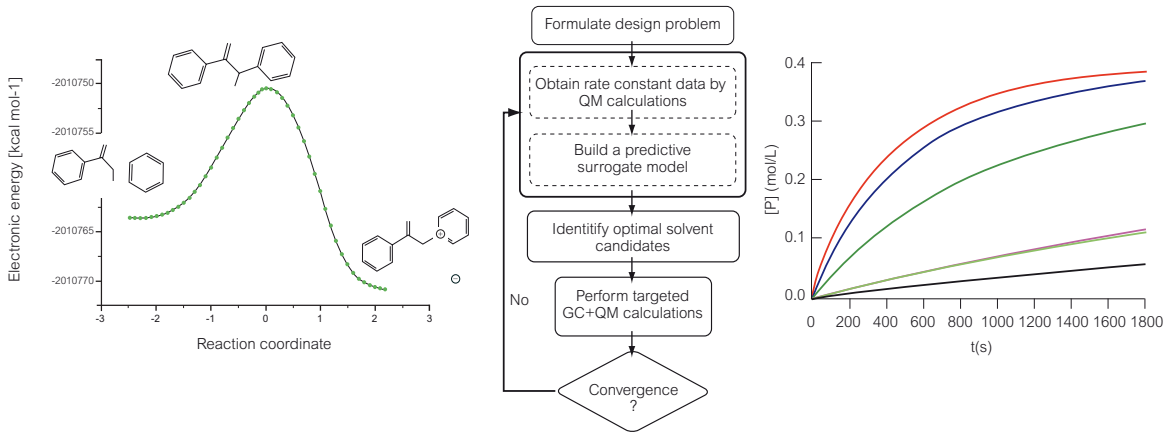
SAFT-g force fields for simulation of molecular fluids

C. Avendaño, T. Lafitte, V. Papaioannou, A. Galindo, C. S. Adjiman, G. Jackson, E. A. Müller

Many interesting and important phenomena in soft matter, such as self-assembly of large complex molecules, protein folding or colloidal aggregation, are typically observed in the mesoscale regime. The spatial and time scales involved in these processes are very large, making atomistic simulations very challenging. The growing area of coarse-graining (CG) methods has made possible the use of conventional molecular simulation techniques to study large systems in a reasonable computing time. In generic CG methodologies molecules are described as being formed by segments of bundles of matter (super-atoms) interacting via effective CG potentials. This approach clearly involves a loss in resolution of the description of the system, hence it is important to have an appropriate methodology that preserves a good overall description of the key target properties that one wants to represent after the coarse-graining. We have introduced a new coarse-graining methodology, where the statistical associating fluid theory (SAFT) is used as a link between the experimental fluid phase equilibria data and novel CG force fields based on the Mie potential, thereby facilitating parametrization.

Figure 1. Schematic representation of the SAFT-g CG force field procedure for the study of CO_2 absorption





Accelerating chemical reactions by computer-aided molecular design

Heiko Strübing, Zara Ganase, Eirini Siougkrou, 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. When investigating new liquid phase reactions, it is essential to find a "good" solvent to avoid dismissing a valuable chemistry because of a solvent which suppresses the desired reaction. At the process development level, the problem of solvent choice is further compounded by the numerous safety, environmental and process constraints that the solvent must satisfy. Despite the complexity inherent in solvent selection for reactions, few tools exist to support this decision and researchers are often left to choose on the basis of their intuition and/or extensive and costly experimental investigations. As a result, the improved understanding of liquid phase reactions and the development of solvent selection techniques have recently been highlighted as key priority areas by the ACS Green Chemistry roundtable.

In this series of projects, we have been developing a methodology for optimal solvent design for enhanced reaction kinetics, QM-CAMD, which relies on the integration of continuum solvation quantum mechanical calculations into a computer aided molecular design (CAMD) framework. This approach allows the exploration of a solvent design space consisting of thousands of potential molecules and leads to a shortlist of promising solvents that can then be assessed experimentally. To manage the computational cost, a surrogate model for the quantum mechanical (QM) calculations is built and improved iteratively. As a result, only a small number of QM calculations need to be performed during the course of the QM-CAMD algorithm. This approach has been successfully applied to the S_N2 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.

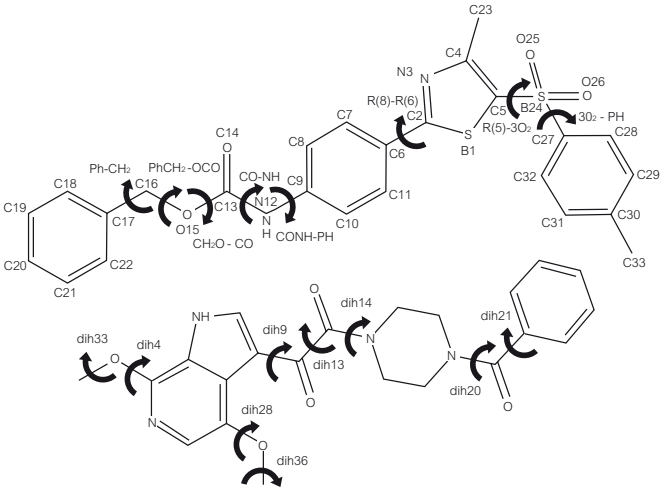
Figure 2 (top). Predictions & experiments within QM-CAMD methodology lead to an improved reaction rate using a designed solvent

Systematic methodologies for crystal structure predictions

Andrei Kazantsev, Manolis Vasileiadis, Claire Adjiman, Costas Pantelides

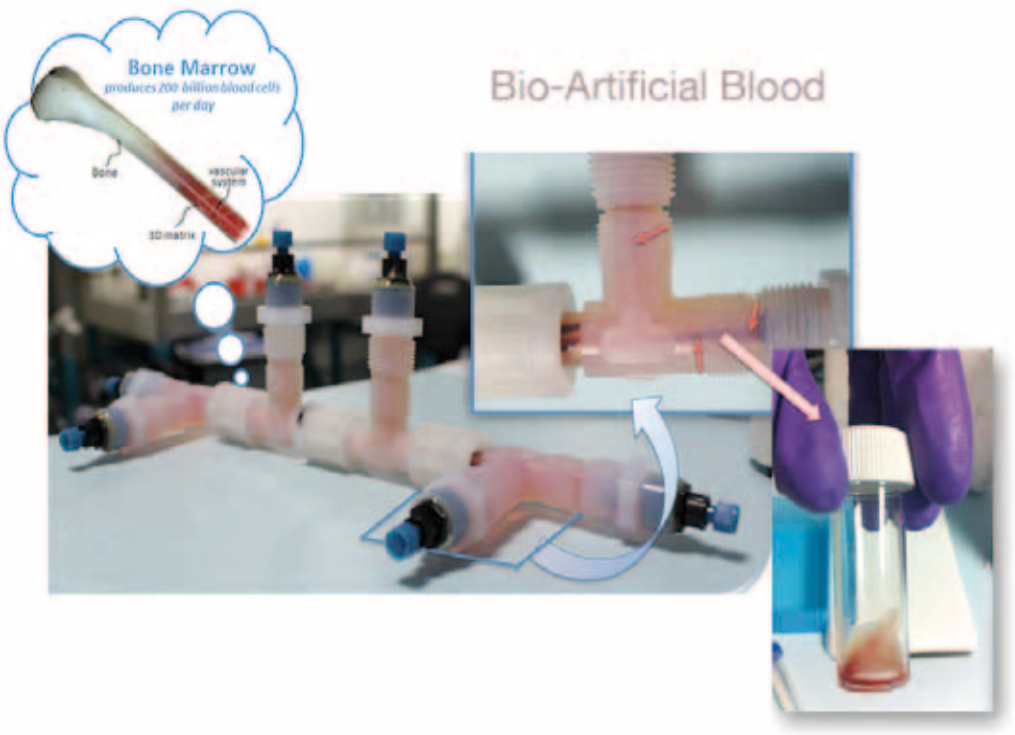
Methodologies for the systematic prediction of the polymorphs of organic molecules solely from the knowledge of the molecular connectivity diagram have undergone rapid improvements in the last few years. Progress has been achieved by combining better models of the different forces at play (e.g., electrostatics, dispersion) with efficient and reliable numerical techniques. In our most recent works, we have significantly extended the range of flexibility that can be handled, by developing local approximate models that allow us to achieve quantum mechanical accuracy at a fraction of the cost. Using an approach based on a global search stage, with our CrystalPredictor code, followed by a more accurate calculation of the lattice energy with our CrystalOptimizer code, we have successfully found experimental structures for large and flexible molecules such as molecule XX of the latest Blind Test (Fig. 1) and a pharmaceutical compound provided by BMS (Fig. 2). We have also been able to identify all seven known polymorphs of ROY, the molecule with the largest number known (anhydrate) polymorphs.

Figure 3. (top figure, below). Molecular diagram of molecule XX in the 2010 Blind Test, with key torsions. Figure 4. (lower figure, below) Molecular diagram of BMS molecule, with key torsions



Application Domains | Biological Systems Engineering

The Biological Systems Engineering group within CPSE focuses on the development of mathematical models for biological/medical problems with the aim of model-based control and optimisation.



Research on model development, model analysis, model reduction as well as multi-scale modelling has been the driving force behind the activities in the Biological Systems Engineering area. Over the past year, the research volume and output has significantly increased as indicated by selected examples listed below:

1. **Prof. Nilay Shah and Dr. Cleo Kontoravdi** secured funding from EPSRC on “Development and application of methods for complexity reduction, metamodelling and optimal experimental design based on global sensitivity analysis” working closely with EDF and Lonza to apply global sensitivity techniques in the identification of critical parameters in the biological models developed.

2. **Dr. Cleo Kontoravdi** working closely with synthetic biologists secured funding from EPSRC on “Engineering a semi-biotic immune system”, which aims to design and fabricate a semi-biotic immune device that will use a consortium of engineered bacteria, composed of a group of detectors that monitor the host for signals of disease onset and responders, that await signals from the detecting bacteria, before initiating the production and release of the relevant small molecule treatment.

3. **Dr. Cleo Kontoravdi** and collaborators from Biochemistry secured funding from BBSRC to work on “a platform for the optimisation of metabolic pathways for glycosylation to achieve a narrow and targeted glycoform distribution”. In this project, a computer model of the metabolism of the cells will be developed that can predict which glycoforms are produced, which will enable the design of new media for the cells to use resulting in a more homogeneous glycoform profile.

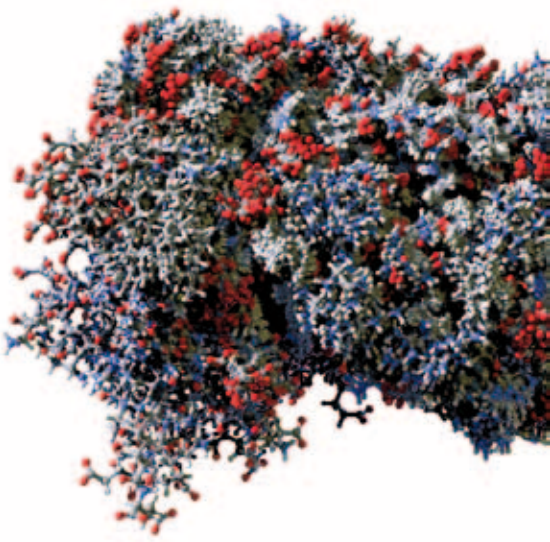
4. **Dr. J. Krishnan** secured funding from BBSRC to work on “Systems modelling of a translational negative feedback loop: an in vivo toolkit to dissect ribosomal termination and mRNA surveillance”. In this project, an integrated systems analysis of the dynamic flux of ribosomes along the mRNA, coupled with a model of the termination process will be developed to identify how mRNA stability is dictated by the interplay between natural mRNA decay, nonsense mediated decay, and translational activity, thus integrating modelling and experimentation to dissect the functional consequences of termination complex remodelling, and to define how stop codon position and translational efficiency govern protein productivity and stability of an mRNA.

5. **Prof. Nina Thornhill and Dr. Lazaros Papageorgiou** are part of the newly formed EPSRC's Centre for Innovative Manufacturing in Emergent Macromolecular Therapies, which aims to greatly reduce the time and costs of developing new treatments, as well as improving the access to drugs with advanced therapeutic properties.

6. **Prof. Stratos Pistikopoulos** and **Prof. Sakis Mantalaris** have received two EU grants, Multimod and OPTICO, which aim to model biological systems: a) "closing the loop from in silico to in vivo: modelling and optimisation of bacterial cell culture systems", whereby mathematical models will be used to optimise the biocatalytic activity for the breakdown of toxic substances of the industrially-relevant Pseudomonas putida bacterium; b) "population balance modelling in cell culture systems" whereby the aim is the development of a framework that integrated experimentation and modelling that facilitates the study of mammalian cell cultures as a sum of subpopulations with individual growth/metabolic and productivity characteristics; c) "population balance modelling of leukemic cells for the optimisation of chemotherapy delivery" whereby the aim is to develop a mathematical model that describes the growth of normal hematopoiesis and acute myeloid leukaemia and to validate it experimentally through the setup of a bioreactor, capable of mimicking the conditions found in human bone marrow during haematopoiesis; d) "molecular dynamics modelling of biological molecules" whereby the aim is the development of highly accurate equation of state for the thermodynamic properties of protein – polyphenol complexes.
Working closely with Unilever, keratin (most of the visual, biomechanical and biophysical properties of hair and skin are related to keratins) were selected as the protein and tea catechin as the active molecule.

7. **Prof. Mantalaris** working closely with the Department of Haematology and the National Blood Service has secured funding from the National Health Service (NHS) to work towards a "bio-inspired, reverse-engineered bioreactor" that will be able to produce blood for transfusions. In the UK, blood is normally provided by registries of volunteer donors, which are nationally funded and maintained to allow maximal flexibility and capacity to meet needs, whilst ensuring highest safety and quality. For patients with very rare blood groups, as well as some patients who have multiple red cell antibodies, finding compatible blood can be extremely difficult and, at times impossible, resulting in compromised compatibility of blood or delays in provision, which can contribute to morbidity or death.

   Prof. Mantalaris' technology has the potential to deliver cost-effective production of clinically-relevant cell numbers with selective cell harvesting in a closed culture system that requires minimal handling and would be ideal for Good Manufacturing Practice (GMP) purposes of cellular therapy. The ultimate goal is to replace blood donation for transfusion. This project was selected as part of RCUK's Big Ideas initiative that included "disruptive technologies". Furthermore, Prof. Mantalaris was selected as a finalist for IChemE's Biorpocessing award.



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.

These include:

Sustainability

- 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;
- Reduction of waste and landfill.

Supporting Healthcare

Meeting the global healthcare needs in an affordable way (e.g. in line with the Millennium Development Goals);

Exploiting the advances in biosciences to develop customised healthcare products

Developing new lean manufacturing approaches to ensuring cost and waste minimisation

Commercialising Innovation

Exploiting rapid advances in the physical and biological sciences (e.g. nanotechnology) along with new manufacturing techniques to translate these into mass customised innovative products.

These challenges will require a holistic approach to the underlying science, the process engineering and the structuring of the supply chain, and therefore fall squarely into the remit of multi-scale process engineering. Two examples of our work (one strategic and one operational) in this area are:

Example 1: Global Supply Chain Planning for Pharmaceuticals

The shortening of patent life periods, generic competition and public health policies, amongst other factors, have changed the operating context of the pharmaceutical industry. In this work we address a dynamic allocation/planning problem that optimises the global supply chain planning of a pharmaceutical company, from production stages at primary and secondary sites to product distribution to markets. The model explores different production and distribution costs and tax rates at different locations in order to maximise the company's net profit value (NPV).

Large instances of the model are not solvable in realistic time scales, so two decomposition algorithms were developed. In the first method, the supply chain is decomposed into independent primary and secondary subproblems, and each of them is optimised separately. The second algorithm is a temporal decomposition, where the main problem is separated into several independent subproblems, one per each time period. These algorithms enable the solution of large instances of the problem in reasonable time with good quality results.

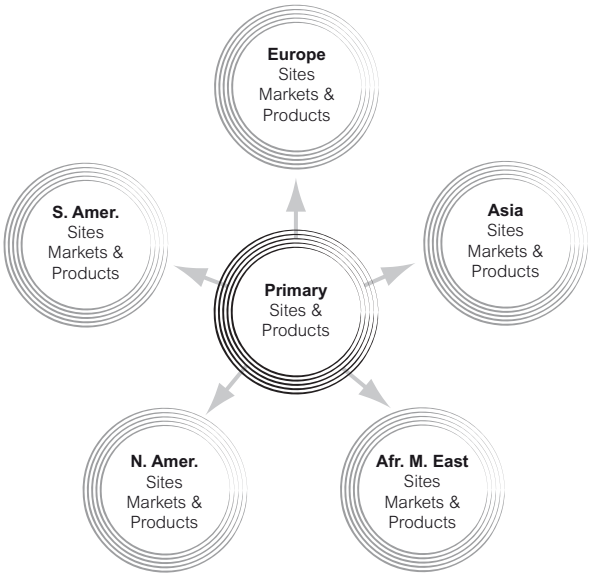


Figure 1. Supply chain structure

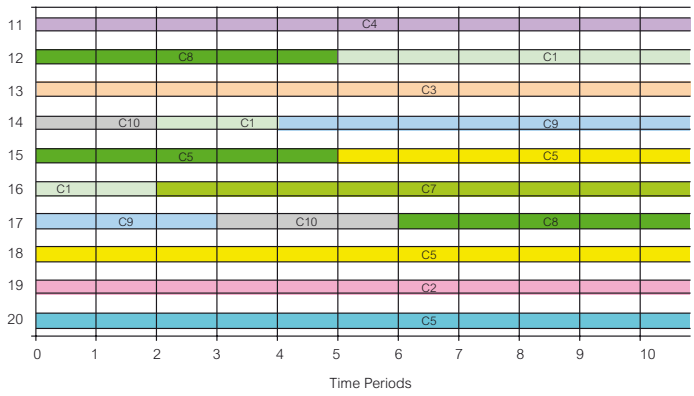


Figure 2. This shows the allocation of different products (I1-I10) to different sites (C1-C10) and the manufacturing campaigns over a year of operation (12 time periods)

Example 2: Model-Predictive Control for Multi-Echelon Supply Chain Management

As a successful optimal control method, Model Predictive Control (MPC) has been applied to many dynamic complex systems in the process industry, including supply chains. This work aims to propose a MPC framework for a multi-echelon multiproduct supply chain under demand uncertainty for the optimal inventory control and pricing. The sequence-dependent changeovers occur at the production plants, and the price elasticity of demand is considered at the markets. A mixed integer liner programming (MILP) model is proposed for the optimisation problem in the MPC, in which the objective function considers the profit, inventory deviations from the trajectories and price changes. The applicability of the proposed approach was illustrated by solving a supply chain example.

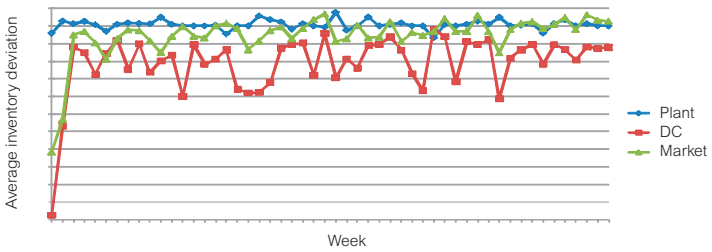


Figure 3. Inventory variations in different echelons. The MPC approach is able to avoid the “bullwhip” effect, whereby large variations are seen in the upstream part of the chain

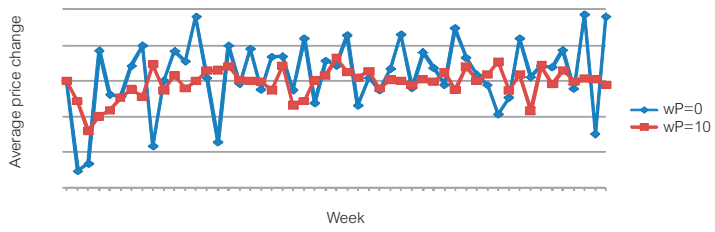
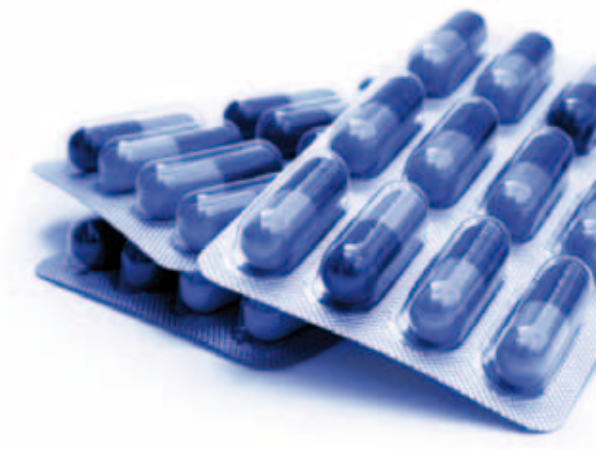


Figure 4. Price variations with time for two cases. In the case of wP = 10, large fluctuations are penalised in the model and the price is relatively stable



Application Domains | Energy Systems Engineering

Energy systems engineering is concerned with improving the way in which energy is generated and distributed to provide the essential energy services of heat, light, power and communication.

The increasing cost of fossil fuels, energy security and government targets to reduce greenhouse gas emissions provide a focus for CPSE's research on bioenergy, more efficient energy conversion and use and CO_2 separation. Essentially we adopt a multi-scale modeling approach with the lower levels corresponding to technologies or sub-processes, for example, Electrochemistry, Fuel cells, Gasifiers, Storage, inter-conversion and distribution options and the higher levels corresponding to networks, systems, space and time variation of supply and demands, large geographical regions, superstructures of sources, sinks, intermediates, conversion and storage technologies.

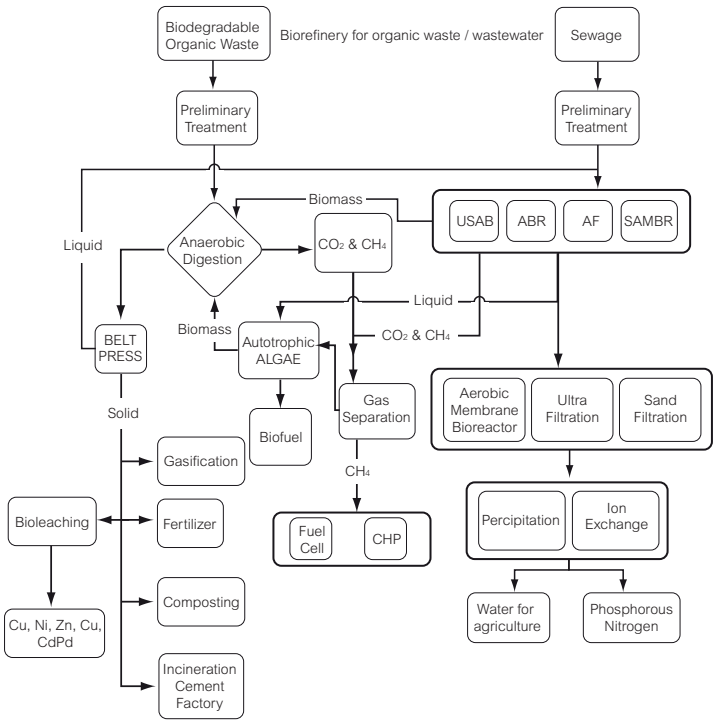
We are currently engaged in four major research projects that encompass the full range of modeling and optimization techniques developed by CPSE. These are; Polygeneration and Hydrogen networks, Bioenergy systems, Urban Energy Systems and CO_2 capture and network systems. Some examples are described in more detail below.

Biopolygeneration

Biological systems show considerable promise both as a source of biomass for energy and as chemical feedstocks, moreover they may provide a means of converting waste material into valuable commodities. However, the systems are complex and require detailed understanding before their economic potential can be assessed.

CPSE is investigating the potential for using microalgae to convert waste streams and carbon dioxide into biodiesel using a photo-bioreactor. Studies of the mechanisms that control microalgae metabolism and their ability to excrete methane or lipids and/or accumulate heavy metals has lead to the conceptual design of a bio-refinery for organic waste and waste water that could produce a number of high value products.

CPSE is also providing computer aided methodologies and tools for a faculty wide research programme on integrated marine resource harvesting.

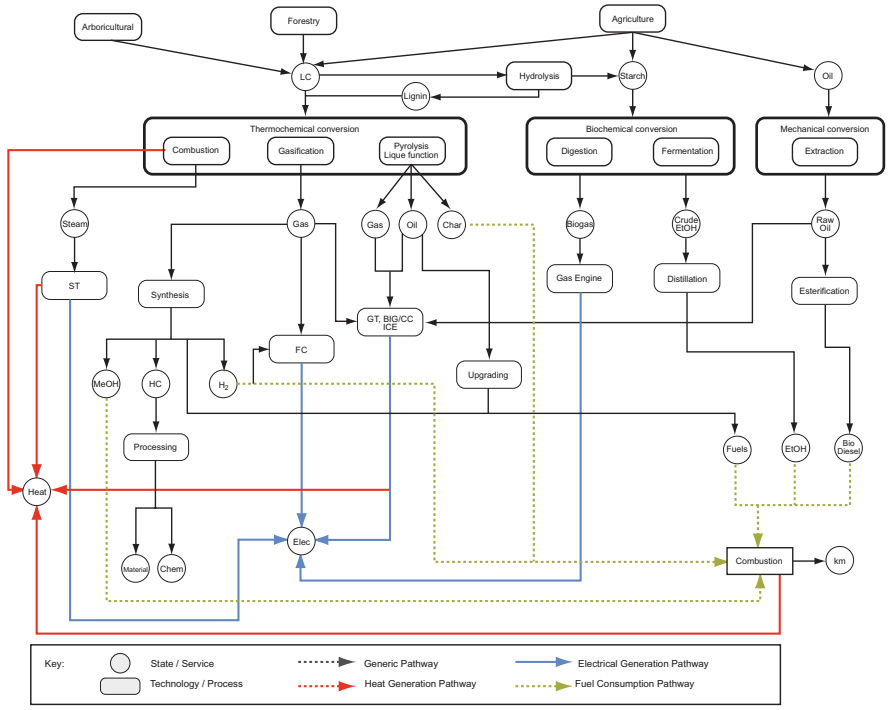


Investigators
B.Chachuat (ICL) D. Stuckey (ICL)

Waste / wastewater treatment,
Methane + biofuels production,

Heavy metals extraction,
Nitrogen / photophorus

Which technologies are the most appropriate?
How to best integrate them?



Bioenergy systems

Bioenergy systems integrates all the processes involved in the biomass supply chain from optimizing the biochemistry that microbial cells use to convert nutrients into biomass, to the supply chain of the biomass and its conversion into electricity or fuels. Recent work has focused on the trade-off between the total supply cost of UK Bioethanol and the total environmental impact of supply chain options. The results provide a detailed breakdown of the relationship between cost and environmental impact of different supply chain configurations.

Figure (above). One view of bioenergy systems

Chemisorption – based, Post combustion CO_2 capture

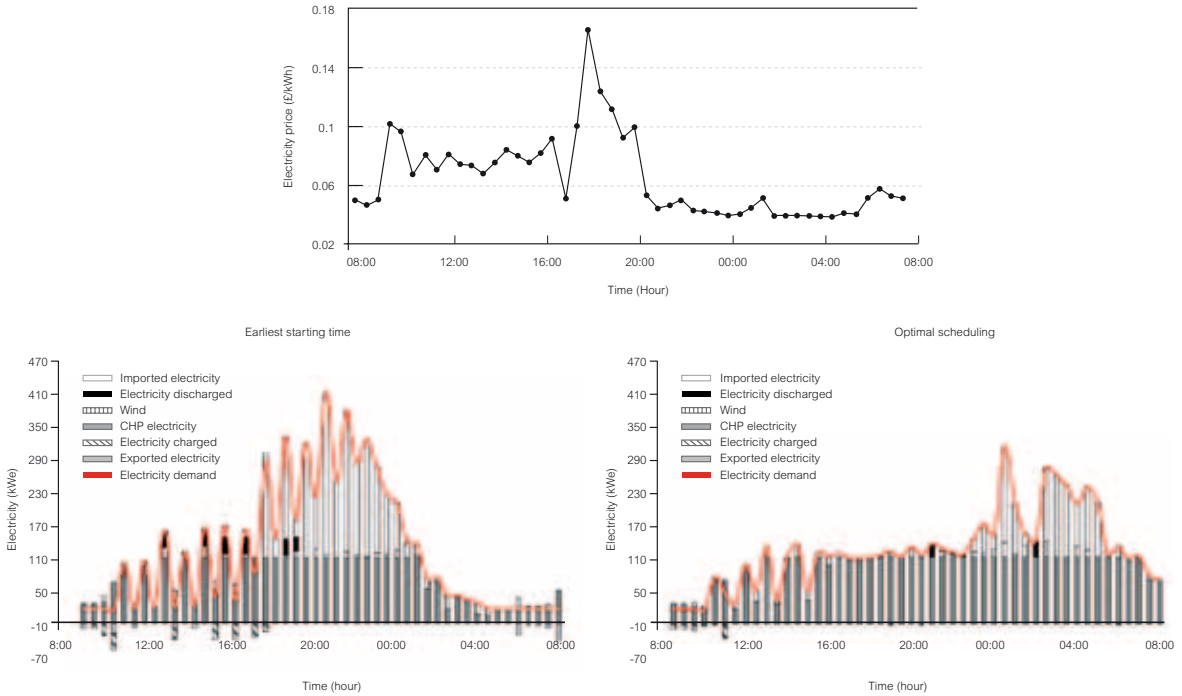
Carbon capture and storage is an important option in the task of reducing global greenhouse gas emissions. Current processes based on the use of amines to absorb CO_2 from flue gases followed by the regeneration of the amine are not economic at present carbon and energy prices. As a consequence, a considerable amount of research is focused on modeling the chemical and physical components of the CO_2 capture process. CPSE has developed a novel rate based CO_2 absorber model based on the statistical fluid association theory for potential of variable range (SAFT-VR). This allows different correlations for the rate-based equations governing heat and mass transfer in the absorber to be examined. The reactions are treated implicitly, with the products of the chemical reactions treated as associated aggregates of the reactant molecules, so that there is no need for explicit rates of reaction.

Urban Energy Systems

The Urban Energy Systems project began several years ago with a study of the way in which energy is supplied to urban regions and subsequently converted to energy services.

The first year's programme assessed the state of the art in urban energy systems modeling and related disciplines, while the second year focused on developing our own modeling framework. More recent work has involved refining and extending this framework, developing an urban energy systems modeling and design tool and performing validation studies. The highlights of the year include the further development and demonstration of a hierarchical modeling framework (SynCity) for urban energy systems based on four interacting layered models, the enhancement of the SynCity tool and the generation of a large range of results via a series of case studies (Toronto, Melbourne, Lingang New City), which have provided useful insights into the design and operation of urban energy systems.

A number of additional projects are concerned with micro-generation, power generation and sustainable development. The introduction of micro-generation is changing the relationship between homeowners and the utilities. The electricity grid could eventually be seen not as a primary power supplier but as a back up to a micro-grid made up of a number of micro CHP generators. The planning and overall management of such micro-grids involves highly sophisticated decision making problems. As a result, we are working on the development of a systematic computer aided modeling framework and tool for optimal energy management and planing of microchip microgrids.



The objective of the Smart neighbourhood project is to optimize the one-day-ahead energy consumption cost of a home, which has access to a number of distributed energy supply options such as CHP and energy storage. Models have been developed which optimize the consumption schedule of domestic electrical appliances and the operation of distributed energy technologies to reduce equipment operation and maintenance costs and minimize the net electricity purchase cost by exporting surplus generation capacity to the grid. The results of a case study based on 90 homes with access to a CHP generator, a wind farm, a boiler and one thermal and one electrical storage unit showed an 11.6% cost saving and 24.6% power demand peak shaving.

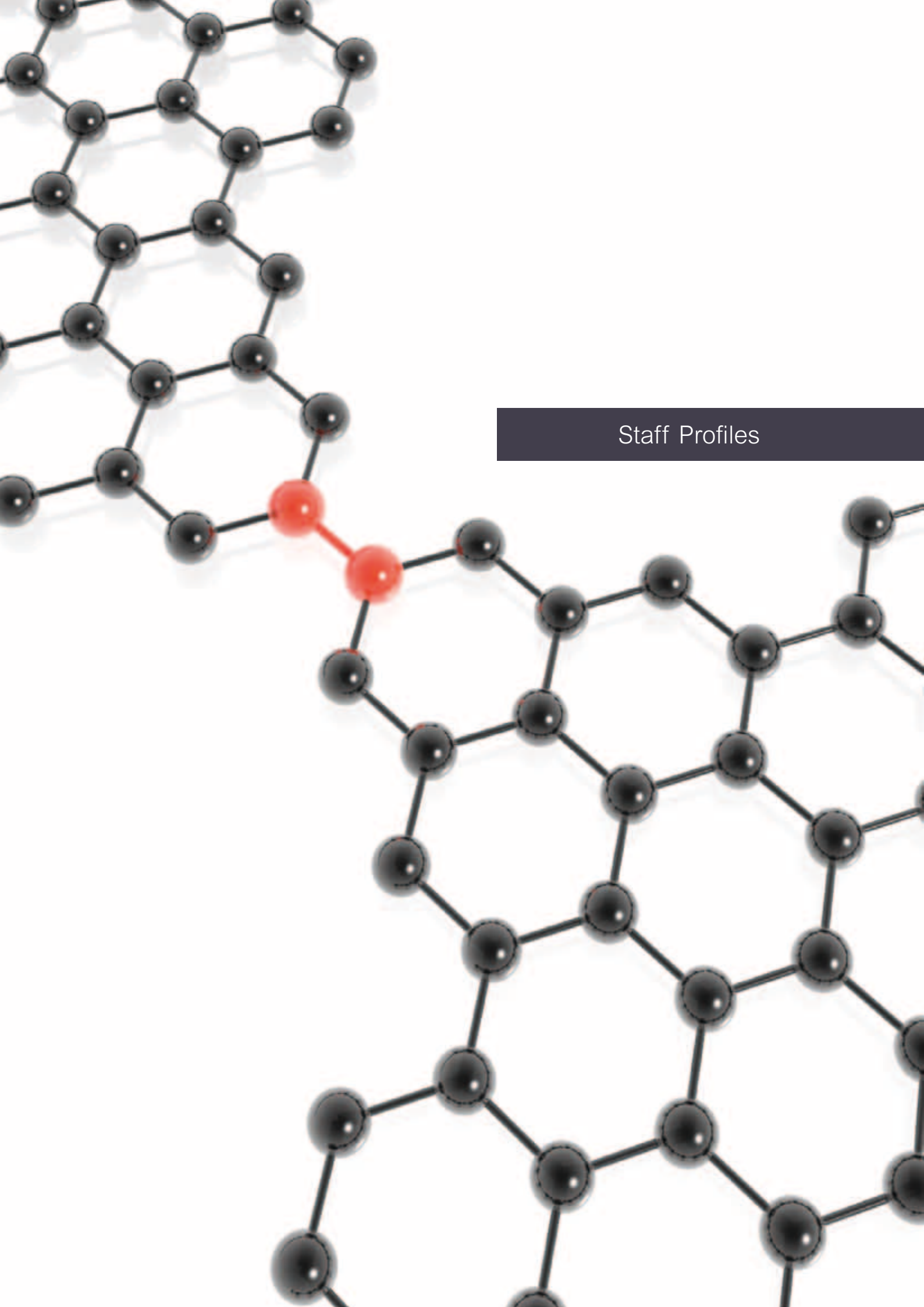
Collaboration with a major retail company to reduce the carbon footprint of commercial buildings has allowed CPSE to study the energy demand of a large state of the art supermarket in considerable detail at the consuming unit level. The resulting analysis revealed a number of control system and operational changes together with new energy supply options that have led to substantial energy cost reductions that can be integrated into other existing and new build stores. The project will continue with the object of arriving at a design for a 'zero carbon store', which appears to be feasible in the relatively short term.

With the size of wind turbine generators (WTG) increasing steadily, there has been a growing interest in alleviating structural fatigue through better control. For multi-megawatt WTG, transient operation such as emergency shut-down (EST) has received far less attention than normal power production operation, despite the fact that EST events can contribute significantly to the overall structural fatigue. This project is concerned with the development of a systematic, optimization-based methodology for fatigue minimization during EST procedures. Both off-line (open loop) and on-line (real-time optimization) aspects are investigated. Case studies show that fatigue reductions as high as 45-60% could be obtained at various above rated wind speeds using an optimised EST strategy.

The breadth of experience and ability to model a diverse range of energy systems has enabled CPSE to tackle the question of the London 2012 Olympic Park's sustainability. The Sustainable Development concept has recently become a part of the strategic plans of many industrial and business projects and operations. Quantitative systems analysis models are becoming one of the most important tools in SA because they can be used for more accurate forecasting in the decision-making processes.

The overall aim of this project is to define a comprehensive methodology of sustainability assessment of large international events. The case study for the project is the London 2012 Olympic Park. The main objectives are to identify the appropriate indicator and tool set for the sustainability assessment of the London Olympics; to develop a multi-objective optimisation model that includes key performance indicators; and to integrate the model with SA tool set in order to define a holistic methodology of sustainability assessment of mega-events such as the London Olympics and hence for the application in the future to similar projects.

The project has so far focused on energy, waste and water management models and has been assessing the value of alternative indicators as objective functions. We aim to consider the full time course from conception through construction, operation to legacy.



Staff Profiles

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
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
Editorial board, *Journal of Global Optimization*
AIChE: Technical area co-chair/chair for CAST10a, 2006-2008
IChemE: Committee Member, Computer-Aided Process Engineering group
EPSRC: Member of Peer Review College.
Member of scientific committee for PSE 2012
Member of organising committee for ESCAPE 22

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.

Industrial Collaborations
BMS, GSK, PSE, P&G, Scottish Power, Syngenta

Books Edited
1. Adjiman, C.S., Galindo, A. (Ed), "*Molecular Systems Engineering*" (Wiley-VCH, Germany), 2010 Includes 3 contributed chapters:

1a. Kazantsev, A.V., Karamertzanis, P.G., Pantelides, C.C., Adjiman, C.S., CrystalOptimizer: **An efficient algorithm for lattice energy minimisation of organic crystals using quantum mechanical calculations** Ch. 1 in "*Molecular Systems Engineering*", Adjiman, C.S., Galindo, A. ed (Wiley-VCH, Germany) 2010, 1-42

1b. Papaioannou, V., Adjiman, C. S., Jackson, G., Galindo, A. **Group contribution methodologies for the prediction of thermodynamic properties and phase behaviour in mixtures** Ch. 4 in "*Molecular Systems Engineering*", Adjiman, C.S., Galindo, A. ed (Wiley-VCH, Germany) 2010, 135-172

1c. Strübing, H., Konstantinidis, S., Karamertzanis, P.G., Pistikopoulos, E.N., Galindo, A., Adjiman, C. S. **Computer-aided methodologies for the design of reaction solvents**, Ch. 9 in "*Molecular Systems Engineering*", Adjiman, C.S., Galindo, A. ed (Wiley-VCH, Germany) 2010, 267-306

Journal Articles
1. Mac Dowell, N., Llovell, F., Adjiman, C.S., Jackson, G., Galindo, A., **Modeling the fluid phase behavior of carbon dioxide in aqueous solutions of monoethanolamine using transferable parameters with the SAFT-VR approach**, *Industrial and Engineering Chemistry Research*, 49 (2010) 1883-1899. DOI:10.1021/ie901014t. (0)
2. Shearing, P. R., Cai, Q., Golbert, J.I., Yufit, V., Adjiman, C.S., Brandon, N.P., **Microstructural analysis of a solid oxide fuel cell anode using focused ion beam techniques coupled with electrochemical simulation**, *Journal of Power Sources*, 195 (2010) 4804-4810
3. Pereira, F.E., Jackson, G., Galindo, A., Adjiman, C.S., **A duality-based optimisation approach for the reliable solution of (P,T) phase equilibrium in volume-composition space**, *Fluid Phase Equilibria*, 299 (2010) 1-23

4. Cai, Q., Luna-Ortiz, E., Adjiman, C.S., Brandon, N.P., **The effects of operating conditions on the performance of a solid oxide steam electrolyser: a model-based study**, *Fuel Cells*, 10 (2010) 1114-1128
5. Mac Dowell, N., Florin, N., Buchard, A., Hallett, J., Galindo, A., Jackson, G., Adjiman, C.S., Williams, C.K., Shah, N., Fennell, P. **An overview of Carbon Capture and Storage**, *Energy and Environmental Science*, 3 (2010) 1645-1669, DOI: 10.1039/c004106h
6. Pereira, F.E., Keskes, E., Galindo, A., Jackson, G., Adjiman, C.S., **Integrated solvent and process design using the SAFT-VR equation of state: high-pressure separation of CO_2 from CH4**, *Computers and Chemical Engineering*, 35 (2011) 474-491, doi:10.1016/j.compchemeng.2010.06.016
7. Kazantsev, A.V., Karamertzanis, P. G., Adjiman, C.S., Pantelides C.C., **Efficient handling of molecular flexibility in lattice energy minimization of organic crystals**, *Journal of Chemical Theory and Computation*, 7 (2011) 1998-2106
8. Artola, P.-A., Pereira, F.E., Adjiman, C.S., Galindo, A., Müller, E.A., Jackson, G., Haslam, A.J., **Understanding the thermodynamic behaviour of crude oil: Asphaltene precipitation**, *Fluid Phase Equilibria*, 306 (2011) 129-136
9. Kazantsev, A.V., Karamertzanis, P.G., Adjiman, C.S., Pantelides, C.C., Price, S.L., Galek, P.T.A., Day, G.M., Cruz-Cabeza, A.G., **Successful Prediction of the Crystal Structure of a Model Pharmaceutical in the 5th Blind Test**, *International Journal of Pharmaceutics*, 418 (2011) 168-178
10. Mac Dowell, N., Llovell, F., Blas, F. J., Adjiman, C.S., Jackson, G., Galindo, A. **Transferable SAFT-VR models for the calculation of the fluid phase equilibria in reactive mixtures of carbon dioxide, water and n-alkylamines in the context of carbon capture**, *J. Physical Chemistry B*, 115 (2011) 8155-8168
11. Papaioannou, V., Adjiman, C.S., Jackson, G., Galindo, A., **Simultaneous prediction of vapour-liquid and liquid-liquid equilibria (VLE and LLE) of aqueous mixtures with the SAFT-group contribution approach**, *Fluid Phase Equilibria*, 306 (2011) 82-96
12. Bardwell, D.A., Adjiman, C.S., Arnautova Y.A., Bartashevich E., Boerrigter S.X., Braun D.E., Cruz-Cabeza A.J., Day G.M., Della Valle R.G., Desiraju G.R., van Eijck B.P., Facelli J.C., Ferraro M.B., Grillo D., Habgood M., Hofmann D.W., Hofmann F., Jose K.V., Karamertzanis P.G., Kazantsev A.V., Kendrick J., Kuleshova L.N., Leusen F.J., Maleev A.V., Misquitta A.J., Mohamed S,. Needs R.J., Neumann M.A., Nikylov D., Orendt A.M., Pal R., Pantelides C.C., Pickard C.J., Price L.S., Price S.L., Scheraga H.A., van de Streek J., Thakur T.S., Tiwari S., Venuti E., Zhitkov I.K., **Towards crystal structure prediction of complex organic compounds – A report on the fifth blind test**, *Acta Crystallogr B*, 67 (2011) 535-551
13. Cai, Q., Adjiman, C.S., Brandon, N.P., **Investigation of the active thickness of solid oxide fuel cell electrodes using a 3D microstructure model**, *Electrochimica Acta*, 56, (2011) 5804-5814
14. Avendaño, C., Lafitte, T., Galindo, A., Adjiman, C. S., Jackson, G., Müller, E. A., **SAFT- force field for the simulation of molecular fluids: I. A single-site coarse grained model of carbon dioxide**, The Journal of Physical Chemistry B 115 (2011) 11154-11169

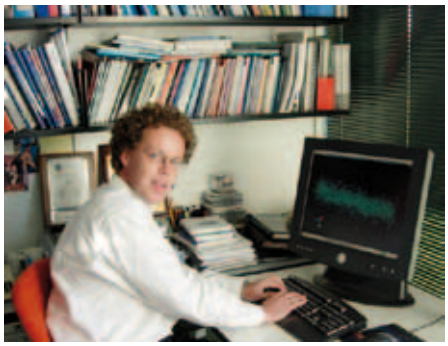
Selected Refereed Conference Publications

1. Cai, Q., Brandon, N.P., Adjiman, C.S., **Modelling the dynamic response of a solid oxide steam electrolyser to transient inputs during renewable hydrogen production**, *Frontiers of Energy and Power Engineering*, China, 2010. DOI 10.1007/s11708-010-0037-6, In press
2. Kazantsev, A.V., Karamertzanis, P.G., Adjiman, C.S., Pantelides, C.C., **Ab initio Crystal Structure Prediction of Flexible Molecules**, ESCAPE20, 6-9 June 2010, Ischia, Italy. pp. 817-822
3. Strübing, H., Karamertzanis, P.G., Pistikopoulos, E.N., Galindo, A., Adjiman, C.S., **Solvent design for a Menschutkin reaction by using CAMD and DFT calculations**, ESCAPE20, 6-9 June 2010, Ischia, Italy. pp. 1291-1296
4. Pereira, F.E., Jackson, G., Galindo, A., Adjiman, C.S., **Robust algorithms for the calculation of phase equilibrium**, ESCAPE20, 6-9 June 2010, Ischia, Italy. pp.79-84
5. Mac Dowell, N., Galindo, A., Jackson, G., Adjiman, C.S., **Integrated solvent and process design for the reactive separation of CO_2 from flue gas**, ESCAPE20, 6-9 June 2010, Ischia, Italy, pp. 1231-1236
6. Cai, Q., Shearing, P. R., Adjiman, C.S., Brandon, N.P., **Design of solid oxide fuel cell electrodes**, European Fuel Cell Forum, 29 June-2 July 2010, Lucerne, Switzerland. In press
7. Kleniati, P. M., Adjiman, C.S. **Global Optimisation of optimistic bi-level programming problems**, 21st European Symposium on Computer-Aided Process Engineering, Pistikopoulos, E.N., Georgiadis, M. C., Kokossis, A.C. (Ed), vol 29A (2011) 602-606
8. Siougkrou, E., Galindo, A., Adjiman, C.S., **Integrated design of a reactor and a gas-expanded solvent**, 21st European Symposium on Computer-Aided Process Engineering, Pistikopoulos, E.N., Georgiadis, M. C., Kokossis, A.C. (Ed), vol 29A (2011) 316-320
9. Papaioannou, V., Lafitte, T., Adjiman, C.S., Galindo, A., Jackson, G., **Simultaneous prediction of phase behaviour and derivative properties with a SAFT-type group contribution method**, 21st European Symposium on Computer-Aided Process Engineering, Pistikopoulos, E.N., Georgiadis, M. C., Kokossis, A.C. (Ed), vol 29B (2011) 1593-1597

Invited lectures and Seminars

1. **Formulations of the molecular design problem**, European Workshop on MINLP, Centre International de Rencontres Mathématiques, Marseille , 13 April 2010
2. **The design of solvent-based reactive systems**, Strathclyde University, Glasgow, Department of Chemical Engineering, 23 January 2010

3. **New formulations of mixture design**, EURO, Lisbon, 14 July 2010
4. **The role of the SAFT equation of state in product and process design**, SAFT 2010, Barcelona, 21 September 20105. **The design of solvent-based reactive systems: from molecules to process**, Northwestern University, IL, USA, Department of Chemical Engineering, 14 October 2010
6. **The reliable solution of (P,T) phase equilibrium and stability in the volume-composition space**, Argonne National Laboratory, Argonne, IL, 15 October 2010
7. **Process design: don't take the molecules for granted**,
8. **The integrated design of optimal molecules and processes**, Thermodynamics 2011, Athens, September 2011
9. **The expanding envelope of process design: from molecules to processes**, Universitat Rovira i Virgili, 25 November 2011



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-

Industrial Research experience
Schlumberger Cambridge Research, Senior Research Scientist, 1994-2009

Research Interests
My research is aimed at complex fluids and flow in porous media. Applications include Enhanced Oil Recovery (EOR), Carbon Capture and Storage (CCS), flow assurance and oilfield fluids for drilling and hydraulic fracturing. Our team investigates how the complex flow behaviour emerges from the underlying fluid properties combined with pore scale physics and chemistry. For this purpose, we are developing a combination of experimental and computer simulation techniques. The experiments include multi-scale imaging of multi-component flow in porous media using micro CT, medical CT and confocal microscopy; micro-fluidic flow of reservoir fluids in etched 2D micro-models; and rheology of complex fluids. The computer simulations are aimed at explaining the complex fluid behaviour observed and include a range of statistical mechanical simulation techniques, across length and time scales, including Multi-Particle Collision Dynamics (MPCD), Lattice-Boltzmann (LB), Molecular Dynamics, Dissipative Particle Dynamics and Brownian Dynamics.

Other Activities
Member, Editorial Advisory Board of Energy and Fuels, American Chemical Society
Chairman and organiser of Petrophase Conference 2011 – Imperial College London
Member, International Advisory Committee 8th Liquid Matter Conference Universität Wien, Vienna, Austria September 2011, European Physical Society
member of management committee, Statistical Mechanics and Thermodynamics Group, Royal Society of Chemistry
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

Journal Articles

1. Lawal KA, Vesovic V, Boek ES, **Modeling Permeability Impairment in Porous Media due to Asphaltene Deposition under Dynamic Conditions**, *ENERG FUEL*, 2011, Vol:25, Pages:5647-5659, ISSN:0887-0624
2. Stukan MR, Ligneul P, Crawshaw JP, Boek ES, **Spontaneous imbibition in nanopores of different roughness and wettability**, *Langmuir*, 2010, Vol:26, Pages:13342-13352

3. Boek ES, Venturoli M, **Lattice-Boltzmann studies of fluid flow in porous media with realistic rock geometries**, *COMPUT MATH APPL*, 2010, Vol:59, Pages:2305-2314, ISSN:0898-1221

Conference Contributions

1. Headen TF, Boek ES, **Molecular Dynamics Simulations of Asphaltene Aggregation in Supercritical Carbon Dioxide with and without Limonene**, 2011, Pages:503-508, ISSN:0887-0624
2. Headen TF, Boek ES, **Potential of Mean Force Calculation from Molecular Dynamics Simulation of Asphaltene Molecules on a Calcite Surface**, 2011, Pages:499-502, ISSN:0887-0624

I David L. Bogle

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

Qualifications
BSc (Eng) Hons MSc PhD DIC CEng

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. Member of College of Engineering for the Engineering & Physical Sciences Research Council (EPSRC). Member of BBSRC Integration and Systems Biology Strategy Panel. Member of BBSRC Bioscience Skills and Careers Panel. 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 Board of Engineering Council UK. Chair Engineering Council Working Groups on Sustainability and on Risk. Member of Royal Academy Research and Secondments Committee, Chair Royal Academy of Engineering Distinguished Visiting Fellowship Scheme. Chair League of European Research Universities Doctoral Studies Community.

Reviewer for
BBSRC, EPSRC, Royal Academy of Engineering, Industrial and Engineering Chemistry Research, Computers and Chemical Engineering, Fluid Phase Equilibria, J Process Control, Int J of Systems Science.

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

Industrial Collaborations
PricewaterhouseCoopers

Journal Articles

1. BOGLE I.D.L., ALLEN R., and SUMNER T. (2010) **The role of Computer Aided Process Engineering in Physiology and Clinical Medicine**. *Comp Chem Engng*. 34 763-769
2. MA K., VALDES GONZALES H., and BOGLE I.D.L. (2010) **Process design in SISO systems with input multiplicity using bifurcation analysis and optimisation**. *Journal of Process Control*, 20,/3 241-247
3. ALLEN R., RIDLEY A. and BOGLE I.D.L. (2011) **A Model of Localised Rac1 Activation in Endothelial Cells due to Fluid Flow**. *J Theoretical Biology* 280/1 7 July 34-42
4. HETHERINGTON J., SUMNER T., SEYMOUR R.M., LI L., VARELA REY M., MARGONINSKI O., BOGLE I.D.L., FINKELSTEIN A., and WARNER A. (2011) **A composite computational model of liver glucose homeostasis. Part 1: Building the composite model**. *J Roy Soc Interface* June 15, 2011, doi: 10.1098/rsif.2011.0141

Invited Talks

1. **Engineering Council UK Guidelines for Risk' Engineering** Professors Council Annual Congress, London, April 2011

Nigel Brandon

Director of the Energy Futures Lab, Department of Chemical Engineering, Imperial College London

Qualifications

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

Awards and Distinctions

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
2007 PI of £4.2 million 'New and Renewable Solar Routes to Hydrogen Energy', the largest grant awarded by EPSRC in this field
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
2005 Management hub of £2.1 million EPSRC 'Supergen' fuel cell consortia

Research Interests

Nigel Brandon's research is focused on electrochemical power sources such as fuel cells, batteries, and hybrid systems. He collaborates extensively with industry in this field, as well with other research centres and universities around the world, and he leads the EPSRC 'Supergen' Fuel Cell consortia. He is the Director of the Energy Futures Lab at Imperial College (www.imperial.ac.uk/energyfutureslab), which is leading cross-faculty, interdisciplinary energy research programmes across the College. He is a founder of Ceres Power (www.cerespower.com), an AIM listed fuel cell company spun out from Imperial College.

Other Activities

Fellow, Royal Academy of Engineering
Fellow, The City and Guild of London Institute
Fellow, Royal Society of arts, manufacturing and commerce
Fellow, Energy Institute
Fellow, Institute of Materials, Minerals and Mining

Reviewer for

Frontier of Energy and Power Engineering in China, Editorial Board
Journal of Power and Energy, Editorial Board
ChemSusChem - energy and materials, Editorial Board
Fuel cells - from fundamentals to systems, Editorial Board

Journal Articles

1. Brandon NP, **Understanding solid oxide fuel cell microstructure**, *Abstracts Of Papers Of The American Chemical Society*, 2010, Vol:239, ISSN:0065-7727
2. Cai Q, Adjiman CS, Brandon NP, **Investigation of the active thickness of solid oxide fuel cell electrodes using a 3D microstructure model**, *Electrochimica Acta*, 2011, Vol:56, Pages:10809-10819, ISSN:0013-4686
3. Ang SMC, Fraga ES, Brandon NP, et al, **Fuel cell systems optimisation – Methods and strategies**, *INT J HYDROGEN ENERG*, 2011, Vol:36, Pages:14678-14703, ISSN:0360-3199
4. Kehrwald D, Shearing PR, Brandon NP, et al, **Local Tortuosity Inhomogeneities in a Lithium Battery Composite Electrode**, *J ELECTROCHEM SOC*, 2011, Vol:158, Pages:A1393-A1399, ISSN:0013-4651
5. Zhang XQ, Su SH, Chen JC, et al, **A new analytical approach to evaluate and optimize the performance of an irreversible solid oxide fuel cell-gas turbine hybrid system**, *INT J HYDROGEN ENERG*, 2011, Vol:36, Pages:15304-15312, ISSN:0360-3199
6. Liso V, Zhao YR, Brandon N, et al, **Analysis of the impact of heat-to-power ratio for a SOFC-based mCHP system for residential application under different climate regions in Europe**, *INT J HYDROGEN ENERG*, 2011, Vol:36, Pages:13715-13726, ISSN:0360-3199
7. Zhao YR, Sadhukhan J, Lanzini A, et al, **Optimal integration strategies for a syngas fuelled SOFC and gas turbine hybrid**, *J POWER SOURCES*, 2011, Vol:196, Pages:9516-9527, ISSN:0378-7753
8. Liu M, Millan MG, Aravind PV, et al, **Influence of Operating Conditions on Carbon Deposition in SOFCs Fuelled by Tar-Containing Biosyngas**, *J ELECTROCHEM SOC*, 2011, Vol:158, Pages:B1310-B1318, ISSN:0013-4651
9. Thiedmann R, Stenzel O, Spettl A, et al, **Stochastic simulation model for the 3D morphology of composite materials in Li-ion batteries**, *COMP MATER SCI*, 2011, Vol:50, Pages:3365-3376, ISSN:0927-0256
10. Shearing PR, Bradley RS, Gelb J, et al, **Using Synchrotron X-Ray Nano-CT to Characterize SOFC Electrode Microstructures in Three-Dimensions at Operating Temperature**, *ELECTROCHEM SOLID ST*, 2011, Vol:14, Pages:B117-B120, ISSN:1099-0062
11. Clague R, Shearing PR, Lee PD, et al, **Stress analysis of solid oxide fuel cell anode microstructure reconstructed from focused ion beam tomography**, *J POWER SOURCES*, 2011, Vol:196, Pages:9018-9021, ISSN:0378-7753
12. Zhao YR, Shah N, Brandon N, **Comparison between two optimization strategies for solid oxide fuel cell-gas turbine hybrid cycles**, *INT J HYDROGEN ENERG*, 2011, Vol:36, Pages:10235-10246, ISSN:0360-3199

13. Yufit V, Shearing P, Hamilton RW, et al, **Investigation of lithium-ion polymer battery cell failure using X-ray computed tomography**, *ELECTROCHEM COMMUN*, 2011, Vol:13, Pages:608-610, ISSN:1388-2481
14. Cai Q, Adjiman CS, Brandon NP, **Modelling the 3D microstructure and performance of solid oxide fuel cell electrodes: Computational parameters**, *Electrochimica Acta*, 2011, Vol:56, Pages:5804-5814, ISSN:0013-4686
15. Millichamp J, Ali E, Brandon NP, et al, **Application of a GaPO4 Crystal Microbalance for the Detection of Coke Formation in High-Temperature Reactors and Solid Oxide Fuel Cells**, *IND ENG CHEM RES*, 2011, Vol:50, Pages:8371-8375, ISSN:0888-5885
16. Matian M, Marquis A, Brandon N, **Model based design and test of cooling plates for an air-cooled polymer electrolyte fuel cell stack**, *INT J HYDROGEN ENERG*, 2011, Vol:36, Pages:6051-6066, ISSN:0360-3199
17. Somalu MR, Yufit V, Cumming D, et al, **Fabrication and characterization of Ni/ScSZ cermet anodes for IT-SOFCs**, *INT J HYDROGEN ENERG*, 2011, Vol:36, Pages:5557-5566, ISSN:0360-3199
18. Konda NVSNM, Shah N, Brandon NP, **Optimal transition towards a large-scale hydrogen infrastructure for the transport sector: The case for the Netherlands**, *INT J HYDROGEN ENERG*, 2011, Vol:36, Pages:4619-4635, ISSN:0360-3199
19. Mermelstein J, Milian M, Brandon NP, **The interaction of biomass gasification syngas components with tar in a solid oxide fuel cell and operational conditions to mitigate carbon deposition on nickel-gadolinium doped ceria anodes**, *J POWER SOURCES*, 2011, Vol:196, Pages:5027-5034, ISSN:0378-7753
20. Brandon N, **Special issue on fuel cells for stationary applications,** *P I MECH ENG A-J POW*, 2011, Vol:225, Pages:151-151, ISSN:0957-6509
21. Hawkes AD, Brett DJL, Brandon NP, **Role of fuel cell based micro-cogeneration in low carbon heating**, *P I MECH ENG A-J POW*, 2011, Vol:225, Pages:198-207, ISSN:0957-6509
22. Offer GJ, Contestabile M, Howey DA, et al, **Techno-economic and behavioural analysis of battery electric, hydrogen fuel cell and hybrid vehicles in a future sustainable road transport system in the UK**, *Energy Policy*, 2011, Vol:39, Pages:1939-1950, ISSN:0301-4215
23. Patcharavorachot Y, Brandon NP, Paengjuntuek W, et al, **Analysis of planar solid oxide fuel cells based on proton-conducting electrolyte**, *SOLID STATE IONICS*, 2010, Vol:181, Pages:1568-1576, ISSN:0167-2738
24. Cai Q, Luna-Ortiz E, Adjiman CS, et al, **The Effects of Operating Conditions on the Performance of a Solid Oxide Steam Electrolyser: A Model-Based Study**, *Fuel Cells*, 2010, Vol:10, Pages:1114-1128, ISSN:1615-6854
25. Cai Q, Adjiman CS, Brandon NP, **Modelling the dynamic response of a solid oxide steam electrolyser to transient inputs during renewable hydrogen production**, *Frontiers of Energy and Power* Engineering in China, 2010, Vol:4, Pages:211-222
26. Matian M, Marquis A, Brett D, et al, **An experimentally validated heat transfer model for thermal management design in polymer electrolyte membrane fuel cells**, *P I MECH ENG A-J POW*, 2010, Vol:224, Pages:1069-1081, ISSN:0957-6509
27. Shearing PR, Brett DJL, Brandon NP, **Towards intelligent engineering of SOFC electrodes: a review of advanced microstructural characterisation techniques**, *INT MATER REV*, 2010, Vol:55, Pages:347-363, ISSN:0950-6608
28. Iora P, Taher MAA, Chiesa P, et al, **A novel system for the production of pure hydrogen from natural gas based on solid oxide fuel cell-solid oxide electrolyzer**, *INT J HYDROGEN ENERG*, 2010, Vol:35, Pages:12680-12687, ISSN:0360-3199
29. Matian M, Marquis A, Brandon NP, **Application of thermal imaging to validate a heat transfer model for polymer electrolyte fuel cells**, *INT J HYDROGEN ENERG*, 2010, Vol:35, Pages:12308-12316, ISSN:0360-3199
30. Sadhukhan J, Zhao YR, Leach M, et al, **Energy Integration and Analysis of Solid Oxide Fuel Cell Based Microcombined Heat and Power Systems and Other Renewable Systems Using Biomass Waste Derived Syngas**, *IND ENG CHEM RES*, 2010, Vol:49, Pages:11506-11516, ISSN:0888-5885
32. Yufit V, Brandon NP, **Development and application of an actively controlled hybrid proton exchange membrane fuel cell-Lithium-ion battery laboratory test-bed based on off-the-shelf components**, *J POWER SOURCES*, 2011, Vol:196, Pages:801-807, ISSN:0378-7753
33. Cai Q, Brett DJL, Browning D, et al, **A sizing-design methodology for hybrid fuel cell power systems and its application to an unmanned underwater vehicle**, *Journal of Power Sources*, 2010, Vol:195, Pages:6559-6569, ISSN:0378-7753
34. Ivey DG, Brightman E, Brandon N, **Structural modifications to nickel cermet anodes in fuel cell environments**, *J POWER SOURCES*, 2010, Vol:195, Pages:6301-6311, ISSN:0378-7753
35. Brett DJ, Kucernak AR, Aguiar P, et al, **What happens inside a fuel cell? Developing an experimental functional map of fuel cell performance.**, *Chemphyschem*, 2010, Vol:11, Pages:2714-2731
36. Shearing PR, Cai Q, Golbert JI, et al, **Microstructural analysis of a solid oxide fuel cell anode using focused ion beam techniques coupled with electrochemical simulation**, *J POWER SOURCES*, 2010, Vol:195, Pages:4804-4810, ISSN:0378-7753
37. Shearing PR, Gelb J, Yi J, et al, **Analysis of triple phase contact in Ni-YSZ microstructures using non-destructive X-ray tomography with synchrotron radiation**, *ELECTROCHEM COMMUN*, 2010, Vol:12, Pages:1021-1024, ISSN:1388-2481
38. Shearing PR, Gelb J, Brandon NP, **X-ray nano computerised tomography of SOFC electrodes using a focused ion beam sample-preparation technique**, *J EUR CERAM SOC*, 2010, Vol:30, Pages:1809-1814, ISSN:0955-2219

39. Weng X, Brett D, Yufit V, et al, **Highly conductive low nickel content nano-composite dense cermets from nano-powders made via a continuous hydrothermal synthesis route**, *Solid State Ionics*, 2010, Vol:181, Pages:827-834
40. Sadhukhan J, Zhao YR, Shah N, et al, **Performance analysis of integrated biomass gasification fuel cell (BGFC) and biomass gasification combined cycle (BGCC) systems**, *CHEM ENG SCI*, 2010, Vol:65, Pages:1942-1954, ISSN:0009-2509
41. Shearing PR, Howard LE, Jorgensen PS, et al, **Characterization of the 3-dimensional microstructure of a graphite negative electrode from a Li-ion battery**, *ELECTROCHEM COMMUN*, 2010, Vol:12, Pages:374-377, ISSN:1388-2481
42. Bidault F, Brett DJL, Middleton PH, et al, **An improved cathode for alkaline fuel cells**, *INT J HYDROGEN ENERG*, 2010, Vol:35, Pages:1783-1788, ISSN:0360-3199
43. Offer G, Howey D, Contestabile M, et al, **Comparative analysis of battery electric, hydrogen fuel cell and hybrid vehicles in a future sustainable road transport system**, *Energy Policy*, 2010, Vol:38, Pages:24-29
44. Panos C, Kouramas KI, Georgiadis MC, et al, **Modelling and Explicit MPC of PEM Fuel Cell Systems**, *Computer Aided Chemical Engineering*, 2010, Vol:28, Pages:517-522

Invited Lectures and Seminars

Alternative energy – looking into the future, The British lecture series, Qongqing, China, 2010

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

Automatica Outstanding Reviewer Award, 2007
Lavoisier Postdoctoral Fellowship, 2003–2004
Outstanding PhD Thesis Award, INPL, 2002

Research Interests

- Environmental systems engineering, especially synthesis and design of biorefineries for wastewater, integrated design and operation of miroalgae photobioreactors
- Systematic methodologies for design and operation under uncertainty
- Real time optimization of dynamic and complex processes
- Development of new methods and tools for deterministic global optimization

Other Activities

- International Energy Agency (IEA), Annex IX, Leader for Task 2: Design & Operation Methodologies for Separation
- International Scientific Committee & Theme Coordinator, ESCAPE21
- Guest Editor, Optimal Control Applications and Methods (OCAM), special issue on Optimal Process Control (Volume 31, Issue 5)
- Advisory Committee, Industrial Optimization Seminar Series, Fields Institute, University of Toronto
- International Scientific Committee, ESCAPE20
- Invited Lecturer, PASI Workshop, Two-Day Course on “Global Optimization Methods and Tools”, Angra dos Reis, Brazil
- Adjunct Professor, Department of Chemical Engineering, McMaster University, Canada

Reviewer Activities

AIChE Journal; Automatica; Applied Numerical Mathematics; Chemical Engineering Research & Design; Computers & Chemical Engineering; Industrial & Engineering Chemistry Research; Journal of Global Optimization; Journal of Optimization Theory & Applications; Journal of Process Control; Mathematical Programming; Optimal Control Applications & Methods; Optimization & Engineering.

Academic Collaborations

MIT, USA, Dpt Chemical Engineering (Prof. Barton),
Dpt Mechanical Engineering (Prof. Mitsos)
EPFL, Swtizerland, Automatic Control Lab (Prof. Bonvin)
INRIA Sophia Antipolis, France, BIOCORE Group (Dr. Bernard)
INRA, France, LBE Narbonne (Dr. Steyer)
STUBA, Slovakia, Dpt Chemical Engineering (Prof. Fikar)

Industrial Collaborations

Petrobras, Praxair, Syngenta

Journal Articles

1. Khor, C.S., S. Giarola, B. Chachuat, N. Shah, **An Optimization-based Framework for Process Planning under Uncertainty with Risk Management**, *Chemical Product & Process Modeling*, 6(2):4, 2011
2. Shalodin, A.M., B. Chachuat, **Convex/concave relaxations of parametric ODEs using Taylor models**, *Computers & Chemical Engineering*, 35(5):844-857, 2011
3. Shalodin, A.M., B. Chachuat, **Discretize-then-Relax Approach for Convex/Concave Relaxations of the Solutions of Parametric ODEs**, *Applied Numerical Mathematics*, 61(7):803-820, 2011

4. Marchetti, A., A. Gopalakrishnan, B. Chachuat, D. Bonvin, L. Tsikonis, A. Nakajo, Z. Wuillemin, J. Van Herle, **Real-Time Optimization of a Solid Oxide Fuel Cell Stack**, *Journal of Fuel Cell Science & Technology*, 8(5):051001, 2011
5. Marchetti, A., B. Chachuat, D. Bonvin, **A Dual Modifier-Adaptation Approach for Real-Time Optimization**, *Journal of Process Control*, 20(9):1027-1037, 2010
6. Chachuat, B., A. Mitsos, P.I. Barton, **Optimal Start-up of Micro Power Generation Processes Employing Fuel Cells**, *Optimal Control Applications & Methods*, 31(5):471-495, 2010. Chachuat B., "Introduction to the Special Issue on Optimal Process Control," Optimal Control Applications & Methods, 31(5):391-392

Book Chapters

1. Chachuat, B., **Optimal Design and Steady-State Operation**. In: Mitsos A., Barton P.I., (Eds.), Microfabricated Power Generation Devices. *Design and Technology*, Chapter 11, pp. 199-222, Wiley-VCH, 2010 (ISBN: 978-3-527-32081-3)

Conference Contributions

1. Cameron, E.T., Mairet F., Bernard O., Ras M., Lardon L., Steyer J.-P., Chachuat B., **Anaerobic Digestion of Microalgae: Identification for Optimization and Control**, 18th IFAC World Congress (IFAC'11), Aug 28 - Sep 2, 2011, Milano, Italy
2. Rodger E., Chachuat B., **Design Methodology of Modifier Adaptation for On-Line Optimization of Uncertain Processes**," 18th IFAC World Congress (IFAC'11), Aug 28 - Sep 2, 2011, Milano, Italy
3. Podmajersky, M., Chachuat B., Fikar M., **Integrated Two-Time-Scale Scheme for Real-time Optimisation of Batch Processes**, 18th IFAC World Congress (IFAC'11), Aug 28 - Sep 2, 2011, Milano, Italy
4. Sahlodin, A.M., Chachuat B. **Tight Convex and Concave Relaxations via Taylor Models for Global Dynamic Optimization**, 21th European Symposium on Computer Aided Process Engineering (ESCAPE21), May 28 - Jun 1, 2011, Porto Caras, Greece
5. Deshpande, S., Bonvin D., Chachuat B. **Selective Input Adaptation in Parametric Optimal Control Problems Having Path Constraints**, 8th IFAC Symposium on Nonlinear Control Systems (NOLCOS), Sep 1 - 3, 2010, Bologna, Italy
6. Sahlodin, A.M., Chachuat B. **Discretize-then-Relax Approach for State Relaxations in Global Dynamic Optimization**, 20th European Symposium on Computer Aided Process Engineering (ESCAPE20), Jun 6 – 9, 2010, Ishia, Italy
7. Deshpande, S., Bonvin D., Chachuat B. **Selective Input Adaptation in Parametric Optimal Control Problems Involving Terminal Constraints**, American Control Conference (ACC), Jun 30 - Jul 2, 2010, Baltimore, MD

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, Refinery-wide optimization, Solvent Extraction based Water Desalination, Synthetic Biology

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

Reviewer for
Industrial and Engineering Chemistry Research, Computers and Chemical Engineering, Journal of Global Optimization, Automatica

Journal Articles

1. Gueddar, T. and Dua, V. (2012). **Novel model reduction techniques for refinery-wide energy optimisation**. *Applied Energy* 89, 117–126
2. 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*, in press
3. Gueddar, T. and Dua, V. (2011). **Disaggregation–aggregation based model reduction for refinery-wide Optimization**. *Computers and Chemical Engineering*, 35, 1838– 1856
4. Dua, V. (2011). **An artificial neural network approximation based decomposition approach for parameter estimation of system of ordinary differential equations**. *Computers and Chemical Engineering*, 35, 545-553

Conference Contributions

1. Polykarpou, E.M. and Dua, V. (2012) **Sustainable water desalination: Model-based optimisation of a low-temperature liquid-liquid extraction process**, accepted for publication in the proceedings of the 22nd European Symposium on Computer-Aided Process Engineering
2. Dua, V. (2012) **Model-Based Optimal Control of Non-Viral Gene Delivery**, accepted for publication in the proceedings of the 22nd European Symposium on Computer-Aided Process Engineering
3. Gueddar, T. and Dua, V. (2011) **Approximate Multi-Parametric Programming based B&B Algorithm for MINLPs**, 21st European Symposium on Computer-Aided Process Engineering Book Series: Computer-Aided Chemical Engineering, Pistikopoulos EN; Georgiadis MC; Kokossis AC (editors), 29, 798-802
4. Thanapalan, K. and Dua, V. (2011) **Using Low-Grade Heat for Solvent Extraction based Efficient Water Desalination**, 21st European Symposium on Computer-Aided Process Engineering Book Series: Computer-Aided Chemical Engineering, Pistikopoulos EN; Georgiadis MC; Kokossis AC (editors), 29, 1703-1707

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

Journal Articles

1. S M C Ang, D J L Brett, I Staffell, A D Hawkes, E S Fraga & N P Brandon (to appear), **Design of fuel cell micro-cogeneration systems through modelling and optimisation**, review article, Wiley Interdisciplinary Reviews: *Energy and Environment*.
2. S M C Ang, E S Fraga, N P Brandon, NJ Samsatli & D J L Brett (2011), **Fuel cell systems optimisation – methods and strategies**, review article in the *International Journal of Hydrogen Energy* 36 (22):14678-14703.
3. S M C Ang, D J L Brett & E S Fraga (2011), **Optimal design of fuel cell systems**, in A E Johnson and E C Williams (editors), *Fuel Cell Efficiency* (Nova Science Publishers), to appear

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

Computer aided process engineering, specializing in automated process synthesis and the use of Internet related tools for collaborative design. The use of visualisation and knowledge discovery methods for the generation of insight in process design.

Other Activities

EPSRC: Member of Peer Review College
Member of the International Editorial Board for the Information Technology and Control journal

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)

Reviewer for

AIChE Journal
Fluid Phase Equilibria
Indian Journal of Pure and Applied Physics and Journal of Molecular Liquids.
Industrial and Engineering Chemistry Research
Journal of Chemical Engineering Data
Journal of Chemical Physics
Journal of Physical Chemistry B
Molecular Physics
Journal of Supercritical Fluids

Academic Collaborations

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

Industrial Collaborations

IFP, BMS, P&G, PSE Ltd, QatarPetroleum, Shell, Syngenta, Total

Books

1. **Molecular Systems Engineering**, Vol. 6 of *Process Systems Engineering Series*, Volume editors, C. Adjiman and A. Galindo, Wiley-VCH (2010)

Book Chapters

1. V. Papaioannou, C. S. Adjiman, G. Jackson, A. Galindo, **Group contribution methodologies for the prediction of thermodynamic properties and phase behaviour in mixtures**, in *Molecular Systems Engineering*, C.S. Adjiman and A. Galindo (Eds), Wiley-VCH, 2010
2. H. Strübing, S. Konstantinidis, P.G. Karamertzanis, E.N. Pistikopoulos, A. Galindo, C. S. Adjiman, **Computer-aided methodologies for the design of reaction solvents**, in *Molecular Systems Engineering*, C.S. Adjiman and A. Galindo (Eds), Wiley-VCH, 2010
3. C. McCabe and A. Galindo, **SAFT Associating Fluids and Fluid Mixtures**, In *Applied Thermodynamics* of Fluids; Goodwin, A. R. H. and Sengers, J. V., Eds.; Royal Society of Chemistry (2010)

Journal Articles

1. C. Avendaño, T. Lafitte, A. Galindo, C. S. Adjiman, G. Jackson and E. A. Müller, **SAFT-g force field for the simulation of molecular fluids:I. A single-site coarse-grained model of carbon dioxide**, *Journal of Physical Chemistry B*, 115, 11154-11169 (2011)
2. E. Forte, A. Galindo, and J. P. M. Trusler, **Experimental and molecular modeling study of the three-phase behavior of (n-decane + carbon dioxide + water) at reservoir conditions**, *Journal of Physical Chemistry B*, 115, 14591–14609 (2011)
3. F. E. Pereira, G. Jackson, A. Galindo and C. S. Adjiman, **The HELD algorithm for multicomponent, multiphase equilibrium calculations with generic equations of state**, *Computers and Chemical Engineering*, 36, 99-118 (2012)
4. L. Morales-Anda, H. H. Wensink, A. Galindo and A. Gil-Villegas, **Anomalous columnar order of charged colloidal platelets**, *The Journal of Chemical Physics*, 136, 034901 (2012)
5. Mac Dowell N, Pereira FE, Llovell F, et al, **Transferable SAFT-VR models for the calculation of the fluid phase equilibria in reactive mixtures of carbon dioxide, water, and n-alkylamines in the context of carbon capture.**, *J Phys Chem B*, 2011, Vol:115, Pages:8155-8168
6. Forte E, Llovell F, Vega LF, et al, **Application of a renormalization-group treatment to the statistical associating fluid theory for potentials of variable range (SAFT-VR)**., *J Chem Phys*, 2011, Vol:134
7. Pereira FE, Keskes E, Galindo A, et al, **Integrated solvent and process design using a SAFT-VR thermodynamic description: High-pressure separation of carbon dioxide and methane**, *COMPUTERS & CHEMICAL ENGINEERING*, 2011, Vol:35, Pages:474-491, ISSN:0098-1354
8. Macchietto S, Hewitt GF, Coletti F, et al, **Fouling in Crude Oil Preheat Trains: A Systematic Solution to an Old Problem**, *HEAT TRANSFER ENGINEERING*, 2011, Vol:32, Pages:197-215, ISSN:0145-7632
9. Mac Dowell N, Galindo A, Jackson G, et al, **Integrated solvent and process design for the reactive separation of CO(2) from flue gas**, *20TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING*, 2010, Vol:28, Pages:1231-1236, ISSN:1570-7946
10. Pereira FE, Jackson G, Galindo A, et al, **Robust algorithms for the calculation of phase equilibrium**, *20TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING*, 2010, Vol:28, Pages:79-84, ISSN:1570-7946

12. Georgiadis A, Llovell F, Bismarck A, et al, **Interfacial tension measurements and modelling of (carbon dioxide plus n-alkane) and (carbon dioxide plus water) binary mixtures at elevated pressures and temperatures**, *JOURNAL OF SUPERCRITICAL FLUIDS*, 2010, Vol:55, Pages:743-754, ISSN:0896-8446
17. Pereira FE, Jackson G, Galindo A, et al, **A duality-based optimisation approach for the reliable solution of (P, T) phase equilibrium in volume-composition space**, *FLUID PHASE EQUILIBRIA*, 2010, Vol:299, Pages:1-23, ISSN:0378-3812
20. Mac Dowell N, Florin N, Buchard A, et al, **An Overview of CO_2 capture technologies**, *Energy and Environmental Science*, 2010, Vol:3, Pages:1645-1669
23. Llovell F, Galindo A, Blas FJ, et al, **Classical density functional theory for the prediction of the surface tension and interfacial properties of fluids mixtures of chain molecules based on the statistical associating fluid theory for potentials of variable range.**, *J Chem Phys*, 2010, Vol:133
26. Karamertzanis PG, Raiteri P, Galindo A, **The Use of Anisotropic Potentials in Modeling Water and Free Energies of Hydration**, *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*, 2010, Vol:6, Pages:1590-1607, ISSN:1549-9618
29. Mac Dowell N, Llovell F, Adjiman CS, et al, **Modeling the Fluid Phase Behavior of Carbon Dioxide in Aqueous Solutions of Monoethanolamine Using Transferable Parameters with the SAFT-VR Approach**, *INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH*, 2010, Vol:49, Pages:1883-1899, ISSN:0888-5885

Refereed Conference Contributions

1. Siougkrou E, Galindo A, Adjiman CS, **Integrated Design of a Reactor and a Gas-Expanded Solvent, 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21)**, *ELSEVIER SCIENCE BV*, 2011, Pages:316-320, ISSN:1570-7946
2. Cuevas J, Llovell F, Galindo A, et al, **Solid-liquid equilibrium using the SAFT-VR equation of state: Solubility of naphthalene and acetic acid in binary mixtures and calculation of phase diagrams**, Symposium on 20 Years of the SAFT Equation of State Recent Advances and Challenges, *ELSEVIER SCIENCE BV*, 2011, Pages:137-147, ISSN:0378-3812
3. Struebing H, Karamertzanis PG, Pistikopoulos EN, et al, **Solvent design for a Menschutkin reaction by using CAMD and DFT calculations**, 20th European Symposium on Computer Aided Process Engineering (ESCAPE), *ELSEVIER SCIENCE BV*, 2010, Pages:1291-1296, ISSN:1570-7946
4. F.E. Pereira, G. Jackson, A. Galindo, C.S. Adjiman, "**Robust algorithms for the calculation of phase equilibrium**", ESCAPE20, 6-9 June 2010, Ischia, Italy, in press (2010)
5. N. Mac Dowell, A. Galindo, G. Jackson, C. S. Adjiman, "**Integrated solvent and process design for the reactive separation of CO_2 from flue gas**", ESCAPE20, 6-9 June 2010, Ischia, Italy, in press (2010)

Invited Lectures and Seminars

1. **Modelling aqueous solutions: SAFT and computer simulation results**, ESAT2011, June 2011, St Petersburg, Russia
2. **Modelling aqueous solutions with SAFT approaches: past successes and future challenges**, SAFT2010, September 19-21, 2010, Barcelona, Spain
3. **Alkane molecules in aqueous solution: phase behaviour, solubility and salting out**, PPEPPD, 16-21 May 2010, Suzhou, Jiangsu, China

Michael C. Georgiadis

Associate Professor of Process Optimization, Department of Chemical Engineering, Aristotle University of Thessaloniki, Thessaloniki 54124, Greece

Qualifications

Diploma of Chemical Engineering, Aristotle University of Thessaloniki, Greece
Master of Science (with Distinction) in Advanced Chemical Engineering, Imperial College London
Ph.D. in Chemical Engineering, Imperial College London

Awards and Distinctions

Honorary Research Fellow, Department of Chemical Engineering, Centre for Process Systems Engineering, Imperial College London

Research Interests

Dynamic Process Modelling and Simulation. Optimisation of Energy Systems. Production Scheduling. Advanced Process Control. Supply Chain Optimisation. Energy Planning.

Other Activities

Independent Expert of the European Commission (evaluator of RTD projects under the NMP/FP7, PEOPLE/FP7 and ENERGY/FP7 programmes)
Independent Expert for the EYREKA Programme
Independent project reviewer for the European Commission – DG Research
Member of the Scientific Committee of ESCAPE series and PRES series
Guest editor – Computers and Chemical Engineering

Reviewer for

Chemical Engineering Research and Design; AIChE Journal; Computational Management Science, Computers and Chemical Engineering; Chemical Engineering Science, European Journal of Operational Research; Chemical Engineering Research and Design; Computers and Operations Research; International Journal of Hydrogen Energy; OMEGA; Control Engineering in Pracrice

Academic Collaborations

University College London
Universitad Politechnica de Catalunua
Josef Stefan Institute
University of Pannonia

Industrial Collaborations

KOTHALI S.A. (Greece), MITOL S.A. (Slovenia), ESTIA Engineering (Greece), Atlantis Engineering (Greece)

Books

1. M.C. Georgiadis, J.R. Banga, E.N. Pistikopoulos (2010). **Process Systems Engineering**. Volume VII. *Dynamic Process Modeling*, WILEY-VCH, ISBN: 978-3-527-31696-0

Chapters in Books

1. Georgiadis, M. C., & Longinidis, P. 2011. **Optimal design and operation of supply chain networks under demand uncertainty**. In I. Minis, V. Zeimpekis, G. Dounias, & N. Ampazis (Eds.), *Supply Chain Optimization, Design, and Management: Advances and Intelligent Methods*. Hershey, Pennsylvania: IGI Global (2011)

Journal Articles

1. P. Christos, K. Kouramas, M.C. Georgiadis and E.N. Pistikopoulos (2010). **Dynamic Optimization and Robust explicit model predictive control of hydrogen storage tanks**. *Computers & Chemical Engineering*, 34, 1341,1347
2. M.C. Georgiadis, P. Tsiakis, P. Logginidis and M. Sofioglou (2010). **Optimal design of supply chain networks under uncertain transient demand variations** In Press; *OMEGA – The international journal of management science*
3. P. Logginidis and M.C. Georgiadis (2011). **Integration of Financial Issues in the Optimal Design of Supply Chains**. *International Journal of Production Economics*, 129, 262-276
4. M. C. Georgiadis, P. Tsiakis, P. Longinidis, M.K. Sofioglou (2011), **Optimal design of supply chain networks under uncertain transient demand variations**. *OMEGA*, 39, 254-272
5. P. Liu, M.C. Georgiadis and E.N. Pistikopoulos (2011). **Advances in Energy Systems Engineering**. *Ind. Eng. Chem.* Res., 50, 4916-4926
6. Kopanos GM, Puigjaner L, Georgiadis M.C. (2010). **Optimal Production Scheduling and Lot-Sizing in Dairy Plants: The Yogurt Production Line** , *Ind. Eng. Chem.* Res., 49 701-718
7. Kopanos GM, Puigjaner L, Georgiadis M.C (2011). **Production Scheduling in Multiproduct Multistage Semicontinuous Food Processes**, *Ind. Eng. Chem.* Res., 50, 6116-6324
8. C. Ziogou, S. Voutetakis, S. Papadopouloua,c, M.C.Georgiadis (2011). **Modeling, simulation and experimental validation of a PEM fuel cell system**. *Computers and Chemical Engineering*, 35, 1886-1900
9. Kopanos, G.M.; Puigjaner, L.; Georgiadis, M.C **Resource-constrained production planning in semicontinuous food industries**. *Computers & Chemical Engineering* 35 (12), 2929{2944 (2011)
10. Kopanos, G.M.; Puigjaner, L.; Georgiadis, M.C. **Simultaneous production and logistics operations planning in semicontinuous food industries**. OMEGA - *The International Journal of Management Science* 40 (5), 634 650 (2012)
11. Kopanos, G.M.; Puigjaner, L.; Georgiadis, M.C. **Effcient mathematical frameworks for detailed production scheduling in food processing industries**. *Computers & Chemical Engineering*, in Press, doi:10.1016/j.compchemeng.2011.12.015
12. T. S. Kyriakidis, G. M. Kopanos, M. C. Georgiadis (2011). **MILP formulations for single- and multi-mode resource-constrained project scheduling problems**, *Computers and Chemical Engineering*, In Press

Refereed Conference Contributions

1. Zavitsanou, S., Panoskaltsis, N., Mantalaris, A., Georgiadis, M.C., Pistikopoulos, E.N. (2011). **Modelling of the Insulin Delivery System for patients with Type 1 Diabetes Mellitus** *Computer-Aided Chemical Engineering*, 29,1500-1505
2. Krieger, A., Panoskaltsis, N., Mantalaris, A., Georgiadis, M.C., Pistikopoulos, E.N.. (2011). **A novel physiological based compartmental model for volatile anaesthesia**. *Computer-Aided Chemical Engineering*, 29,1495-1500
3. Pefani, E, Panoskaltsis, N Mantalaris, A, Georgiadis M.C, Pistikopoulos, E (2011). **Towards a high-fidelity model for model based optimisation of drug delivery systems in acute myeloid leukemia** *Computer-Aided Chemical Engineering*, 29,1505-1509
4. E.N. Pistikopoulos, Pei Liu, M.C. Georgiadis **Modelling and Optimisation Issues of the Energy Systems of the Future**. Invited Presentation in the PRES'2010 conference, Prague, 29 August – 1 September 2010
5. C. Ziogou, S. Voutetakis, S. Papadopoulou, M. Georgiadis, **Experimental Validation of a PEM Fuel Cell Dynamic Model**, 7th Symposium on Fuel Cell Modeling and Experimental Validation (MODVAL7), March 2010, Lausanne, Switzerland

6. Kopanos, G.M.; Puigjaner, L.; Georgiadis, M.C. **Optimal production scheduling and lot-sizing in yoghurt production lines**. *European Symposium on Computer Aided Process Engineering* (ESCAPE-20), Ischia - Naples, Italy, 2010
7. Kyriakidis, T.S., Kopanos, G.M, Georgiadis, M.C., 2011. **MILP Formulation for Resource-Constrained Project Scheduling Problems**. In Proceedings of *21st European Symposium on Computer Aided Process Engineering* (ESCAPE-21), Chalkidiki, Greece, pp. 880-884
8. C. Ziogou, S. Voutetakis, S. Papadopoulou, M. Georgiadis, **Development of a Nonlinear Model Predictive Control Framework for a PEM Fuel Cell System**, In E. N. Pistikopoulos, M. C. Georgiadis, & A. C. Kokossis (Eds.), *21st European Symposium on Computer-Aided Process Engineering*. N. Marmaras-Chalkidiki, Greece, May 29 - June 1, 2011, 743-747
9. M. Kostoglous and M.C. Georgiadis. **Three-moments conserving sectional techniques for the solution of coagulation and breakage population balances**. In E. N. Pistikopoulos, M. C. Georgiadis, & A. C. Kokossis (Eds.), *21st European Symposium on Computer-Aided Process Engineering*. N. Marmaras-Chalkidiki, Greece, May 29 - June 1, 2011, 41-45
10. C. Ziogou, C. Panos, K. Kouramas, S. Papadopoulou, M. Georgiadis, S. Voutetakis, E. N. Pistikopoulos, **Multi-Parametric Model Predictive Control of an Automated Integrated Fuel Cell Testing Unit**, *Computer Aided Chemical Engineering*, Volume 29, 2011, Pages 744-747
11. C. Ziogou, S. Voutetakis, S. Papadopoulou, M. Georgiadis, **Dynamic Modeling and Experimental Validation of a PEM Fuel Cell System**, *Chemical Engineering Transactions*, Volume 21, 2010, Pages 565-570
12. C. Ziogou, S. Voutetakis, S. Papadopoulou, M. Georgiadis, **Modeling and Experimental Validation of a PEM Fuel Cell System**, *Computer Aided Chemical Engineering*, Volume 29, 2010, Pages 721-726
13. C. Ziogou, S. Voutetakis, S. Papadopoulou, M. Georgiadis, **Design of an Integrated Model Predictive Control Framework for a PEM Fuel Cell System**, *European Fuel Cell Conference (EFC11)*, 12-14 Dec 2011, Rome, Italy
14. Longinidis, P., Georgiadis, M. C., & Tsiakis, P. **Integration of financial statement analysis in the optimal design and operation of supply chain networks**. In E. N. Pistikopoulos, M. C. Georgiadis, & A. C. Kokossis (Eds.), *21st European Symposium on Computer-Aided Process Engineering*. N. Marmaras-Chalkidiki, Greece, May 29 - June 1, 2011
15. Longinidis, P., & Georgiadis, M. C. **Integration of financial statement analysis in the optimal design of supply chain networks under demand uncertainty** *International Conference on Computational Management Science*. Vienna, Austria, July 28-30, 2010

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 (Ludwigshafen, Germany); BCURA (Cheltenham); Borealis AS (Stathelle, Norway); Britest Ltd. (Runcorn); BP Exploration (Sunbury); BP Gas (Sunbury); ICI Research (Wilton); Ineos fluor (Runcorn); P&G (Cincinnati, USA); Schlumberger Cambridge Research (Cambridge); Syngenta (Huddersfield); Unilever Research (Port Sunlight).

Journal Articles

1. Avendaño C, Lafitte T, Galindo A, et al, **SAFT- force field for the simulation of molecular fluids. 1. A single-site coarse grained model of carbon dioxide**., *J Phys Chem B*, 2011, Vol:115, Pages:11154-11169
2. Artola PA, Pereira FE, Adjiman CS, et al, **Understanding the fluid phase behaviour of crude oil: Asphaltene precipitation**, *FLUID PHASE EQUILIBRIA*, 2011, Vol:306, Pages:129-136, ISSN:0378-3812
3. Papaioannou V, Adjiman CS, Jackson G, et al, **Simultaneous prediction of vapour-liquid and liquid-liquid equilibria (VLE and LLE) of aqueous mixtures with the SAFT-gamma group contribution approach**, *FLUID PHASE EQUILIBRIA*, 2011, Vol:306, Pages:82-96, ISSN:0378-3812
4. Vega LF, Jackson G, **20 Years of the SAFT equation of state-Recent advances and challenges Symposium held in Bellaterra**, Barcelona, 19-21 September 2010 Foreword, *FLUID PHASE EQUILIBR*, 2011, Vol:306, Pages:1-3, ISSN:0378-3812
5. Mac Dowell N, Pereira FE, Llovell F, et al, **Transferable SAFT-VR models for the calculation of the fluid phase equilibria in reactive mixtures of carbon dioxide, water, and n-alkylamines in the context of carbon capture**., *J Phys Chem B*, 2011, Vol:115, Pages:8155-8168
6. Wensink HH, Jackson G, **Cholesteric order in systems of helical Yukawa rods**, *J PHYS-CONDENS MAT*, 2011, Vol:23, ISSN:0953-8984
7. Varga S, Jackson G, **A study of steric chirality: the chiral nematic phase of a system of chiral two-site HGO molecules**, *MOL PHYS*, 2011, Vol:109, Pages:1313-1330, ISSN:0026-8976
8. Pereira FE, Keskes E, Galindo A, et al, **Integrated solvent and process design using a SAFT-VR thermodynamic description: High-pressure separation of carbon dioxide and methane**, *COMPUT CHEM ENG*, 2011, Vol:35, Pages:474-491, ISSN:0098-1354
9. Macchietto S, Hewitt GF, Coletti F, et al, **Fouling in Crude Oil Preheat Trains: A Systematic Solution to an Old Problem**, *HEAT TRANSFER ENG*, 2011, Vol:32, Pages:197-215, ISSN:0145-7632
10. Jackson G, Nezbeda I, 8th Liblice **Conference on the Statistical Mechanics of Liquids - Brno, Czech Republic**, 13-18 June 2010 FOREWORD, *MOL PHYS*, 2011, Vol:109, Pages:1-2, ISSN:0026-8976
11. Brumby PE, Haslam AJ, de Miguel E, et al, **Subtleties in the calculation of the pressure and pressure tensor of anisotropic particles from volume-perturbation methods and the apparent asymmetry of the compressive and expansive contributions**, *MOLECULAR PHYSICS*, 2011, Vol:109, Pages:169-189, ISSN:0026-8976
12. Pereira FE, Jackson G, Galindo A, et al, **A duality-based optimisation approach for the reliable solution of (P, T) phase equilibrium in volume-composition space**, *FLUID PHASE EQUILIBR*, 2010, Vol:299, Pages:1-23, ISSN:0378-3812
13. Georgiadis A, Llovell F, Bismarck A, et al, **Interfacial tension measurements and modelling of (carbon dioxide plus n-alkane) and (carbon dioxide plus water) binary mixtures at elevated pressures and temperatures**, *J SUPERCRIT FLUID*, 2010, Vol:55, Pages:743-754, ISSN:0896-8446
14. Sampayo JG, Blas FJ, de Miguel E, et al, Monte Carlo **Simulations of the Liquid-Vapor Interface of Lennard-Jones Diatomics for the Direct Determination of the Interfacial Tension Using the Test-Area Method**, *J CHEM ENG DATA*, 2010, Vol:55, Pages:4306-4314, ISSN:0021-9568
15. Llovell F, Galindo A, Blas FJ, et al, **Classical density functional theory for the prediction of the surface tension and interfacial properties of fluids mixtures of chain molecules based on the statistical associating fluid theory for potentials of variable range**., *J Chem Phys*, 2010, Vol:133

16. Sampayo JG, Malijevský A, Müller EA, et al, **Communications: Evidence for the role of fluctuations in the thermodynamics of nanoscale drops and the implications in computations of the surface tension**., *J Chem Phys*, 2010, Vol:132
17. Mac Dowell N, Llovell F, Adjiman CS, et al, **Modeling the Fluid Phase Behavior of Carbon Dioxide in Aqueous Solutions of Monoethanolamine Using Transferable Parameters with the SAFT-VR Approach**, *IND ENG CHEM RES*, 2010, Vol:49, Pages:1883-1899, ISSN:0888-5885
18. Mac Dowell N, Florin N, Buchard A, et al, **An Overview of CO_2 capture technologies**, *Energy and Environmental Science*, 2010, Vol:3, Pages:1645-1669
19. Pereira FE, Jackson G, Galindo A, et al, **Robust algorithms for the calculation of phase equilibrium**, *20TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING*, 2010, Vol:28, Pages:79-84, ISSN:1570-7946
20. Mac Dowell N, Galindo A, Jackson G, et al, **Integrated solvent and process design for the reactive separation of CO_2 from flue gas**, *20TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING*, 2010, Vol:28, Pages:1231-1236, ISSN:1570-7946

Cleo Kontoravdi

Lecturer (Lonza/RCUK Academic Fellowship), Department of Chemical Engineering, Imperial College London

Qualifications
MEng, PhD

Research Interests
Bioprocessing, Biotechnology, Ageing

Reviewer for
Biotechnology and Applied Biochemistry
Biotechnology and Bioengineering
Biochemical Engineering Journal
Biotechnology Progress

Academic Collaborations
School of Chemistry, University of Southampton
School of Chemical Engineering and Analytical Science at the University of Manchester
Bioelectronics Centre at the University of Glasgow
Department of Civil and Structural Engineering, University of Sheffield
School of Mathematics, University of Exeter

Industrial Collaborations
Lonza Biologics
MedImmune Plc

Book Chapters
1. Polizzi K. and Kontoravdi C. **Vaccine production**, In: *Handbook of Healthcare Delivery Systems*. Edited by Y. Yih, Taylor & Francis Group, FL, U.S.A., 2010

Journal Articles
1. Jimenez del Val I, Nagy JM, Kontoravdi C, **A dynamic mathematical model for monoclonal antibody N-linked glycosylation and nucleotide sugar donor transport within a maturing Golgi apparatus**, *Biotechnology Progress*, 2011, Vol:27, Pages:1730-1743
2. Kiparissides A, Koutinas M, Kontoravdi C, Mantalaris A, Pistikopoulos EN. **Closing the loop in biological systems modelling - From the in Silico to the in Vitro**, *AUTOMATICA* Special Issue on Systems Biology, 2011, Vol:47, Pages:1147-1155
3. Jimenez del Val I, Kontoravdi C, Nagy JM, **Towards the implementation of quality by design to the production of therapeutic monoclonal antibodies with desired glycosylation patterns**, *Biotechnology Progress*, 2010, Vol:26, Pages:1505-1527
4. Kontoravdi C, Pistikopoulos EN, Mantalaris A, **Systematic development of predictive mathematical models for animal cell cultures**, *Computers & Chemical Engineering*, 2010, Vol:34, Pages:1192-1198

Conference Contributions
1. Jimenez del Val I, Nagy JM, Kontoravdi C, **Quantification of intracellular nucleotide sugars and formulation of a mathematical model for prediction of their metabolism**, *22nd European Society for Animal Cell Technology (ESACT)* Meeting on Cell Based Technologies, BMC Proceedings. 5(Suppl 8): P10, 2011
2. Ning Chen, Karen M. Polizzi, Cleo Kontoravdi, **Kinetic modelling of cytosolic glucose metabolism**, *21st European Symposium on Computer Aided Process Engineering* / Elsevier, May 2011
3. Sarantos Kyriakopoulos, Karen M. Polizzi, Cleo Kontoravdi, **Ubiquitous Amino Acid Transporters Expressed During CHO Cell Culture**, *BioProcessing, Biologics & Biotherapeutics Congress*, 2011
4. Ioscani Jiménez del Val and Cleo Kontoravdi, **Towards the Implementation of Quality by Design to the Production of Therapeutic Monoclonal Antibodies with Desired Glycosylation Patterns**, *Annual AIChE Meeting,* 2011

Invited Seminars
European Symposium of Animal Cell Technology, U.K. meeting, January 2012
MedImmune Plc, October 2011
University of Kent Molecular Processing Conference, July 2011

J Krishnan

Lecturer, Department of Chemical Engineering, Imperial College London

Qualifications
PhD

Research Interests
Mathematical and computational modelling of cellular processes of biological and biomedical relevance focussing on signal transduction, both spatial and temporal; systems analysis of signal processing in natural and synthetic cellular systems; systems and synthetic biology; complex networked dynamical systems; non-linear dynamics and pattern formation in biological and physico-chemical systems.

The research in my group largely focuses on signal transduction in cellular systems and has two strands. One strand involves the mathematical and computational modelling of cellular signalling networks, using a combination of detailed and qualitatively simplified models, Modelling (both deterministic and stochastic) is undertaken in a range of systems involving spatial (eg gradient perception, cellular guidance, polarity generation) and purely temporal signal transduction (eg translation regulation, drug resistance). A complementary strand involves systems approaches and abstractions aimed at elucidating complex signal processing in natural and synthetic cellular systems, especially using approaches from dynamical systems, systems and control engineering and signal processing.

Reviewer for
Journal of Theoretical Biology, IEEE Transactions in Automatic Control, Interface Journal of the Royal Society, PLOS Computational Biology, Biochemical Engineering Journal, Automatica, Wiley Interdisciplinary Reviews in Systems Biology and Medicine, Computers and Chemical Engineering, BMC Systems Biology, BMC Research Notes, Advances in Systems Biology, Annals of Biomedical Engineering, BBSRC, AVIESAN/French National Cancer Institute.

Academic Collaborations
School of Medical Sciences Univ. of Aberdeen, Dept. of Molecular Biosciences, Imperial College, Division of Experimental Medicine, Hammersmith Hospital.

Journal Articles

1. C. Liu, J. Krishnan and X.Y.Xu **An systems-based mathematical modelling approach for elucidating the effect of drugs on solid tumours** *Theoretical Biology and Medical Modelling*, 2011
2. C. Liu, J. Krishnan, X.Y.Xu and J. Stebbing **The use of mathematical models in elucidating the effect of drugs on solid tumours**, *Pharmacogenomics*, 2011.
3. D. Seaton and J. Krishnan **The coupling of pathways and processes through shared components**, *BMC Systems Biology*, 2011
4. J.Krishnan **Chemical Engineering at the cellular scale: cellular signal processing**
5. **Industrial and Engineering Chemistry Research**, 2011
6. J. Krishnan **The effect of saturation in feedforward adaptive signal transduction**, *IET Systems Biology*, 2011.
7. J. Krishnan and A. Alam-Nazki **An investigation of design principles underlying repulsive and attractive gradient sensing and their switching**, *Journal of Theoretical Biology*, 2011
8. D. Seaton and J. Krishnan **A modular systems approach to the interaction of adaptive and monostable and bistable threshold modules**, *IET Systems Biology* 2011
9. Alam-Nazki and J. Krishnan **A mathematical modelling framework for elucidating chemorepulsive gradient sensing in Dictyostelium**, *Journal of Theoretical Biology* 2010
10. J. Krishnan and D. Seaton **The role of feedback regulation in irreversible reaction networks**, *Int. Rev. Automatic Control*, 2010
11. R. Betney, E. de Silva, J. Krishnan, I.Stansfield **Auto-regulatory systems controlling translation efficiency: thermostat-like control of translation efficiency**, *RNA*, 2010
12. E. de Silva, J. Krishnan, R. Betney, I.Stansfield **A modelling framework for elucidating the role of feedback control in translation termination**, *Journal of Theoretical Biology*, 2010

Invited Lectures and Seminars

1. Oxford University, Indian Institute of Science, Systems Biology Network, University of Sheffield, Angionet Conference, (other lecture at Cold Spring Harbour Engineering Principles of Biological Systems)

Daniel Kuhn

Senior Lecturer, Department of Computing, Imperial College London

Qualifications
PhD in Economics, University of St. Gallen (2004), MSc in Physics, ETH Zurich (1999)

Awards and Distinctions
Fellowships from Swiss National Science Foundation (2004-2006), Polya Award of ETH Zurich for Best MSc Examination Result in Theoretical Physics (1999)
Research Interests - Optimal decision making under uncertainty, stochastic programming, robust optimisation, optimal control
Other Activities - Member of Mathematical Programming Society, Associate Editor for Computational Management Science, Energy Systems and Operations Research

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 Industrial Management and Optimization, Journal of Mathematical Analysis and Applications, 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 Applied Mathematics, SIAM Journal on Control and Optimization, SIAM Journal on Discrete Mathematics, SIAM Journal on Optimization, The Computer Journal

Book

1. Daniel Kuhn. **Generalized Bounds for Convex Multistage Stochastic Programs**, vol. 548 of *Lecture Notes in Economics and Mathematical Systems*. Springer-Verlag, Berlin, 2004

Journal Articles

1. Steve Zymler, Daniel Kuhn, and Berç Rustem. **Distributionally Robust Joint Chance Constraints with Second-Order Moment Information**. *Mathematical Programming* (accepted 2011)
2. Phebe Vayanos, Daniel Kuhn, and Berç Rustem. **A Constraint Sampling Approach for Multistage Robust Optimization**. *Automatica* (accepted 2011)
3. Wolfram Wiesemann, Daniel Kuhn, and Berç Rustem. **Robust Resource Allocations in Temporal Networks**. *Mathematical Programming* (accepted 2011)
4. Simon A. Spacey, Wolfram Wiesemann, Daniel Kuhn, and Wayne Luk. **Robust Software Partitioning with Multiple Instantiation**. *INFORMS Journal on Computing* (accepted 2011)
5. Michael Hadjiyiannis, Paul Goulart, and Daniel Kuhn. **An Efficient Method to Estimate the Suboptimality of Affine Controllers**. *IEEE Transactions on Automatic Control* 56(12), 2841-2853 (2011)
6. Daniel Kuhn, Wolfram Wiesemann, and Angelos Georghiou. **Primal and Dual Linear Decision Rules in Stochastic and Robust Optimization**. *Mathematical Programming* 130(1), 177-209 (2011)
7. Steve Zymler, Berç Rustem, and Daniel Kuhn. **Robust Portfolio Optimization with Derivative Insurance Guarantees**. *European Journal of Operational Research* 210(2), 410-424 (2011)
8. Daniel Kuhn and David G. Luenberger. **Analysis of the Rebalancing Frequency in Log-Optimal Portfolio Selection**. *Quantitative Finance* 10(2), 221-234 (2010)
9. Wolfram Wiesemann, Daniel Kuhn, and Berç Rustem. **Maximizing the Net Present Value of a Project under Uncertainty**. *European Journal of Operational Researc*h 202(2), 356-367 (2010)

Conference Papers

1. Dimitra Bampou and Daniel Kuhn. **Scenario-Free Stochastic Programming via Polynomial Decision Rules**. IEEE Conference on Decision and Control and European Control Conference, Orlando, USA, December 2011
2. Phebe Vayanos, Daniel Kuhn, and Berç Rustem. **Decision Rules for Information Discovery in Multistage Stochastic Programming**. IEEE Conference on Decision and Control and European Control Conference, Orlando, USA, December 2011
3. Michael Hadjiyiannis, Paul Goulart, and Daniel Kuhn. **A Scenario Approach for Measuring the Suboptimality of Linear Decision Rules in Two-Stage Robust Optimization**. IEEE Conference on Decision and Control and European Control Conference, Orlando, USA, December 2011
4. Phebe Vayanos, Wolfram Wiesemann, and Daniel Kuhn. **Hedging Electricity Swing Options in Incomplete Markets**. 18th IFAC World Congress, Milan, Italy, August 2011
5. Fook Wai Kong, Daniel Kuhn, and Berç Rustem. Welfare-Maximizing Correlated Equilibria with an

Application to Wireless Communication. 18th IFAC World Congress, Milan, Italy, August 2011

6. Evangelia Kalyvianaki, Wolfram Wiesemann, Quang Hieu Vu, Daniel Kuhn, and Peter Pietzuch. **SQPR: Stream Query Planning with Reuse**. IEEE International Conference on Data Engineering (ICDE), Hannover, Germany, April 2011
7. Fook Wai Kong, Daniel Kuhn, and Berç Rustem. **A Cutting-Plane Method for Mixed-Logical Semidefinite Programs with an Application to Multi-Vehicle Robust Path Planning.** IEEE Conference on Decision and Control, Atlanta, USA, December 2010
8. Michael Hadjiyiannis, Paul Goulart, and Daniel Kuhn. **An Efficient Method to Estimate the Suboptimality of Affine Controllers**. UKACC International Conference on Control, Coventry, UK, September 2010

Book Chapters

1. Karl Frauendorfer, Daniel Kuhn, and Michael Schürle. **Barycentric Bounds in Stochastic Programming: Theory and Application**. In *Stochastic Programming*: The State of the Art, In Honor of George B. Dantzig (Gerd Infanger, ed.), Springer, New York, 67-96 (2011)
2. Daniel Kuhn, Panos Parpas, and Berç Rustem. **Threshold Accepting Approach to Improve Bound-Based Approximations for Portfolio Optimization**. In *Computational Methods in Financial Engineering* (E. Kontoghiorghes, B. Rustem, and P. Winker, eds.), Springer Verlag, Berlin, 3-26 (2008)
3. Daniel Kuhn, Panos Parpas, and Berç Rustem. **Stochastic Optimization of Investment Planning Problems in the Electric Power Industry**. In *Process Systems Engineering*: Volume 5: Energy Systems Engineering, (M. Georgiadis, E. Kikkinides, and E. Pistikopoulos, eds.), Wiley-VCH, Weinheim, 215-230 (2008)

Editorial

1. Daniel Kuhn. Guest Editorial: **Special Issue on Computational Finance**. *Computational Management Science* 8(1-2), 1-2 (2011)

Invited Lectures and Seminars

1. Charles University, Seminar of the Department of Probability and Mathematical Statistics, Prague (Czech Republic), December 2011
2. National University of Singapore, Seminar of the Department of Decision Sciences, Singapore (Singapore), September 2011
3. ABB Corporate Research Switzerland, IT Seminar, Baden-Dättwil (Switzerland), July 2011
4. MAN Investments, AHL Research Seminar, London (UK), June 2011
5. Lancaster University, LANCS Workshop on Modeling and Solving Complex Optimization Problems, Lancaster (UK), April 2011
6. Vienna University of Economics and Business, Seminar of the Department of Finance, Accounting and Statistics, Vienna (Austria), March 2011
7. PhD Winter School on “Managing uncertainty in energy infrastructure investments” organized by Norwegian University of Science and Technology, Oppdal (Norway), March 2011
8. University College London, Seminar of the Centre for Computational Statistics and Machine Learning, London (UK), January 2011
9. Institute for Pure and Applied Mathematics at UCLA, Invited lecture in workshop on Robust Optimization, Los Angeles (USA), November 2010
10. ETH Zurich, Optimization and Applications Seminar, Zurich (Switzerland), October 2010

Geoffrey C. Maitland

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
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

Research Interests

Clean production and use of fossil fuels
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
Chemical characterisation of multicomponent fluids
The development of new hydrocarbon recovery processes
The application of biological processes to oil recovery

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 Shell Grand Challenge Programme in Clean Fossil Fuels and of the Qatar Carbonates and Carbon Storage Research Centre. Existing research projects include:
– Measurement of the thermophysical properties of CO_2
– 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 crudeoils 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 CO_2 storage.
– Renewable production of hydrogen from water using green algae photocatalysis.
– The rheology and systematic design of colloidal fluids and gelling soft solids for industrial (especially oilfield) applications.

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

Reviewer for
ACS Petroleum Research Fund
Chemical Engineering Research and Development
Chemical Engineering Science
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
Foster Wheeler Energy, Qatar Petroleum, Schlumberger, Shell

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. **Capillary trapping in carbonate rocks** C. Lamy, S. Iglauer, C.H. Pentland, M.J. Blunt and G.C. Maitland Proc. Society of Petroleum Engineers Europe/EAGE Annual Conference, Barcelona Spain, 14th-17th June 2010, Paper SPE 130720
3. **Interfacial tension measurements of the (H_2O + CO_2) system at elevated pressures and temperatures** A. Georgiadis, G.C. Maitland, J.P.M. Trusler and A. Bismarck J. Chem. Eng. Data, 2010, 55, 4168–4175. Part of the Sir John Rowlinson Festschrift.
4. **Interfacial tension measurements of (carbon dioxide plus n-alkane) and (carbon dioxide plus water) binary systems at elevated pressures and temperatures** A. Georgiadis, F. Llovell, A. Bismarck, F.J. Blas, A. Galindo, G.C. Maitland, J.P.M. Trusler and G. Jackson J. Supercrit. *Fluids*, 2010, 55, 743-754 (J.D. van der Waals special issue)
5. **Interfacial Tension Measurements of the (H_2O + n-Decane + CO_2) Ternary System at Elevated Pressures and Temperatures** Apostolos Georgiadis, Geoffrey Maitland, J. P. Martin Trusler, and Alexander Bismarck J. *Chem. Eng. Data* 2011, 56, 4900–4908
6. **Interfacial Tension of (Brines + CO_2): (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** Xuesong Li, Edo Boek, Geoffrey C. Maitland, and J. P. Martin Trusler J. *Chem. Eng. Data*, 2012, dx.doi.org/10.1021/je201062r
7. **Mutual Diffusion Coefficients of Aqueous KCl at High Pressures Measured by the Taylor Dispersion Method** Catinca Secuianu, Geoffrey C. Maitland, J. P. Martin Trusler, and William A. Wakeham J. *Chem. Eng. Data* 2011, 56, 4840–4848
8. **Solubility of carbon dioxide in aqueous solution of monoethanolamine or 2-amino-2-methyl-1-propanol: Experimental measurements and modelling** Danlu Tong J.P. Martin Trusler, Geoffrey C. Maitland, Jon Gibbins, Paul S. Fennell International *Journal of Greenhouse Gas Control* 6 (2012) 37–47
9. **Parameters affecting the growth and hydrogen production of the green alga Chlamydomonas reinhardtii** Bojan Tamburic*, Fessehaye W. Zemichael, Geoffrey C. Maitland, Klaus Hellgardt International *J of Hydrogen Energy*, 36, 7827-7876, 2011
10. **Design of a novel flat-plate photobioreactor system for green algal hydrogen production Bojan Tamburic**, Fessehaye W. Zemichael, Paul Crudge, Geoffrey C. Maitland, Klaus Hellgardt International J of Hydrogen Energy, 36, 6578-6591, 2011

Athanasios Mantalaris

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

Qualifications
BSc(Hon) in Biochemistry (UWO)
MSc in Chemical Engineering (University of Rochester)
PhD in Chemical Engineering (University of Rochester)

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

Research Interests
My research aims to utilise and implement engineering principles to Biological/Biomedical applications. The philosophy of my research approach is to productively link mathematical modelling to experiments in a systematic manner. My research focuses on two main areas:

a) Stem Cell Bioprocessing and Tissue Engineering: The development of bioprocess technology for the successful transfer of laboratory-based practice of stem cell & tissue culture to the clinic as therapeutics through the application of engineering principles and practices in order to achieve control, reproducibility, automation, validation, safety, and cost-effectiveness.
b) Biological Systems Engineering: The advancement of an integrated systems engineering platform for the generation of solutions/strategies through the development of adaptive algorithms for the model-based design of experiments, prediction, control, and optimisation of complex biological/biomedical problems.

Other Activities
EPSRC: Member of Peer Review College
MRC Stem Cell User Liaison Committee
Review Panel for ETP in Nanomedicine

Reviewer for
Tissue Engineering
Biotechnology & Bioengineering
Biotechnology & Applied Biochemistry
Blood Cells, Molecules & Diseases
Food & Bioproducts Processing
Biomaterials
Biochemical Engineering Journal
Regenerative Medicine
Journal of Membrane Science
Industrial & Engineering Chemistry Research
Biomacromolecules
Stem Cells & Development
Biotechnology Progress
Journal of Microscopy
Process Biochemistry
Journal of Zhejiang University Science

Academic Collaborations
Nanyang Technological University, Singapore
National University of Singapore, Singapore
University of Tokyo
University of Athens Medcical School

Industrial Collaborations
GSK

Journal Articles

1. Quero, F., M. Nogi, K-Y. Lee, G.V. Poel, A. Bismarck, A. Mantalaris, H. Yano, S.J. Eichorn (2011). **Cross-Linked Bacterial Cellulose Networks Using Glyoxalization**, *ACS Applied Materials & Interfaces* 3(2):490-499
2. Kiparissides, A., M. Koutinas, T. Moss, J. Newman, E.N. Pistikopoulos, and A. Mantalaris (2011). **Modelling the Delta1/Notch1 Pathway: In Search of the Mediator(s) of Neural Stem cell Differentiation**, *Plos One* 6(2):e14668
3. Kuzin, I. HL. Sun, S. Moshkani, CY. Feng, A. Mantalaris, J.H.D. Wu, and A. Bottaro (2011). **Long-Term Immunologically Competent Human Peripheral Lymphoid Tissue Cultures in a 3D Bioreactor**, *Biotechnology & Bioengineering* 108(6): 1430-1440
4. Mantalaris, A. (2011). **Bioprocess Systems Engineering: bridging the "scales" between "molecules, cells & processes"**, *Microbial Biotechnology* 4(2):212-124
5. Koutinas, M., A. Kiparissides, M-C. Lam, R. Silva-Rocha, M. Godinho, V. de Lorenzo, V.A.P. Martins dos Santos, E.N. Pistikopoulos, and A. Mantalaris (2011). **Improving the prediction of Pseudomonas putida mt-2 growth kinetics with the use of a gene expression regulation model of the TOL plasmid**, *Biochemical Engineering Journal* 55(2): 108-118
6. Lim, M., N. Panoskaltsis, H. Ye, and A. Mantalaris (2011). **Optimization of in vitro erythropoiesis from CD34+ cord blood cells using design of experiments (DOE)**, *Biochemical Engineering Journal* 55(3): 154-161

7. Kiparissides, A., M. Koutinas, C. Kontoravdi, A. Mantalaris, E.N. Pistikopoulos (2011). **Closing the loop in biological systems modelling – From the in silico to the in vitro**, *Automatica* 47(6): 1147-1155
8. Koutinas, M., A. Kiparissides, M-C. Lam, R. Silva-Rocha, M. Godinho, V. de Lorenzo, V.A.P. Martins dos Santos, E.N. Pistikopoulos, and A. Mantalaris (2011). **Linking genes to microbial growth kinetics – An integrated biochemical systems engineering approach**, *Metabolic Engineering* 13:401-413
9. Ripamonti, U., E. Tsiridis, C. Ferretti, C.J. Kerawala, A. Mantalaris, and M. Heliotis (2011). **Perspectives in regenerative medicine and tissue engineering of bone**, *British Journal of Oral & Maxillofacial Surgery* 49(7):507-509
10. Mortera-Blanco, T., A. Mantalaris, A. Bismarck, N. Aqel, and N. Panoskaltsis (2011). **Long-term cytokine-free expansion of cord blood mononuclear cells in three-dimensional scaffolds**, *Biomaterials* 32(35):9263-70
11. Graham, S.M., D. Howgate, W. Anderson, C. Howes, M. Heliotis, A. Mantalaris, E. Tsiridis, E. Tsapakis (2011). **Risk of osteoporosis and fracture incidence in patients on antipsychotic medication**, *Expert Opinion on Drug Safety* 10(4):575-602

Book Chapters

1. Ye H, Cui Z, Ellis M, Chaudhuri J, Macedo H, Mantalaris A. **Hollow fibre membrane bioreactor technology for tissue engineering and stem cell therapy**. In: Drioli E, Giorno L, editors. *Comprehensive Membrane Science and Engineering*. Rende, Italy: Elsevier, 2011

Conference Contributions

1. **Mechanics of bacterial cellulose composite interfaces** Author(s): Eichhorn, SJ (Eichhorn, Stephen J.); Quero, F (Quero, Franck); Lee, KY (Lee, Koon-Yang); Mantalaris, A (Mantalaris, Ananasios); Bismarck, A (Bismarck, Alexander) Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY Volume: 241 Meeting Abstract: 24-CELL Published: MAR 27 2011
2. **Predicting microbial growth kinetics with the use of genetic circuit models** Author(s): Koutinas, M (Koutinas, Michalis)1; Kiparissides, A (Kiparissides, Alexandros)1; de Lorenzo, V (de Lorenzo, Victor); dos Santos, VAPM (Martins dos Santos, Vitor A. P.); Pistikopoulos, EN (Pistikopoulos, Efstratios N.)1; Mantalaris, A (Mantalaris, Athanasios)1 Editor(s): Pistikopoulos, EN; Georgiadis, MC; Kokossis, AC Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1321-1325 Published: 2011
3. **A combined growth kinetics, metabolism and gene expression model for 3D ESC bioprocesses** Author(s): Yeo, D (Yeo, David)1; Kiparissides, A (Kiparissides, Alexandros)1; Pistikopoulos, E (Pistikopoulos, Efstratios)1; Mantalaris, A (Mantalaris, Athanasios)1 Editor(s): Pistikopoulos, EN; Georgiadis, MC; Kokossis, AC Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1326-1330 Published: 2011
4. **Towards a high-fidelity model for model based optimisation of drug delivery systems in acute myeloid leukemia** Author(s): Pefani, E (Pefani, Eleni)1; Panoskaltsis, N (Panoskaltsis, Nicki); Mantalaris, A (Mantalaris, Athanasios)1; Georgiadis, MC (Georgiadis, Michael C.)1; Pistikopoulos, E (Pistikopoulos, EfstratiosN.)1 Editor(s): Pistikopoulos, EN; Georgiadis, MC; Kokossis, AC Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1505-1509 Published: 2011

Invited Lectures and Seminars

1. **Modelling of Mammalian Cell Culture Systems**, Modular Training for the Bioprocess Industries, Advanced Centre for Biochemical Engineering, UCL, London, February 2011
2. **Functional, Controllable, Automatable, and Scalable Bioprocessing of Stem Cells: The Need for a Paradigm Shift**, Regenerative Medicine: innovations for Clinical Applications, Hilton Head, USA, March 2011
3. **Mammalian Cell Culture Modelling**, Department of Chemical & Biological Engineering, University of Sheffield, Sheffield, April 2011

Keynote Lectures

1. Keynote Lecture at the 13th International Conference on Pseudomonas, **Linking genes to microbial growth kinetics – An integrated biochemical systems engineering approach**, Sydney, Australia, September 2011
2. Keynote Lecture at the 3rd Asian Biomaterials Congress, **Production of Mineralised Cellular Implants fop Translational Bone Tissue Engineering**, Busan, Korea, September 2011

Costas C Pantelides

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

Qualifications
BSc(Eng) in Chemical Engineering. (Imperial College London)
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
Model-based analysis & design methodologies for process safety
Quality-by-Design in pharmaceutical processes
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
Member of the Council of Educational Assessment & Accreditation, Republic of Cyprus

Invited Lectures
1. **Model-Based Innovation: models, optimisation and design space in process development**. Keynote presentation at GlaxoSmithKline's internal Modelling Conference, Ware, June 2010
2. **Process Modelling: Scope, Benefits and Pitfalls**. Invited keynote presentation at Chemistry Innovation KTN Workshop, London, May 2010

Journal Articles
1. Bardwell DA, Adjiman CS, Arnautova YA, et al, **Towards crystal structure prediction of complex organic compounds – a report on the fifth blind test.**, *Acta Crystallogr B*, 2011, Vol:67, Pages:535-551

Contributions in Books
1. A.V. Kazantsev, P.G. Karamertzanis, C.C. Pantelides and C.S. Adjiman, **CrystalOptimizer: An Efficient Algorithm for Lattice Energy Minimization of Organic Crystals Using Isolated Molecule Quantum Mechanical Calculations**, in *Process Systems Engineering. Vol. 6: Molecular Systems Engineering*, Adjiman, C.S. and Galindo, A. eds., Wiley-VCH, 2010

Refereed Conference Proceedings
1. Gao, G-Y., Wang, M., Pantelides, C.C., Li, X-G., and Yeung, H., **Mathematical Modeling and Optimal Operation of Industrial Tubular Reactor for Naphtha Cracking**, in *Computer Aided Process Engineering*, 27, de Brito Alves, R.M., do Nascimento, C.A.O. and Biscaia, Jr , E.C., eds., 501-506, Elsevier (2010)

Lazaros G. Papageorgiou

Reader 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
Supply chain optimisation. Production planning and scheduling. Data mining and network analysis. Optimisation of biological and biochemical systems. Process plant layout. Energy systems engineering.

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

Journal Articles

1. S. Liu, J.M. Pinto and L.G. Papageorgiou, **MILP-based Approaches for Medium-Term Planning of Single-Stage Continuous Multiproduct Plants with Parallel Units**, *Computational Management Science*, 7, 407-435 (2010)
2. S. Liu, J.M. Pinto and L.G. Papageorgiou, **Single-stage Scheduling of Multiproduct Batch Plants: An Edible-oil Deodoriser Case Study**, *Ind. Eng. Chem*. Res., 49, 8657-8669 (2010)
3. G. Xu, L. Bennett, L.G. Papageorgiou and S. Tsoka, **Module Detection in Complex Networks through an Optimisation Framework**, *Algorithms for Molecular Biology*, 5, 36 (2010)
4. F. Konstantopoulou, S. Liu, L.G. Papageorgiou and P. Gikas, **Water resources management for Paros island, Greece**, *International Journal of Sustainable Water and Environmental Systems*, 2, 1-6 (2011)
5. O. Akgul, A. Zamboni, F. Bezzo, N. Shah, and L.G. Papageorgiou, **Optimisation-based Approaches for Bioethanol Supply Chains**, *Ind. Eng. Chem*. Res, 50, 4927-4938 (2011)
6. S. Liu, F. Konstantopoulou, P. Gikas and L.G. Papageorgiou, **A Mixed Integer Optimisation Approach for Integrated Water Resources Management**, *Comput. Chem. Eng.*, 35, 858-875 (2011)
7. S. Liu, L.G. Papageorgiou and P. Gikas, **Water Resources Management for Insular and Geographically Isolated Areas using Optimisation Techniques**, *Desalination and Water Treatment*, 33, 3-13 (2011)
8. R.T. Sousa, S. Liu, N. Shah and L.G. Papageorgiou, **Global Supply Chain Planning for Pharmaceuticals**, *Chem. Eng*. Res. Des., 89, 2396-2409 (2011)
9. E.M. Polykarpou, P.A. Dalby and L.G. Papageorgiou, **Optimal Synthesis of Chromatographic Trains for Downstream Protein Processing**, *Biotechnology Progress*, 27, 1653-1660 (2011)

Conference Contributions

1. S. Liu, P. Gikas and L.G. Papageorgiou, **An Optimisation-based Approach for Integrated Water Resources Management**, Escape-20 conference (2010)
2. F. Konstantopoulou, S. Liu, L.G. Papageorgiou and P. Gikas, **Water Resources Management for Paros Island, Greece**, International Conference on Energy, Water, and Environment (ICEWE 2010)
3. E.M. Polykarpou, P.A. Dalby and L.G. Papageorgiou, **Synthesis of Chromatographic Purification Processes using Optimisation Techniques**, Euro 2010, Portugal (2010).
4. E. Kornelaki, S. Liu, L.G. Papageorgiou and P. Gikas, " **Potential for Water Reclamation and Reuse** at the Municipality of Kasteli, Heraklion, Greece", Orbit 2010, Greece (2010)
5. O. Akgul, N. Shah and L.G. Papageorgiou, **Optimisation-based Approaches for Bioethanol Supply Chains**, 7th International Conference on Computational Management Science, Austria (2010)
6. L. Bennett, S. Liu, L.G. Papageorgiou and S. Tsoka, **Module Detection in Complex Networks**, 18th Annual Conference on Intelligent Systems for Molecular Biology (ISMB), Boston, Massachusettes, USA, 11-13 July 2010
7. S. Padula , J.J. Harou, L.G. Papageorgiou and V. Viros (2010), **Preliminary Formulation and Application of a Minimum Cost Capacity Expansion Model for Water Supply and Demand Systems**, British Hydrological Society, BHS 2010 International Symposium, Newcastle, UK
8. E.M. Polykarpou, P.A. Dalby and L.G. Papageorgiou, **Synthesis of Downstream Processes: Optimal Selection of Chromatographic Sequences**, 14th conference on Recovery of Biological Products, USA (2010)
9. E.D. Mehleri1, H. Sarimveis, N.C. Markatos and L.G. Papageorgiou, **Optimal Design and Operation of Distributed Energy Systems**, Editors: Pistikopoulos EN, Georgiadis MC, Kokossis AC., Escape-21 conference, 1713-1717 (2011)
10. O. Akgul, N. Shah and L.G. Papageorgiou, **An MILP Model for the Strategic Design of the UK Bioethanol Supply Chain**, Editors: Pistikopoulos EN, Georgiadis MC, Kokossis AC., Escape-21 conference, 1799-1803 (2011)
11. C. Ainali, F. Nesltle L.G. Papageorgiou and S. Tsoka, **Disease Classification on the Basis of Biochemical Pathways through Integer Optimisation**, Editors: Pistikopoulos EN, Georgiadis MC, Kokossis AC., Escape-21 conference, 1548-1552 (2011)
12. T. Lastusilta, L.G. Papageorgiou and T. Westerlund, **A Comparative Study of Solving the Problem of Module Identification in a Complex Network**, ICheap-10 (2011).
13. D. Zhang, L.G. Papageorgiou, N.J. Samsatli and N. Shah, **Optimal Scheduling of Smart Homes Energy Consumption with Microgrid**, Energy 2011 (2011)
14. D. Zhang, N.J. Samsatli, D.J.L. Brett, N. Shah and L.G. Papageorgiou, **Fair Electricity Transfer Pricing and Capacity Planning in Microgrid**, 10th International Conference on Sustainable Energy Technologies (SET2011)
15. O. Akgul, N. Shah and L.G. Papageorgiou, **Optimisation of Hybrid First/Second Generation Biofuel Supply Chains**, 10th International Conference on Sustainable Energy Technologies (SET2011)
16. E.D. Mehleri, H. Sarimveis, N.C. Markatos and L.G. Papageorgiou, **Design and Operational Optimisation of a Heating Pipeline Network within a Microgrid**, 10th International Conference on Sustainable Energy Technologies (SET2011)

Efstratios N Pistikopoulos

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

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

Awards and Distinctions
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 and
- energy and the environment - sustainable process, product and network systems development

Other Activities
Director, CPSE, 2002-2009
Chair, International Programme Committee, European Symposium of Computer Aided Process Engineering (ESCAPE) 21, Porto Carras, Chalkidiki, Greece, 2011
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
Guest Co-Editor, Computers & Chemical Engineering, August 2011, Special Issue [on Energy Systems Engineering]
Co-Founder and Senior/ Consultant, PSE Ltd
Founder and Director, PAROS Ltd
Chair, Scientific Advisory Board, CERTH, Thessaloniki, Greece
Plenary Lectures – Benelux Meeting 2011, AMIDIQ 2011 Conference (Mexico)
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, 180 journal publications, over 150 refereed conference publications, over 60 Chapters in books & chapter contributions to encyclopaedias
Formulated, initiated and established an ongoing research programme involving an average of 15 man-years per annum (last ten years) – currently 12 PhD students, 3 Post-Doctorate Associates, 2 MSc students
Involved in (over) 50 research and industrial contracts, as Coordinator and/or PI
Supervised 32 PhD students, 18 Post-doctorate Associates, 40 MSc students and associates

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

Journal Articles

1. Ropponen Aino; Ritala Risto; Pistikopoulos Efstratios N. **Optimization issues of the broke management system in papermaking** *COMPUTERS & CHEMICAL ENGINEERING* 35:11 2510-2520 NOV 15 2011
2. Li Zheng; Liu Pei; He Fen; et al. **Simulation and exergoeconomic analysis of a dual-gas sourced polygeneration process with integrated methanol/DME/DMC catalytic synthesis** *COMPUTERS & CHEMICAL ENGINEERING* 35:9 SI 1857-1862 SEP 14 2011
3. Liu Pei; Whitaker Alan; Pistikopoulos Efstratios N. **A mixed-integer programming approach to strategic planning of chemical centres: A case study in the UK** *COMPUTERS & CHEMICAL ENGINEERING* 35:8 1359- 1373 AUG 10 2011
4. Kouramas K. I.; Faisca N. P.; Panos C. et al. **Explicit/multi-parametric model predictive control (MPC) of linear discrete-time systems by dynamic and multi-parametric programming** *AUTOMATICA* 47:8 1638-1645 AUG 2011

5. Koutinas M, Kiparissides A, Lam MC, et al. **Improving the prediction of Pseudomonas putida mt-2 growth kinetics with the use of a gene expression regulation model of the TOL plasmid** *BIOCHEMICAL ENGINEERING JOURNAL* 55:2 108-118 JUL 15 2011
6. Koutinas M, Kiparissides A, Silva-Rocha R, et al. **Linking genes to microbial growth kinetics-An integrated biochemical systems engineering approach** *METABOLIC ENGINEERING* 13:4 401-413 JUL 2011
7. Kiparissides A, Koutinas M, Kontoravdi C, et al **'Closing the loop' in biological systems modeling - From the in silico to the in vitro** *AUTOMATICA* 47:6 Sp. Iss. SI 1147-1155 JUN 2011
8. Liu P, Georgiadis MC, Pistikopoulos EN **Advances in Energy Systems Engineering** *INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH* 50:9 4915-4926 MAY 2011
9. Kiparissides A, Koutinas M, Moss T, Newman J, Pistikopoulos EN, Mantalaris A **Modelling the Delta1/Notch1 Pathway: In Search of the Mediator(s) of Neural Stem Cell Differentiation** *PLOS ONE* 6:2 e14668 FEB 2011
10. Khajuria H, Pistikopoulos EN **Dynamic modeling and explicit/multi-parametric MPC control of pressure swing adsorption systems** *JOURNAL OF PROCESS CONTROL* 21:1 151-163 JAN 2011
11. Dominguez LF, Pistikopoulos EN **Recent Advances in Explicit Multiparametric Nonlinear Model Predictive Control** *INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH* 50:2 609-619 JAN 2011
12. Dominguez LF, Pistikopoulos EN **Multiparametric programming based algorithms for pure integer and mixed-integer bilevel programming problems** *COMPUTERS & CHEMICAL ENGINEERING* 34:12 2097-2106 DEC 2010
13. Panos C, Kouramas KI, Georgiadis MC, et al. **Dynamic optimization and robust explicit model predictive control of hydrogen storage tank** *COMPUTERS & CHEMICAL ENGINEERING* 34:9 Sp. Iss. SI 1341-1347 SEP 2010
14. Kontoravdi C, Pistikopoulos EN, Mantalaris **A Systematic development of predictive mathematical models for animal cell cultures** *COMPUTERS & CHEMICAL ENGINEERING* 34:8 1192-1198 AUG 2010
15. Liu P, Pistikopoulos EN, Li Z **An energy systems engineering approach to the optimal design of energy systems in commercial building**s *ENERGY POLICY* 38:8 4224-4231 AUG 2010
16. Dua P, Dua V, Pistikopoulos EN **Modelling and multi-parametric control for delivery of anaesthetic agents** *MEDICAL & BIOLOGICAL ENGINEERING & COMPUTING* 48:6 543-553 JUN 2010

Refereed Conference Proceedings

1. Pefani E., Panoskaltsis N., Mantalaris A., Georgiadis M. C., Pistikopoulos E. N.. **Modelling and Simulation of Drug Delivery Systems for the treatment of Acute Myeloid Leukemia**. Accepted for presentation in the 5th European Conference of IFMBE, Budapest, Hungary, 2011
2. **Scenario-Based Strategic Supply Chain Design and Analysis for the Forest Biorefinery** Author(s): Mansoornejad Behrang; Pistikopoulos Efstratios N.; Stuart Paul Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010–2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1025-1029 Published: 2011
3. **On the model based optimization of secreting mammalian cell cultures via minimal glucose provision** Author(s): Kiparissides Alexandros; Pistikopoulos Efstratios N.; Mantalaris Athanasios Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis ACConference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29 JUN 01, 20102011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1210-1214 Published: 2011
4. **Predicting microbial growth kinetics with the use of genetic circuit models** Author(s): Koutinas Michalis; Kiparissides Alexandros; de Lorenzo Victor; et al. Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1321-1325 Published: 2011
5. **A combined growth kinetics, metabolism and gene expression model for 3D ESC bioprocesses** Author(s): Yeo David; Kiparissides Alexandros; Pistikopoulos Efstratios; et al.Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1326-1330 Published: 2011
6. **A Novel Physiologically Based Compartmental Model for Volatile Anaesthesia** Author(s): Krieger Alexandra; Panoskaltsis Nicki; Mantalaris Athanasios; et al. Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1495-1499 Published: 2011

7. **Modelling of the Insulin Delivery System for patients with Type 1 Diabetes Mellitus** Author(s): Zavitsanou Stamatina; Panoskaltsi Nicki; Mantalaris Athanasios; et al. Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1500-1504 Published: 2011
8. **Towards a high-fidelity model for model based optimisation of drug delivery systems in acute myeloid leukemia** Author(s): Pefani Eleni; Panoskaltsis Nicki; Mantalaris Athanasios; et al.Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1505-1509 Published: 2011
9. **A Mixed-Integer Programming Approach to Infrastructure Planning for Chemical Centres: A Case Study in the UK** Author(s): Liu Pei; Whitaker Alan; Pistikopoulos Efstratios N.; et al. Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 1668-1672 Published: 2011
10. **A robust optimization based approach to the general solution of mp-MILP problems** Author(s): Wittmann-Hohlbein Martina; Pistikopoulos Efstratios N.Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 527-531 Published: 2011
11. **Disturbance Estimation via Moving Horizon Estimation for In-flight Model-based Wind Estimation** Author(s): Voelker Anna; Kouramas Konstantinos; Panos Christos; et al.Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 577-581 Published: 2011
12. **Combined nonlinear model reduction and multiparametric nonlinear programming for nonlinear model predictive** control Author(s): Rivotti Pedro; Lambert Romain S. C.; Dominguez Luis; et al. Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 617-621 Published: 2011
13. **Integrated Design and Control of Pressure Swing Adsorption Systems** Author(s): Khajuria Harish; Pistikopoulos Efstratios N. Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 628-632 Published: 2011
14. **A novel approximation technique for online and multi-parametric model predictive control** Author(s): Lambert Romain S. C.; Rivotti Pedro; Pistikopoulos E. N. Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 738-742 Published: 2011
15. **Multi-Parametric Model Predictive Control of an Automated Integrated Fuel Cell Testing Unit** Author(s): Ziogou Chrysovalantou; Panos Christos; Kouramas Konstantinos I.; et al.Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 743-747 Published: 2011
16. **Explicit/Multi-Parametric Model Predictive Control of a Solid Oxide Fuel Cell** Author(s): Kouramas Kostas; Varbanov Petar S.; Georgiadis Michael C.; et al. Editor(s): Pistikopoulos EN; Georgiadis MC; Kokossis AC Conference: 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21) Location: Chalkidiki, GREECE Date: MAY 29-JUN 01, 2010-2011 Source: 21ST EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING Book Series: Computer-Aided Chemical Engineering Volume: 29 Pages: 773-777 Published: 2011

Presentations

1. **A hybrid robust/multi-parametric programming approach to process scheduling under uncertainty**. 8th International Conference on Computational Management - CMS 2011. 28-30 April 2011, Neuchatel, Switzerland
2. **A robust optimization based approach to the general solution of mp-MILP problems**. 21st European Symposium on Computer Aided Process Engineering – ESCAPE-21. 29 May -1 June 2011, Porto Carras, Greece
3. **On the global solution of multi-parametric mixed integer linear programming problems**. 2nd World Congress of Global Optimization in Engineering & Science – WCGO 2012. 3-7 July 2011, Chania, Greece
4. **Advances in multi-parametric mixed integer linear programming**. AIChe Annual Meeting. 16-21 October 2011, Minneapolis, USA
5. **A hybrid approach for process scheduling under uncertainty**. AIChe Annual Meeting. 16-21 October 2011, Minneapolis, USA
6. **Optimization under uncertainty - Recent advances in multi-parametric mixed integer linear programming and its applications**. QUADS Seminar on Optimization. 10 November 2011, Imperial College London, UK
7. Rivotti P., Lambert R., ERC MOBILE: **Algorithms for model reduction and explicit model based control of biomedical drug-delivery systems**, CPSE Consortium Meeting, London, December 2011
8. Zavitsanou S., Krieger A., Pefani E., ERC MOBILE: **Development of optimal drug delivery systems for Anaesthesia, Leukemia and Type 1 Diabetes**, CPSE Consortium Meeting, London, December 2011

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

Editor 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/

Computational Management Science, University of Vienna, July 10 http://www.univie.ac.at/cms2010/

Computing and Statistics (ERCIM'10), University of London, Dec 10
http://www.cfe-csda.org/ercim10/

Invited Speaker
Computational Management Science, Neuchatel, July 11
Computing in Economics and Finance Conference, London, July 10

Book Chapters

1. Tsoukalas, A., W. Wiesemann, B. Rustem (2009), **Global Optimisation of Pessimistic Bi-LevelProblems**, in P.M. Pardalos and T.F. Coleman (Eds), Workshop on Global Optimization, Fields Communications Series, American Mathematical Society Publishers.
2. P. Parpas, B. Rustem (2009). **Algorithms for minimax and expected value optimization**, In the Handbook of Computational Econometrics, (David A. Belsley, Erricos Kontoghiorghes eds.), John Wiley, New York and London

Journal Articles

1. Obasanjo, E., G.T. Regas, B. Rustem (2010). **An interior point algorithm for nonlinear minimax problems**, J of Optimization Theory & Applications, 144, 291-318
2. Kleniati, P. Parpas, B. Rustem (2010). **Partitioning Procedure for Polynomial Optimization**, J of Global Optimization, 48, 549-567
3. Wolfram Wiesemann, Daniel Kuhn, and Berç Rustem (2010). **Maximizing the Net Present Value of a Project under Uncertainty**. European Journal of Operational Research 202(2), 356-367 (2010)
4. P. Kleniati, P. Parpas, B. Rustem (2010). "**Decomposition-based Method for Sparse SDP Relaxations of Polynomial Optimisation Problems**", J of Optimization Theory & Applications, 145, 2, 289-310
5. S. Zymler, B. Rustem, D. Kuhn (2010). "**Robust Portfolio Optimization with Derivative Insurance Guarantees**", European J of Operations Research, 210, 410-424
6. R. J. Fonseca, S. Zymler, W. Wiesemann and B. Rustem (2010) "**Robust Optimization of Currency Portfolios**", J of Computational Finance, 15(1), 3-30
7. George Tzallas-Regas and Berc Rustem (2011) "**Switching Stepsize Strategies for SQP**", J of Optimization Theory & Applications, 149, 269-292
8. Steve Zymler, Berç Rustem, and Daniel Kuhn (2011). **Robust Portfolio Optimization with Derivative Insurance Guarantees**. European Journal of Operational Research 210(2), 410-424
9. N. Papadakos, B. Rustem, G. Tzallas-Regas, and J. Thoms (2011). "**Risky Traveling Salesman Problem**", European Journal of Operational Research, 212(1), 69-73.

Conference Papers

1. 24th European Conference on Operational Research (2010) Lizbon: Fonseca, R., Zymler, S., Wiesemann, W., and Rustem, B. **Linearly Adjustable Rules for International Portfolio Optimization**
2. 7th International Conference on Computational Management Science (2010) Vienna: Wiesemann, W. Kuhn, D., Rustem, **Interdicting a Project to Develop Nuclear Weapons**

Other Activities

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

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)

Research Interests

- Energy systems engineering, especially urban energy systems, bio-energy systems and biofuels, hydrogen infrastructures
- Supply chain and enterprise optimization
- Planning and scheduling
- Process development and design
- Model-based process safety assessment

Other Activities

Co-founder of Process Systems Enterprise Ltd
Defra panel member
EPSRC college member
EPSRC Manufacturing Strategy Advisory Team
BBSRC Industrial Biotechnology and Bioenergy Strategic Advisory Team
IChemE Transactions editorial board member

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, iCPSE
Tsinghua University, Clean Energy Centre

National University of Singapore
Delft University of Technology
Rothamsted Research
DECC
IBERS – University of Aberystwyth

Industrial Collaborations
Ashe Morris (Novel reactor modeling and experimentation)
BP (Urban Energy Systems Project)
Shell (H2-CO2 infrastructure design)
Syngenta (Supply chain network design)
Sainsbury's (Store of the future)
Mycologix (Biomass pretreatment)
Masdar clean energy company (CCS in the UAE)
Unilever (Sustainable supply chains design)
Energy Technologies Institute (Bioenergy Value Chain)
Biosep (Biomass fractionation)

Journal Articles

1. Sousa RT, Liu S, Papageorgiou LG, et al, **Global supply chain planning for pharmaceuticals**, *CHEMICAL ENGINEERING RESEARCH & DESIGN*, 2011, Vol:89, Pages:2396-2409, ISSN:0263-8762
2. Keirstead J, Shah N, **Calculating minimum energy urban layouts with mathematical programming and Monte Carlo analysis techniques**, *COMPUTERS ENVIRONMENT AND URBAN SYSTEMS,* 2011, Vol:35, Pages:368-377, ISSN:0198-9715
3. Zhao Y, Sadhukhan J, Lanzini A, et al, **Optimal integration strategies for a syngas fuelled SOFC and gas turbine hybrid**, *JOURNAL OF POWER SOURCES, 2011*, Vol:196, Pages:9516-9527, ISSN:0378-7753
4. Stefansson H, Sigmarsdottir S, Jensson P, et al, **Discrete and continuous time representations and mathematical models for large production scheduling problems: A case study from the pharmaceutical industry**, *EUROPEAN JOURNAL OF OPERATIONAL RESEARCH*, 2011, Vol:215, Pages:383-392, ISSN:0377-2217
5. Hosseini SA, Shah N, **Modelling enzymatic hydrolysis of cellulose part I: Population balance modelling of hydrolysis by endoglucanase**, *BIOMASS & BIOENERGY*, 2011, Vol:35, Pages:3841-3848, ISSN:0961-9534
6. Hosseini SA, Shah N, **Enzymatic hydrolysis of cellulose part II: Population balance modelling of hydrolysis by exoglucanase and universal kinetic model**, *BIOMASS & BIOENERGY*, 2011, Vol:35, Pages:3830-3840, ISSN:0961-9534
7. Zhao Y, Shah N, Brandon N, **Comparison between two optimization strategies for solid oxide fuel cell-gas turbine hybrid cycles**, *INTERNATIONAL JOURNAL OF HYDROGEN ENERGY*, 2011, Vol:36, Pages:10235-10246, ISSN:0360-3199
8. Zamboni A, Murphy RJ, Woods J, et al, **Biofuels carbon footprints: Whole-systems optimisation for GHG emissions reduction**, *BIORESOURCE TECHNOLOGY*, 2011, Vol:102, Pages:7457-7465, ISSN:0960-8524(publication doi)
9. Liang H, Keirstead J, Samsatli N, et al, **Application of a novel, optimisation-based toolkit ("syncity") for urban energy system design in Shanghai Lingang New City**, ENERGY EDUCATION SCIENCE AND TECHNOLOGY PART A-ENERGY SCIENCE AND RESEARCH, 2011, Vol:28, Pages:311-318, ISSN:1308-772X
10. Konda NVSNM, Shah N, Brandon NP, **Optimal transition towards a large-scale hydrogen infrastructure for the transport sector: The case for the Netherlands**, INTERNATIONAL JOURNAL OF HYDROGEN ENERGY, 2011, Vol:36, Pages:4619-4635, ISSN:0360-3199
11. Akgul O, Zamboni A, Bezzo F, et al, **Optimization-Based Approaches for Bioethanol Supply Chains**, INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, 2011, Vol:50, Pages:4927-4938, ISSN:0888-5885
12. Kucherenko S, Feil B, Shah N, et al, **The identification of model effective dimensions using global sensitivity analysis**, RELIABILITY ENGINEERING & SYSTEM SAFETY, 2011, Vol:96, Pages:440-449, ISSN:0951-8320
13. Weber C, Shah N, **Optimisation based design of a district energy system for an eco-town in the United Kingdom**, ENERGY, 2011, Vol:36, Pages:1292-1308, ISSN:0360-5442
14. Sadhukhan J, Zhao Y, Leach M, et al, **Energy Integration and Analysis of Solid Oxide Fuel Cell Based Microcombined Heat and Power Systems and Other Renewable Systems Using Biomass Waste Derived Syngas**, INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, 2010, Vol:49, Pages:11506-11516, ISSN:0888-5885
15. Mac Dowell N, Florin N, Buchard A, et al, **An Overview of CO2 capture technologies, Energy and Environmental Science**, 2010, Vol:3, Pages:1645-1669
16. Hosseini SA, Lambert R, Kucherenko S, et al, **Multiscale Modeling of Hydrothermal Pretreatment: From Hemicellulose Hydrolysis to Biomass Size Optimization**, ENERGY & FUELS, 2010, Vol:24, Pages:4673-4680, ISSN:0887-0624
17. Sadhukhan J, Zhao Y, Shah N, et al, **Performance analysis of integrated biomass gasification fuel cell (BGFC) and biomass gasification combined cycle (BGCC) systems**, CHEMICAL ENGINEERING SCIENCE, 2010, Vol:65, Pages:1942-1954, ISSN:0009-2509
18. Zhao Y, Shah N, Brandon NP, **The Development and Application of a Novel Optimisation Strategy for Solid Oxide Fuel Cell-Gas Turbine Hybrid Cycles**, Fuel Cells, 2010, Vol:10, Pages:181-193

Refereed Conference Proceedings

1. M. Kostantinidis, N. J. Samsatli, J. E. Keirstead and N. Shah, **Modelling of integrated municipal solid waste to energy technologies in the urban environment**, 3rd International Conference on Engineering for Waste and Biomass Valorisation, May 17-19, 2010 – Beijing, China
2. Acha, S., Green, T., Shah, N. (2010) **Effects of Optimised Plug-in Hybrid Vehicle Charging Strategies on Electric Distribution Network Losses**. IEEE PES Transmission and Distribution Conference and

Exposition, New Orleans, USA. April 19-22 2010
3. Acha S, van Dam KH, Keirstead J, et al, **Integrated modelling of agent-based electric vehicles into optimal power flow studies**, Frankfurt, Germany
4. Khor CS, Shah N, **A superstructure optimization approach for optimal refinery water network systems synthesis with membrane-based regenerators**, 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21), ELSEVIER SCIENCE BV, 2011, Pages:361-365, ISSN:1570-7946
5. Patel MP, Shah N, Ashe R, **Plant-wide optimisation and control of a multi-scale pharmaceutical process**, 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21), ELSEVIER SCIENCE BV, 2011, Pages:713-717, ISSN:1570-7946
6. Patel MP, Shah N, Ashe R, **Robust optimisation methodology for the process synthesis of continuous technologies**, 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21), ELSEVIER SCIENCE BV, 2011, Pages:351-355, ISSN:1570-7946
7. Mehdizadeh A, Shah N, Bongers PMM, et al, **Complex Network Optimization in FMCG**, 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21), ELSEVIER SCIENCE BV, 2011, Pages:890-894, ISSN:1570-7946
8. Mac Dowell N, Alhajaj A, Konda M, et al, **Multiscale whole-systems design and analysis of CO(2) capture and transport networks**, 21st European Symposium on Computer Aided Process Engineering (ESCAPE-21), ELSEVIER SCIENCE BV, 2011, Pages:1205-1209, ISSN:1570-7946

Invited/Keynote Lectures
1. N. Shah, J. Keirstead, SynCity: **New Tools, Methods and Business Models for future urban sustainability**, Communities for Advanced Distributed Energy Resources, San Diego, April 2010
2. N. Shah, **Supply chain optimisation in the process industries**, Advances In Process Analytics And Control Technologies, Manchester, April 2010
3. N. Shah, **Planning for Low Carbon Urban Energy Systems: Olympic Park Legacy Committee Workshop**, October 2011.
4. N. Shah, **Multiscale modelling and optimisation for scale-up: Commercialisation of Nanomaterials - Overcoming the Scale-up Challenge Event**, Leeds, October 2011

Eva Sørensen

Reader in Chemical Engineering, Department of Chemical Engineering, UCL

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)
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
Treasurer of IChemE's Education Special Interest Group
Member of IChemE's Fluid Separations Special Interest Group Committee
Member of American Institute of Chemical Engineers (AIChE)

Member of European Siciety 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

Industrial Collaborations
Novasep, Pfizer, Yorkshire Water

Journal Articles
1. Lam K.F., E. Cao, E. Sorensen and A. Gavriilidis (2011), **Development of multistage distillation in a microfluidic chip,** *Lab on a Chip - Miniaturisation for Chemistry and Biology*, 11 (7), 1311-1317
2. Lam K.F., E. Sorensen and A. Gavriilidis (2011), **Towards an understanding of the effects of operating conditions on separation by microfluidic distillation**, *Chemical Engineering Science*, 66 (10), 2098-2106

Conference Contributions
3. Osuna-Sanchez, H., C. Ng, E. Sørensen, D. Bracewell and E. Valery (2010), **High performance affinity chromatography to optimize purification via Protein A capture**, presented at International Symposium on Preparative and Process Chromatography (PREP 2010), Philadelphia, May 2010
4. Lam, K.F., E. Sørensen and A. Gavriilidis (2010), **On-chip microscale distillation for acetone-water separation**, presented at The Fourteenth International Conference on Miniaturized Chemical and Biochemical Analysis Systems (uTAS 2010), Groningen, October 2010
5. Lam, K.F., E. Sørensen and A. Gavriilidis (2011), **Microscale distillation for acetone-water separation**, presented at The 3rd European Process Intensification Conference, Manchester, June 2011
6. Förster, M., K.F. Lam, E. Sorensen and A. Gavriilidis, **Separation of toluene and benzaldehyde by microchannel** distillation, presented at European Congress of Chemical Engineering (ECCE 2011), Berlin, September 2011
7. Ng, C., H. Osuna-Sanchez, E. Valery, E. Sorensen and D. Bracewell (2011), **Optimisation of antibody capture by protein A chromatography**, presented at International Chemical and Biological Engineering Conference (ChemPor), Lisbon, September 2011
8. Close, E.J., T. Iskra, J. Salm, E. Sorensen and D. Bracewell (2011), **Characterising the Fouling of An Industrial Anion Exchange Polishing Step During the Manufacturing Process of a Commercial Therapeutic Protein**, presented at AIChE 2011 Annual Meeting, Minneapolis, November 2011, paper 444fe
9. Close, E.J., J. Salm, J. Lyons, D. Bracewell and E Sorensen (2011), **Model Based Experimental Design and Parameter Estimation for An Industrial Hydrophobic Interaction Chromatography Step From a Quality by Design (QbD) Perspective**, presented at AIChE 2011 Annual Meeting, Minneapolis, November 2011, paper 700e

N.F. Thornhill

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
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: Member of Process Management & Control Subject Group.
EPSRC: Member of Peer Review College.
Member of the International Editorial Board of the Journal of Process Control.
Associate Editor of Control Engineering Practice.

Reviewer for
AIChE Journal
Biotechnology and Bioengineering
Chemical Engineering Research and Design
Computers & Chemical Engineering
Control Engineering Practice
IEE Proceedings D
Industrial and Engineering Chemistry Research
Institution of Mechanical Engineers Journal of Systems and Control Engineering
International Journal of Adaptive Control and Signal Processing
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
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. Sharifzadeh, M., and Thornhill, N.F., 2012, **Optimal selection of control structures using a steady-state inversely controlled process model**, *Computers & Chemical Engineering*, accepted for publication. DOI: 10.1016/j.compchemeng.2011.12.007
2. Meland, E., Thornhill, N.F., Lunde, E., and Rasmussen, M., 2012, **Quantification of valve leakage rates**, *AIChE Journal*. Available as Early View article. DOI: 10.1002/aic.12630
3. Turunen, J., Thambirajah, J., Larsson, M., Pal, B.C., Thornhill, N.F., Haarla, L., Hung., W., Carter, A., Rauhala, T., 2011, **Comparison of four electromechanical oscillation damping estimation methods**, *IEEE Transactions on Power Systems*. 26, 2398-2407. DOI:10.1109/TPWRS.2011.2155684
4. Sharifzadeh, M., Rashtchian, D., Pishvaie, M.R., and Thornhill, N.F., 2011, **Energy induced separation network synthesis of an olefin compression section: a case study**, *Industrial Engineering and Chemistry Research*, 50, 1610–1623
5. Thambirajah, J., Thornhill, N.F., and Pal, B.C., 2011, **A multivariate approach towards interarea oscillation damping estimation under ambient conditions via independent component analysis and random decrement**, *IEEE Transactions on Power Systems*, 26, 315-322
6. Thambirajah, J., Barocio, E.B., and Thornhill, N.F., 2010, **A comparative review of methods for stability monitoring in electrical power systems and vibrating structures**, *IET Generation Transmission & Distribution*, 4, 1086-1103

Conference Presentations
1. Cecilio, I.M., Chen, S-L., and Thornhill, N.F., 2011, **Importance of auxiliary systems for process fault detection and diagnosis**, 19th IEEE Mediterranean Conference on Control and Automation (MED'11), Corfu, Greece, June 20-23, 952-957
2. Di Geronimo Gil, G.J., Alabi, D.B., Iyun, O.E. and Thornhill, N.F., 2011, **Merging process models and plant topology, Advanced Control of Industrial Processes** (ADCONIP 2011), Hangzhou, China, May 23-26, Invited keynote paper
3. Stonier, A., Pain, D., Westlake, A., Hutchinson, N., Thornhill, N.F., Farid, S.S., 2011 **Integration of stochastic simulation with advanced multivariate and visualisation analyses for rapid prediction of facility fit issues in biopharmaceutical processes**, 21st European Symposium on Computer Aided Process Engineering. 29:1356-1360
4. Sharifzadeh, M., and Thornhill, N.F., 2011, **Optimal controlled variable selection using a nonlinear simulation-optimization framework**, 21st European Symposium on Computer Aided Process Engineering. 29:597-601
5. Ikram, W., Stoianov, I., and Thornhill N.F., 2010, **Towards a radio-controlled time synchronized wireless sensor network: a work in-progress paper**, IEEE EFTA Conference, September 2010

CPSE | Academics 2010–11

Imperial College London

Department of Chemical Engineering
Professor Claire Adjiman
Dr Edo Boek
Dr Benoit Chachuat
Professor Amparo Galindo
Professor Michael Georgiadias
Professor George Jackson
Dr Cleo Kontoravdi
Dr J Krishnan
Professor Geoffrey Maitland
Professor Sakis Mantalaris
Professor Costas Pantelides
Professor Stratos Pistikopoulos
Professor Nilay Shah
Professor Nina Thornhill

Department of Computing
Dr Daniel Kuhn
Professor Berc Rustem

Department of Earth Science & Engineering
Professor Nigel Brandon

Emeritus and Honorary Academics
Professor Roger Benson
Dr Graham Elkes
Dr Alexandr Malijevsky
Professor Paul Rutter
Professor Roger Sargent

University College London

Department of Chemical Engineering
Professor David Bogle
Dr Vivek Dua
Professor Eric Fraga
Dr Lazaros Papageorgiou
Dr Eva Sørensen

CPSE | Staff Directory

Academic Staff

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Emeritus and Honorary Academics

Professor Roger Benson	roger.s.benson@btinternet.com
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Professor Paul Rutter	p.rutter@imperial.ac.uk
Professor Roger Sargent	r.w.h.sargent@imperial.ac.uk

Research Associates

Dr Afshin Anssari-Benham	a.anssari-benam@ucl.ac.uk
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Academic Support Staff

Miss Cristina Romano	c.romano@imperial.ac.uk
Miss Senait Selassie	s.selassie@imperial.ac.uk
Mr Graham Stuart	g.stuart@imperial.ac.uk

CPSE | Research Project List 2010–2011

Name: **Barakat Arinola Abiola**
Supervisor: Prof E Fraga & Dr P Lettieri
(Chemical Engineering, UCL)
Title of thesis: *Life cycle analysis for bioethanol production*
Start date: October 2006
Finish date: September 2010

Name: **Ozlem Akgul**
Supervisors: Dr L.G Papageorgiou and Prof N Shah
Title of Thesis: *Optimization-based approaches for bioethanol supply chains*
Start Date: September 2009
Finish Date: September 2012

Name: **Shade Akinmolayan**
Supervisor: Dr Eva Sorensen and Prof N. Thornhill
Title: *Real time Operational Risk management through Advanced Multi-Scale Modelling*
Start Date: August 2011
Finish Date: August 2014

Name: **Hala Al Fulaij**
Supervisor: Prof D Bogle
Title of Thesis: *Dynamic modelling and control of multi stage flash (MSF) desalination plant*
Start Date: April 2007
Finish Date: July 2011

Name: **Tareg Al Soudani**
Supervisor: Prof D Bogle
Title of Thesis: *Multiscale modelling for operation and control of PSA units*
Start Date: April 2005
Finish Date: November 2012

Name: **Aiman Alam-Nazki**
Supervisor: Dr J Krishnan
Title of Thesis: *Mathematical modelling and systems approaches to investigating intracellular processes with spatial signal transduction*
Start Date: January 2010
Finish Date: July 2013

Name: **Ahmed Alhajaj**
Supervisor: Prof N Shah, Prof N Brandon & Dr V Vesovic
Title of Thesis: *Design & analysis of CO2 capture, transport & storage (CCTS) networks*
Start Date: December 2008
Finish Date: May 2012

Name: **Bruno Amaro**
Supervisors: Dr C Immanuel & Prof E.N Pistikopoulos
Title of Thesis: *Modelling and optimisation of molecular weight distribution for free-radical aolution polymerisation in batch reactors*
Start Date: December 2005
Finish Date: April 2010

Name: **Sheila MC Ang**
Supervisor: Prof E Fraga & Dr D Brett (UCL Chemical Engineering)
Title of Thesis: *Optimal design of fuel cell systems*
Start Date: September 2008
Finish Date: September 2011

Name: **Afshin Anssari-Benham**
Supervisor: Dr Eva Sorensen and Prof N. Thornhill
Title: *Real time Operational Risk management through Advanced Multi-Scale Modelling*
Start Date: October 2011
Finish Date: October 2013

Name: **Mohd Azua Mohd Azrin**
Supervisor: Prof E.N Pistikopoulos
Title of Thesis: *Optimization and advanced control of solar photovoltaic systems*
Start Date: October 2008
Finish Date: April 2012

Name: **Joakim Bäck**
Supervisor: Prof E Fraga & Dr S Guillas (Statistics, UCL)
Title of thesis: *Carbon capture process modelling and optimisation*
Start Date: October 2009
Finish Date: March 2013

Name: **Alireza Behjousiar**
Supervisor: Dr C Kontoravdi & Dr K Polizzi
Title of Thesis: *Improved cell line selection through in situ metabolic profiling and offline product analysis*
Start Date: October 2009
Finish Date: April 2013

Name: **Asif Bhatti**
Supervisor: Dr V Dua
Title of Thesis: *Design and synthesis of biological systems under uncertainty*
Start Date: October 2010
Finish Date: October 2013

Name: **Charles Brand**
Supervisor: Prof C Adjiman, Prof A Galindo & Prof G Jackson
Title of Thesis: *Development of an innovative process model for carbon capture*
Start Date: October 2009
Finish Date: April 2013

Name: **Paul Brumby**
Supervisor: Prof G Jackson
Title of Thesis: *Modelling and understanding confinement and chirality in liquid-crystalline systems*
Start Date: March 2006
Finish Date: March 2010

Name: **Sara Budinis**
Supervisor: Nina Thornhill
Title of Thesis: *Control systems for centrifugal compressors with emphasis on CO2 compression*
Start date: September 2011
End date: September 2014

Name: **Inês Cecilio**
Supervisor: Prof N.F Thornhill
Title of Thesis: *Integrated performance analysis of plant operation*
Start Date: January 2010
Finish Date: January 2014

Name: **Ning Chen**
Supervisor: Dr C Kontoravdi and Dr Colin Jaques (Lonza Biologics)
Title of Thesis: *Modelling of protein-producing Chinese hamster ovaries cells*
Start Date: October 2008
Finish Date: April 2012

Name: **Edward Close**
Supervisor: Dr E Sorensen & Dr D Bracewell (UCL)
Title: *Process modelling approaches to biological complexity in the production of therapeutic proteins*
Start Date: September 2009
Finish Date: September 2013

Name: **Andrew Crane**
Supervisors: Dr E Muller
Title of Thesis: *Coarse-grained simulation of the self-assembly and mesophase behaviour of polyphilic liquid crystals*
Start Date: July 2007
Finish Date: July 2011

Name: **Luis Dominguez**
Supervisor: Prof E.N Pistikopoulos
Title of Thesis: *Multiparametric mixed integer dynamic optimization of process systems*
Start Date: July 2007
Finish Date: July 2010

Name: **Simon Dufal**
Supervisor: Dr C Adjiman, Dr A Galindo & Prof G Jackson
Title of Thesis: *Modelling the phase behaviour and surface properties of complex*
reservoir fluids
Start Date: October 2009
Finish Date: April 2013

Name: **Alexander Dunnett**
Supervisors: Prof N Shah & Dr C Adjiman
Title of Thesis: *Biofuel supply chain*
Start Date: October 2005
Finish Date: May 2010

Name: **Kealan Exley**
Supervisors: Dr Karen Polizzi & Prof. Paul Freemont (Centre for Synthetic Biology), Dr Cleo Kontoravdi
Title of Thesis: *Towards cell-free synthesis of biopharmaceuticals using a synthetic biology approach*
Start Date: October 2011
Finish Date: October 2014

Name: **Osama Omar M. Fallata**
Supervisor: Dr. A. Mantalaris
Title of Thesis: *Bioprocessing of haematopietic stem cells*
Start Date: 19 November 2006
Finish Date: 19 March 2011

Name: **Iliana Fauzi**
Supervisor: Prof A. Mantalaris
Title of Thesis: *Stem Cell Bioprocessing*
Start Date: May 2006
Finish Date: August 2011

Name: **Hendrik Fentrup**
Supervisors: Dr E Muller
Title of Thesis: *Adsorption and diffusion in nanoporous materials*
Start Date: July 2011
Finish Date: July 2014

Name**: Giovanna Fiandaca**
Supervisors: Prof E Fraga & Prof S Brandani (University of Edinburgh)
Title of Thesis: *Optimal design of pressure swing adsorption for CO2 capture*
Start Date: April 2006
Finish Date: March 2009

Name: **María Fuentes Garí**
Supervisor: Prof. A. Mantalaris & Prof. E.N. Pistikopoulos
Title of thesis: *Population balance modelling of leukemic cells for the optimisation of chemotherapy delivery*
Start date: September 2011
Finish date: September 2014

Name: **Zara Ganase**
Supervisor: Prof C. S. Adjiman, Prof A Galindo & Prof A Armstrong (Imperial Chemistry)
Title of Thesis: *The effects of solvents on organic reactions*
Start Date: October 2009
Finish Date: March 2013

Name: **David Garcia Munzer**
Supervisor: A. Mantalaris, E.F. Pistikopoulos
Title of thesis: *Population Balance Modelling in Cell Culture Systems*
Start date: October 2010
Finish date: October 2014

Name: **Taoufiq Gueddar**
Supervisor: Dr V Dua
Title of Thesis: *Optimization under uncertainty*
Start Date: March 2008
Finish Date: February 2013

Name: **Seyed Ali Hosseini**
Supervisor: Prof N Shah
Title of Thesis: *Multiscale modelling of biorefineries*
Start Date: September 2007
Finish Date: January 2010

Name: **Waqas Ikram**
Supervisor: Prof N.F Thornhill
Thesis of Thesis: *Plant-wide and wireless process control and automation*
Start Date: Oct 2008
Finish Date: Sept 2011

Name: **Oluwatope Ebenezer Iyun**
Supervisor: Prof N.F Thornhill
Title of Thesis: *Plant-wide fault diagnosis: cause-and-effect analysis using process connectivity using process connectivity*
Start Date: December 2007
Finish Date: November 2011

Name: **Jamal Jamil**
Supervisor: Dr V Dua
Title of Thesis: *Process integration for reducing energy consumption and the cost*
Start Date: May 2009
Finish Date: May 2014

Name: **Philip Jedrzejewski**
Supervisors: Dr Cleo Kontoravdi, Dr Karen Polizzi (Centre for Synthetic Biology)
Title of Thesis: *A platform for the optimisation of metabolic pathways for glycosylation to achieve a narrow and targeted glycoform distribution*
Start Date: October2011
Finish Date: October 2015

Name: **Mark Jennings**
Supervisor: Prof N Shah and Prof D Fisk (Department of Civil Engineering)
Title of Thesis: *Optimal retrofits of urban energy systems*
Start Date: October 2009
Finish Date: December 2012

Name: **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*
Start Date: October 2008
Finish Date: April 2012

Name: **Andrei Kazantsev**
Supervisors: Dr C Adjiman & Prof C.C Pantelides
Title of Thesis: *Design of organic crystals for enhanced bioavailability*
Start Date: October 2007
Finish Date: October 2011

Name: **Harish Khajuria**
Supervisor: Prof E.N Pistikopoulos
Title of Thesis: *Advanced control and optimization of PSA hybrid system*
Start Date: October 2007
Finish Date: January 2011

Name: **Cheng Seong Khor**
Supervisor: Prof N Shah, Dr B Chachuat
Title of thesis: *Optimization of Water Network Systems Synthesis and Design*
Start date: October 2010
Finish date: September 2013

Name: **Alexandros Kiparissides**
Supervisor: Prof E.N Pistikopolus & Dr S Mantalaris
Title of Thesis: *Development of a combined mathematical and experimental framework for the control and optimisation of mammolian cell cultures*
Start Date: January 2007
Finish Date: February 2012

Name: **Alexandra Krieger**
Supervisor: Prof E.N Pistikopoulos
Title: *Model and multi-parametric control based drug delivery systems for anaesthesia*
Start Date: October 2009
Finish Date: September 2013

Name: **Sarantos Kyriakopoulos**
Supervisor: Dr Cleo Kontoravdi
Title of Thesis: *Amino Acid Metabolism in Chinese hamster ovary cells*
Start Date: October 2010
Finish Date: October 2013

Name: **Koon Fung Lam**
Supervisor: Dr E Sorensen & Prof A Gavriilidis (UCL)
Title: *Microdistillation*
Start Date: April 2009
Finish Date: April 2011

Name: **Romain Lambert**
Supervisor: Prof E.N Pistikopoulos
Title of Thesis: *Approximation of dynamical systems for application to parametric control*
Start Date: October 2009
Finish Date: September 2013

Name: **Chang-Gun (Colin) Lee**
Supervisor: Prof N Shah
Title of Thesis: *Optimisation of closed-loop supply chain*
Start Date: June 2007
Finish Date: June 2012

Name: **Vivien Li**
Supervisors: Professor D Bogle and Professor R Jalan (Hepatology, UCL)
Title of Thesis: *The Role of Connexin 43 in pathogenesis of liver disease. A Systems Engineering Approach*
Start Date: October 2011
Finish Date: September 2014

Name: **Cong Liu**
Supervisors: Dr Krishnan
Title of Thesis: *Mathematical modelling of drug delivery in cancer tumors*
Start Date: January 2008
Finish Date: June 201262

Name: **Songsong Liu**
Supervisor: Dr L.G Papageorgiou
Title of Thesis: *Optimisation for the process industry*
Start Date: September 2007
Finish Date: September 2010

Name: **Niall MacDowell**
Supervisors: Prof G Jackson, Dr C Adjiman & Dr A Galindo
Title of Thesis: *Improvements in amine based absorption systems for post combustion CO2 capture*
Start Date: October 2006
Finish Date: Jun 2010

Name: **Jan Marzinek**
Supervisors: Prof E.N Pistikopoulos, Prof A. Mantalaris
Title: *Molecular Dynamics Simulations of Protein-Ligand Interactions*
Start Date: October 2010
Finish Date: October 2013

Name: **Ali Mehdizadeh**
Supervisor: Prof N Shah
Title of Thesis: *Complex network global optimisation*
Start Date: October 2009
Finish Date: April 2013

Name: **Candy Ng**
Supervisor: Dr E Sorensen & Dr D Bracewell (UCL)
Title: *Optimal design, operation and control of continuous separation of biomolecules*
Start Date: September 08
Finish Date: September 12

Name: **Andreas Nikolaou**
Supervisor: Dr Benoit Chachuat, Dr Klaus Hellgardt
Title of thesis: *Optimal Design and Operation of an Integrated Process Delivering Multiple Energy Vectors: Photobioreactor, Anaerobic Digestion, Gasification*
Start date: November 2011
End date: November 2014

Name: **Olusola Osunkoya**
Supervisor: Dr E Sorensen
Title: *Modelling and optimisation of hybrid refinery separations based on shape-selective membranes*
Start date: November 2010
Finish Date: November 2013

Name: **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*
Start Date: January 2009
Finish Date: January 2012

Name: **Idtisak Paopo**
Supervisors: Dr S Mantalaris & Dr Xu
Title of Thesis: *Design and modelling of the airlift bioreactor for stem cell bioprocessing*
Start Date: October 2007
Finish Date: February 2011

Name: **Nicole Papaioannou**
Supervisor: Prof N Shah & Prof E.N Pistikopoulos
Title of Thesis: *Urban energy systems: environmental impact assessment and optimization*
Start Date: October 2008
Finish Date: April 2012

Name: **Vasileios Papaioannou**
Supervisor: Dr C Adjiman, Dr A Galindo & Prof G Jackson
Title of Thesis: *Design of solvents and fluid formulations using molecular-based group contribution methods*
Start Date: October 2008
Finish Date: September 2012

Name: **Olga Parkes**
Supervisors: Professor D Bogle and Dr P Lettieri (Chemical Engineering, UCL)
Title of Thesis: *Sustainability and Decision Support for Major Events – the London Olympics*
Start Date: October 2010
Finish Date: September 2013

Name: **Mayank Patel**
Supervisor: Prof N Shah
Title of Thesis: *Design, operation & control of the next generation flexible process plant*
Start Date: June 2007
Finish Date: June 2012

Name: **Eleni Pefani**
Supervisor: Prof E.N Pistikopoulos & Dr N Panoskaltsis
Title of Thesis: *Modelling, Optimisation and Multi-Parametric Control (MPC) based drug delivery systems for the treatment of Acute Myeloid Leukaemia (AML)*
Start Date: October 2009
Finish Date: September 2013

Name: **Frances Pereira**
Supervisors: Prof G Jackson, Dr C Adjiman and Dr A Galindo
Title of Thesis: *Duality-based algorithms for the global solution of fluid phase equilibria with molecular equations of state*
Start Date: October 2006
Finish Date: October 2010

Name: **Eleftheria Polykarpou**
Supervisor: L.G Papageorgiou & P.A Dalby (UCL Biochemical Engineering)
Title of Thesis: *Optimisation of chromatography for the purification of proteins*
Start Date: November 2007
Finish Date: November 2010

Name: **Channarong Puchongkawarin**
Supervisor: Dr Benoit Chachuat & Prof David Stuckey
Title of thesis: *Design of Wastewater Bioferinery for Energy and Nutrient Recovery*
Start date: 15 November 2011
Finish date: 14 November 2014

Name: **Jai Rajyaguru**
Supervisor: Dr. Benoit Chachuat
Title of thesis: *Global optimisation of chemical processes described by differential-algebraic equations.*
Start date: October 2011
Finish date: October 2015

Name: **Melanie Teresa Ramirez-Jaramillo**
Supervisor: Prof E Fraga
Title of Thesis: *Comparative modelling and optimisation of different pretreatment technologies for bioethanol production*
Start Date: March 2008
Finish Date: March 11

Name: **Nina Soraya Ramrattan**
Supervisor: Dr A Galindo & Dr E Muller
Title of Thesis: *Molecular models for the description of solid-fluid behaviour of chain-like molecules*
Start Date: October 2009
Finish Date: April 2013

Name: **Pedro Rivotti**
Supervisor: Prof E.N Pistikopoulos
Title of Thesis: *Advances in multi-parametric model predictive control with application to biomedical drug-delivery systems*
Start Date: October 2009
Finish Date: September 2013

Name: **Kate Elisabeth Royle**
Supervisors: Dr David Leak (Department of Life Sciences) and Dr Cleo Kontoravdi
Title of Thesis: *Modelling as a guide to improving Pichia pastoris protein production*
Start Date: October 2009
Finish Date: October 2012

Name: **Jose Guillermo Sampayo-Hernandez**
Supervisor: Prof G Jackson
Title of Thesis: *Theory and simulation of interfacial systems*
Start Date: October 2005
Finish Date: September 2010

Name: **Jens Schreckenberg**
Supervisors: Prof G Jackson, Dr C Adjiman & Dr A Galindo
Title of Thesis: *Modelling aqueous polymers microemulsions and micelles*
Start Date: July 2007
Finish Date: June 2011

Name: **Daniel Seaton**
Supervisor: Dr Krishnan
Title of Thesis: *Mathematical modelling and systems-based* understanding of cell polarity
Start Date: October 2008
Finish Date: October 2012

Name: **Mahdi Sharifzadeh**
Supervisor: Prof N.F Thornhill
Title of Thesis: *Plant-wide control structure selection*
Start Date: October 2009
Finish Date: September 2012

Name: **Sou Si**
Supervisors: Dr Cleo Kontoravdi, Dr Karen Polizzi (Centre for Synthetic Biology) and Dr Chris Sellick (MedImmune)
Title of Thesis: *Development of a computation model for predicting the impacts of bioprocess condition on protein glycosylation patterns in monoclonal antibody-producing mammalian cell cultures*
Start Date: October 2011
Finish Date: October 2015

Name: **Erini Siougkrou**
Supervisor: Dr C Adjiman, Dr A Galindo
Title of Thesis: *Design of solvent mixtures for organic reactions*
Start Date: October 2009
Finish Date: October 2013

Name: **Roochi Solanki**
Supervisor: Dr A Galindo & Dr C Markides
Title of Thesis: *Novel thermofluidic oscillator devices for low-grade heat utilisation*
Start Date: October 2009
Finish Date: April 2013

Name: **Ioanna Stefani**
Supervisors: Dr Cleo Kontoravdi and Dr Karen Polizzi (Centre for Synthetic Biology)
Title of Thesis: *Endoplasmatic reticulum stress & neurodegeneration in model systems of familial Alzheimer's disease*
Start Date: October 2010
Finish Date: September 2014

Name: **Heiko Strubing**
Supervisors: Dr C Adjman, Prof E.N Pistikopolous & Dr A Galindo
Title of Thesis: *Design of solvents for organic reactions*
Start Date: Nov 07
Finish Date: Nov 10

Name: **Vikram Sundara**
Supervisors: Prof D Bogle
Title: *Interval methods for bounding dynamic biological models*
Start date September 2010
End Date September 2011

Name: **Panthot Suwanapal**
Supervisor: Prof N Shah
Title of Thesis: *Energy systems with application to Thailand*
Start Date: October 2005
Finish Date: September 2010

Name: **Pasant Suwanapal**
Supervisor: Prof N Shah
Title of Thesis: *Chemical complex supply chain*
Start Date: October 2005
Finish Date: September 2010

Name: **Supacharn Tangviriyasirikul**
Supervisor: Dr S Mantalaris
Title of Thesis: *Development of a perfusion bioreactor with mechanical stimulation for bone or cartolage tissue engineering*
Start Date: October 2007
Finish Date: October 2010

Name: **Jegatheeswaran Thambirajah**
Supervisor: Prof N.F Thornhill
Title of Thesis: *A wide-area system for power transmission security*
enhancement using a process systems approach
Start Date: July 2007
Finish Date: July 2010

Name: **Cristina Triana**
Supervisor: Prof E. Fraga and Dr E Sorensen
Title: *Operation and control of bioethanol production*
Start Date: October 11
Finish Date: October 14

Name: **Argyro Tsipa**
Supervisors: Prof. E.N Pistikopoulos and Prof. A. Mantalaris
Title of thesis: *Closing the loop from in silico to in vivo: Modelling and Optimisation of bacterial cell culture systems*
Start date: September 2011
Finish date: December 2013

Name: **Manolis Vasileiadis**
Supervisor: Dr C Adjiman & Prof C.C Pantelides
Title of Thesis: *Design of organic crystals for enhanced bioavailability*
Start Date: October 2009
Finish Date: April 2013

Name: **Mario Eduardo Villanueva**
Supervisor: Dr. Benoit Chachuat
Title of thesis: *Global optimisation methodology for uncertain dynamic processes*
Start date: October 2011
Finish date: October 2015

Name: **Anna Voelker**
Supervisor: Prof E.N Pistikopoulos
Title of Thesis: *Control of MUAVs*
Start Date: October 07
Finish Date: October 10

Name: **Wolfram Wiesemann**
Supervisor: Prof B Rustem
Title of Thesis: *Optimisation of temporal networks under uncertainty*
Start Date: Sept 2006
Finish Date: September 2010

Name: **Liang Wu**
Supervisor: Prof G. Jackson and Dr E. Muller
Title of Thesis: *Modelling ordering in fluid mixtures*
Start Date: October 2009
Finish Date: April 2013

Name: **Dionysios Xenos**
Supervisor: Nina Thornhill
Title of Thesis: *Methods and tools for online process monitoring, diagnosis and optimization of integrated systems*
Start date: September 2011
End date: September 2014

Name: **Omolara Yaroson**
Supervisor: Prof G Jackson, Dr E Muller & Dr A Galindo
Title of Thesis: *A study of chains of molecules interacting vie Mie-type potentials and comparison with the SAFT EOS*
Start Date: January 2009
Finish Date: January 2012

Name: **Stamatina Zavitsanou**
Supervisor: Prof E.N Pistikopoulos
Title of Thesis: *Modeling and multi parametric control drug delivery systems for diabetes type 1*
Start Date: December 2009
Finish Date: December 2013

Name: **Di Zhang**
Supervisor: Dr L.G Papageorgiou
Title of Thesis: *Optimal design and planning of energy microgrid*
Start Date: September 2009
Finish Date: September 2012

Centre for
Process
Systems
Engineering

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