



Centre for
Process
Systems
Engineering

CPSE07

The Centre for Process Systems Engineering Annual Report 2007

Imperial College
London



CPSE07

The Centre for Process Systems Engineering Annual Report 2007

CPSE Contents

2007

Contents

CPSE Profile	05
Introduction and Review of the Year	06
CPSE Research Programme	07
CPSE Industrial Consortium	07

Competence Areas

Product and Process Design	09 - 10
Operations and Control	11 - 12
Modelling and Model Solution Tools	13 - 14

Application Domains

Chemical Manufacturing Systems	17 - 18
Molecular Systems Engineering	18 - 20
Biological Systems Engineering	21 - 22
Supply Chains of the Future	23 - 24
Energy Systems Engineering	25 - 27

Personal Profiles	28 - 41
CPSE Academics	42
List of Publications	43 - 59
Staff Directory	60
Research Project List	61 - 64

“..international research leader in Process Systems Engineering concerned with the management of complexity in uncertain systems, modelled across many time and scale lengths..”

CPSE Profile

2007

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 the Imperial College London South Kensington campus.

The Centre is an international research leader in Process Systems Engineering concerned with 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 tools and techniques required for this. The tools enable Process Systems Engineers to be able 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 to related business processes.

The Centre is dedicated to performing research and to developing 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 and review of the year 2007

Welcome to our Annual Review of the Centre for Process Systems Engineering. Inside you will find a wide range of information including summaries of research activities, the titles of projects being carried out by PhD students, and the profiles of academic staff.

The Centre for Process Systems Engineering (CPSE) is a multi-institutional research centre that was founded in August 1989. It involves Imperial College London and University College London, and is primarily based at the Imperial College London South Kensington campus.

Process engineers are concerned with systems involving physical and chemical change and aim to manage the complexity and uncertainty of such systems. The Centre's research takes a Process Systems Engineering approach to modelling and optimization across many time and scale lengths. Process systems engineering is the study of approaches to analysis and design of processes & systems and the development of tools and techniques required for this. Examples that you will find in this Review include modelling and optimisation of gas separation processes to recover CO₂ or H₂; interactive tools with visualization for process design; tools for robust parametric control; novel methods for data mining and classification; stem cell bio-processing; and modelling and optimization in a systems approach to urban energy integration.

The Centre involves 22 academic staff from Imperial College and UCL, 54 PhD students and 11 research fellows and associates. In the last five years we have been managing a portfolio of grants worth more than £6 million. Of this around 45% of the awards are from industry, 15% from the European Commission, 35% from the Research Councils and the remainder from TSB (previously the DTI) and charities. I am pleased to report that 2007 has been an exciting and memorable year for the CPSE with a prestigious award, new academic members and a major research grant.

PSE, a spinout from the CPSE, received the 2007 Royal Academy of Engineering MacRobert Award for its cutting-edge mathematical modelling system, gPROMS. PSE was established in 1997 and its Managing Director, directors and technical consultants are CPSE members. The MacRobert award is the UK's premier award for innovation in engineering and it recognizes that PSE has been a great example of successful technology transfer. In the last ten years PSE has grown substantially to employ 40 people internationally and has established a global client base in the chemicals, fuel cell, petrochemical, pharmaceuticals, consumer products, minerals & mining, food and other process industry sectors. We welcome new academic members to CPSE. Dr Cleo Kontoravidi has joined as Academic Fellow/Lecturer, a post funded jointly by RCUK and Lonza Biologics. Prof Geoffrey

Maitland, Professor of Energy Engineering, Dr Krishnan who works in systems biology and Dr. Daniel Kuhn, in Computing, have added to our strengths in energy systems engineering, biological systems engineering and stochastic programming respectively; Prof Nina Thornhill, who has been a CPSE member for many years, has moved from UCL to take up the ABB/RAEng Chair of Process Automation at Imperial College. Ms Janice Thomson has joined as Industrial Liaison Officer and manager of the Industrial Consortium.

The Molecular Systems Engineering Group within CPSE has been awarded a £3M EPSRC grant for a proposal entitled: "Molecular Systems Engineering: from generic tools to industrial applications". Major corporations support this research, including BASF, Procter & Gamble, and Bristol Myers Squibb Co. In my opinion, this grant is a great example of how innovative and relevant research grows from the interaction between the CPSE and its industrial partners and gains leverage from public funding.

CPSE has hosted and co-organised an EPSRC-sponsored International Workshop on Global Optimization, partially also supported by the Systems Engineering initiative within Imperial College, in which CPSE plays a leading role. The CPSE's industrial consortium gives privileged access for its members to CPSE academics, research staff and post-graduate students, and opportunities to network with other members. The member companies have a wide range of interests: Shell, BP and Petrobras have particular interests in the oil and gas business; Bristol Myers Squibb, and Bayer are interested in pharmaceutical manufacture; Dow, Ineos-Fluor, BASF, Air Products, Bayer and ICI are active in chemicals and polymers manufacture, while Procter and Gamble have interests in consumer products. ABB has activity in many of these areas as a major technology supplier.

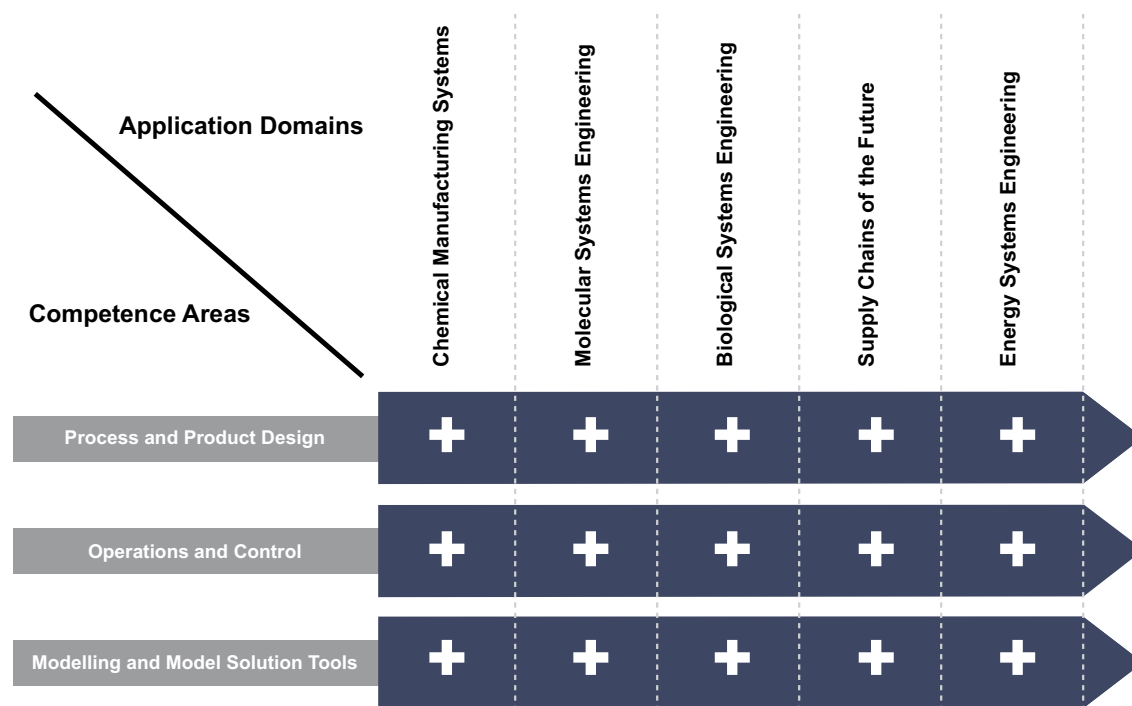
The industrial consortium also provides opportunities for member companies to become involved in the specification, development, validation and final commercial implementation of algorithms and software tools derived from the research performed in the Centre. Other member benefits include specialist technology focus briefings, pre-publication access to reports and papers, student secondments and opportunities for in depth discussions (Open-Days) with PhD students.

I hope you will enjoy reading this report. We are always keen to collaborate with companies (large and small), the non-profit sector, and academia worldwide.

Prof Stratos Pistikopoulos
Director, Centre for Process Systems Engineering
<http://www3.imperial.ac.uk/centreforprocesssystemsengineering>

CPSE Research Programme

2007



CPSE Industrial Consortium

The CPSE Industrial Consortium currently consists of 13 members who are all major companies in their different industries. They are;

- ABB Corporate Research
- Air Products
- BASF
- Bayer AG
- Bristol-Myers Squibb
- BP Exploration
- Dow Benelux B.V.
- GlaxoSmithKline
- ICI
- INEOS
- Petrobras
- Procter & Gamble
- Shell Research & Technology



Product and Process Design

Competence Area 1

The Product and Process Design competence area develops systematic model-based methodologies for the rational design of processes. 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 aim to enable engineers to meet the constraints and objectives imposed by today's business environment, in particular, in the field of sustainable development. They consider not only economic aspects, but also environmental, safety and health factors. 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 optical displays and fuel cells, distributed energy systems, integrated biomass/fuel cell plants and CO₂ capture from natural gas.

This wide-ranging activity engages researchers along four main themes:

Materials design for process synthesis:

The design of products and processing materials is tackled by development of a range of techniques from new property prediction techniques to their use in the design of environmentally benign, yet functional systems. This leads to design problems with an increasing number of degrees of freedom, such as molecular structure, microstructure or formulation variables.

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 projects and noteworthy achievements in the past years include:

The successful launch of a £4.6M Molecular Systems Engineering activity:

The Molecular Systems Engineering programme is described in detail in the application area reports in this Annual Review.

Systematic methodologies for modelling and optimisation of chromatographic separation processes:

Detailed models and systematic design techniques have been developed to consider processes across a range of industries including refining (distillation from petroleum or biofuels), fine-chemical separations (batch distillation, membrane separations such as pervaporation), food & drink (ultrafiltration for milk and whey protein, batch distillation for whisky and extractive distillation for essential oils) and Bioprocessing (chromatographic separations including simulated moving beds for proteins and biomolecules). An example of this is in the area of chromatographic separations, where a new project has just started to model and optimise their design and operation.

The tremendous development of biotechnology in recent years has resulted in the production of more and more new active compounds such as purified sugars, enzymes, peptides, antibiotics and therapeutic macromolecules. In parallel, the constraints on product purity in drug manufacture (e.g. for optical isomers) have become increasingly stringent and this has led to an intensified demand for efficient and economical separation technologies. For chromatographic separations, conducting the separation continuously instead of batch-wise can dramatically improve separation efficiency as well as production capacity and thereby reduce purification costs. This is particularly important for industrial applications of preparative chromatography.

Continuous chromatography involves the simultaneous use of several columns. Simulating moving bed, the basic continuous chromatographic technology, simulates a counter-current contact between a solid and a mobile phase

Product and Process Design

Competence Area 1

whereby the feed, eluent and product removal locations are switched at given intervals thus simulating the movement of the solid phase.

Systematic methodologies for modelling and optimisation of gas separation processes:

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Several projects have focussed on the development of techniques to design gas separation processes to recover CO₂ or H₂, with a focus on pressure swing adsorption (PSA), or hybrid membrane/PSA processes. The techniques developed are based on a combination of detailed models with multi-objective optimisation and/or superstructure optimisation. **The approaches have been demonstrated successfully in several case studies.**

The engineering of flexible reaction systems:

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A systematic approach to developing novel continuous reactors (e.g. Vari-Plate™, micro CSTRs) is under investigation in the field of process intensification, with a view to eventual commercialisation. The methodology is based firstly on gaining an understanding of the fundamental science, including micro and small channel fluid dynamics, unit operation and other design data. This is followed by the multiscale modelling of the dynamic behaviour within the systems through gPROMS® and computational fluid

dynamics and the validation through experimental study. Finally, proposed designs are analysed and evaluated using a process systems engineering approach which includes considerations such as operability and controllability, start-up and shut-down procedures, switching from one steady-state to another, analysis of the safety of processes from large disturbances, planning and on-line scheduling. Other reaction systems of interest have include biomass gasifiers, in which a combined modelling and experimental approach is taken, and organic reactions such as the Grubbs II catalysed ring-closing metathesis, where solvent effects are studied with a view to the computer-based optimisation of reaction conditions.

Methodologies for handling complex networks:

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Problems involving complex structures include the optimisation of heat exchanger networks (high-dimensional structure optimisation), gas production networks (large physical and time scales and complex multi-phase flow and thermodynamics), and N-dimensional allocation problems (flow-shop problems in 1-d, strip packing/cutting problems in 2-d, container packing problems and plant layout in 3-d and combined scheduling and packing problems in 4-d). New iterative approaches have been developed to treat this latter class of problems.

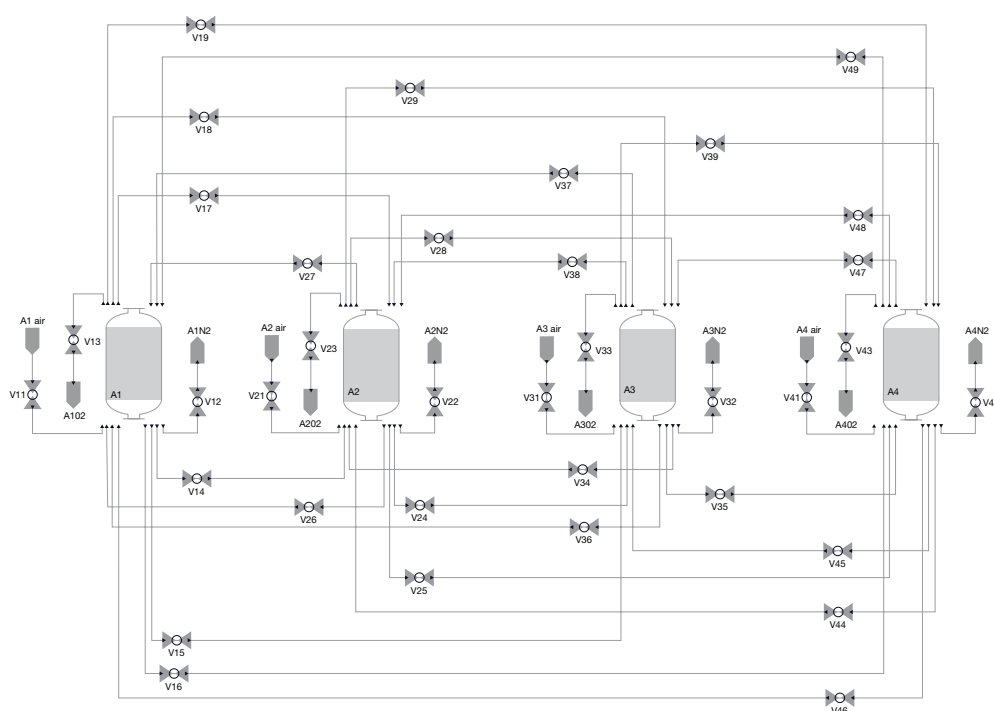


Figure 1. Design of a pressure swing adsorption system showing a superstructure with four units representing all possible interconnections.

Operations and Control

Competence Area 2



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 research 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 in the Centre covers optimization of the operation of existing plants, optimal designs for new plants that take account of dynamic operation at the design stage, and the management of supply chains and 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 projects in oil & gas, reaction and absorption, granulation and polymers. Competencies feeding into applications include integration of design, operation and decision making; multiscale modelling; integrated monitoring of process, electrical and mechanical equipment; and theoretical advances in robust parametric control.

Control at different levels has been understood in the control literature for over a decade leading to applications such as plant-wide planning and scheduling, model predictive control at the supervisory level and PID control at the regulatory level. However, in modern applications it becomes important to utilise explicit multi-scale process details within the control framework. For example, in the particulate area, control of the

individual particle phenomena enables much better and optimal performance at the overall process level. The research challenges in multi-scale control are formidable, not least because the manipulations are limited and sometimes competing, but the reward will be achievement of better performance by explicit consideration within a multi-scale framework.

In May 2007, ABB and the Royal Academy of Engineering established a new Research Chair in Process Automation at Imperial College London with a theme of integrated process operation. Integrated Collaborative Process Automation (CPA) is a strategic concept that will have a major impact over the next five to ten years. One central control system in a site will handle production management, safety and critical control, advanced control, information management, smart instrumentation, smart drives, electrical power, energy management, equipment condition monitoring, asset management, and documentation management. A driver for the change is the desire for the operation and optimization of sites to be undertaken remotely. Work is starting in the Centre into the analysis, monitoring and optimization of the interactions between the process and electrical and mechanical sub-systems to underpin and demonstrate technologies that will emerge in the new CPA environment.

A selection from the broad range of activities and noteworthy achievements in the past year includes:

Robust multi-parametric control:

Parametric control is model-based control which is achieved by formulating an online optimization problem using stored information that is computed offline. The stored information includes sub-regions of the parameter space over which different control action laws apply, together with explicit control laws for each of the sub-regions. Model-based control performs best when the model of the system is accurate, when the disturbances are known and the measurements being used for feedback are accurate. Unfortunately, there are often uncertainties in all of these, and yet safety and operational constraints must be honoured when the process is being controlled. An achievement of recent work has been to immunize parametric control against such uncertainties. Key features are that the constraints are adjusted iteratively to account for worst-case uncertainty at each step. The next control action is then determined using robust multiparametric quadratic programming, giving the benefits of fast computation. The overall effect is a fast, robust controller that can approach constraints more or less cautiously depending on the current level of system uncertainty.

Continued overleaf

Operations and Control

Competence Area 2

Optimal operation and control:

Optimal operation can achieve significant improvements in a wide range of complex processes particularly in fine chemicals and polymer manufacture. In semi-batch emulsion polymerisation, distributed variables such as particle size distribution and molecular weight influence bulk properties of melt index and rheology. Modelling and an experimental programme are underway to identify sensitivities using a multi-scale approach. The work this year has focused on formulating a configuration for the control of distributed variables taking account of their interactions and the limited manipulations available for control of the desired distributions.

Supply chain management:

Supply chain management involves looking at what resources are required and where, how best to use them and getting the right materials to the right place at the right time. The research has a significant societal impact as well as its business impact, for instance in improving the secure and timely supply of flu vaccines. Supply Chains of the Future is one the Centre's highlighted application areas which intersects with the Operations and Control competence area, with a theme of closed loop supply chains and re-manufacturing. Closed loop supply chains are emerging as manufacturers start to take responsibility for the disposal and re-use of components from the products, for instance under the Waste Electrical and Electronic Equipment (WEEE) directive of the EU.

Modelling biological regulatory processes:

Work underway at the intersection of Operations and Control with Biological Systems Engineering involves the analysis of biological pathways from a control point of view. Of particular interest are the mechanisms of chemotaxis, when an organism exhibits a direction response to a gradient in a chemical concentration, and chemokinesis which involves a change of behaviour in response to chemical concentration. The model includes adaptation to homogeneous signals and a persistent response to chemical gradients. The work is giving fundamental insights into gradient perception in eukaryotic cells, the activation of pseudopods and cell migration.

Electric power transmission enhancement:

A project at the intersection of the Energy Systems Engineering application area and the Operations and Control competence area is looking at the operation of electrical

power transmission in collaboration with power systems experts. New wide area measurement technologies using phasor measurement units are starting to be deployed which will give real-time measurements of the high quality that have been available in chemical plants and refineries for many years. The project is investigating and adapting signal analysis methods that have been used successfully in the chemical process industries. The goal is better understanding, early detection and diagnosis of instabilities in a.c. electrical power transmission systems and avoidance of situations leading to large scale power blackouts.

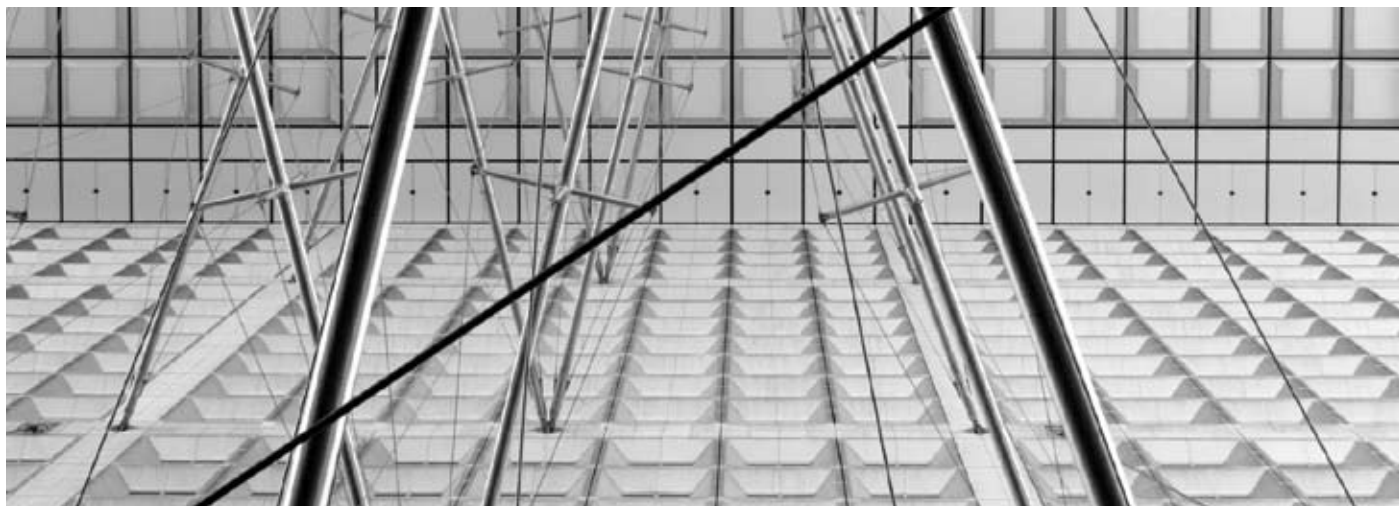
Urban energy systems:

The Operations and Control competence area is involved with the BP Urban Energy Systems project which is described fully elsewhere in this report. The aim is to understand what savings could be achieved if whole cities organized themselves to integrate their energy use. The project draws upon expertise across Imperial College in modelling of complex systems, and the specific contribution from the Optimization and Control competence area is in the application of powerful global optimization techniques from supply chain and logistics, and novel supply strategies.



Modelling and Model Solution Tools

Competence Area 3



The Modelling and Model Solution tools competence area is responsible for underpinning activities within all the application areas in the Centre covering applications across many scales of process and biological systems.

Multiparametric Programming:

The objective here is to obtain the optimal solution vector as an explicit function of the parameters without exhaustively enumerating the entire space of the parameters. New theory and algorithms have been developed and new application areas have been tackled. Due to the generic nature of the problem formulation and solution techniques the optimisation variables and parameters can be defined according to the application under consideration.

For multi-level programming problems where decision making process involves compromises among objectives of several interacting individuals or entities, new multiparametric programming techniques have been developed to solve these problems to global optimality. Multi-level programming problems can be represented by a hierarchical structure of units with independent and perhaps conflicting objectives. Solution of multiparametric programs at each level in a sequential manner provides a complete map of the optimal solution and the global solution can then be computed.

Multi-staged decision making processes can be effectively solved by using the principles of dynamic programming. In the presence of hard constraints and uncertain parameters dynamic programming techniques can not be directly used and new solution techniques are required. New algorithms for such problems based upon multiparametric programming have been developed.

Process design problems simultaneously involving uncertain parameters and control variables can be formulated as min-max-min-max type of optimisation problems. The objective is to find the most economic design (min) for all values of the uncertain parameters (max) by manipulating control variables (min) such that all the constraints are satisfied (max). A two-phase hybrid algorithm for solving such complex process design problems has been developed. In phase I inner min-max problem is solved by using multiparametric programming to obtain an explicit solution. This explicit solution then allows solving the outer min-max problem in phase II by using semi-infinite programming techniques. Novel techniques for solving multi-parametric nonlinear programming problems have been developed. The key contribution here is an efficient procedure for the identification of vertices of the regions characterising the map of the optimal solution.

Global Optimisation:

Many process systems engineering problems are characterised by the presence of nonlinearities which are usually non-convex and therefore potentially have several locally optimal solutions. Computationally efficient solution techniques that can avoid getting trapped in local solutions and converge to global optimal solution are being developed within this topic. Optimisation problems involving uncertainty in the satisfaction of the constraints of the model can be formulated as chance constrained optimisation problems. A global optimisation algorithm based upon addition of noise to negative gradient Lagrangian to escape local minima has been developed.

New global optimisation techniques for computing process conditions in batch thermal sterilization of food have been developed. Conventional food processing techniques over-heat the food to ensure safety, leading to degradation of

Modelling and Model Solution Tools

Competence Area 3

quality. The problem is formulated as an optimisation problem where the objective is to minimise quality reduction subject to constraints on safety. A non-convex optimisation problem is obtained which is solved to global optimality by dividing the time horizon into multiple intervals, the solution is given by temperature profiles in each of these intervals.

Parameter estimation techniques aim to compute the values of the unknown parameters so as to maximise the probability of agreement between the model prediction and experimental data. New global optimisation algorithms for parameter estimation for nonlinear models have been developed. It is shown that the confidence region may not be an ellipsoid, as usually assumed in the standard approaches for linear models. Effect of obtaining a local minimum on the analysis of the model of system has been obtained; it was observed that a local solution may mislead one to believe that the model is incorrect whereas realistic results can be obtained by using global solution for the same model. A multi-start algorithm has been developed that can take advantage of recent multi-core computing architectures.

Data Mining and Classification:

Activities in this topic include finding community structures in complex networks using mixed integer optimisation and multi-class data classification. Many social, technical and biological systems can be represented as networks of interacting components. Community structures are usually found in those systems where nodes are naturally divided into subgroups with dense within-module connections. Detection of such structures can be vitally beneficial to the study of various complex systems since nodes within the same module may share similar functional properties and novel patterns or functions can be deduced through the analysis of the interacting modules. A rigorous mixed integer quadratic programming optimisation model is proposed to identify optimal community structure in complex networks. Symmetry breaking constraints have been introduced to avoid the generation of equivalent solutions thus enhancing the computational performance of the proposed model. Results have shown that global optimal solutions have been achieved for a number of examples studied.

Data classification is one of the fundamental problems in data mining and machine learning. It deals with the identification of patterns and the assignment of new samples into known groups. During the training process, classification functions are generated optimally to separate samples of known class membership into different groups using all attribute values associated with each sample. A new sample is then classified into one of those classes by comparing its discriminant scores derived from classification functions. In this project, a mixed integer linear programming (MILP) model is proposed for the multi-class data classification problem using a hyper-box representation. The latter representation is particularly suitable for capturing disjoint data regions. The objective function used is the minimisation of the total number of misclassified data

samples. According to the computational results obtained, the proposed optimisation-based approach is competitive in terms of prediction accuracy when compared with various standard classifiers.

Population Balance Modelling:

Activities in this area include development of model solution tools for multi-dimensional population balance models and development of dynamic population balance models for a class of particular processes such as emulsion polymerisation and wet granulation, employing these solution tools.

The developed solution tool for multidimensional population balances employs a decomposition solution framework that explicitly accounts for the contributions of the different rate processes (birth, growth and death processes) individually in the first tier of the solution technique, and the amalgamation of the effects in the second tier. This straightforward decomposition framework enables a reduction of time-scale stiffness through the segregation of the various rate processes characterised by different time constants. Secondly, the decomposition framework enables tailoring the discretisation of the population distribution to different extents for the different rate processes, as dictated by the accuracy requirements of the particular rate processes. Thus, continuous processes necessitate a fine discretisation of the population to avoid errors beyond set tolerances, while the discrete processes allow the usage of coarse discretisation (which aids computation times).

The technique is used in the comprehensive modelling of emulsion polymerisation processes towards simultaneous control of multiple control variables – particle size distribution and molecular weight distribution. The technique is also applied for the development of multi-dimensional and rigorous population balance models of wet granulation processes. The future work will include the development of such multi-dimensional and multi-scale population balance models for specific biological processes.

Modelling Biological Regulatory Processes:

The eventual goal here is to develop a modular systems-based modelling framework for the processes of gradient sensing and polarization in eukaryotic chemotaxis, and to understand the regulation and interaction of different sub-processes involved in chemotaxis. Systems approaches are employed to understand and elucidate the nature of signal propagation in this system. Modelling work in collaboration with Dr Stansfield, Institute of Medical Sciences, University of Aberdeen) focuses on modelling pathways involved in the process of translation in yeast. Other current and emerging efforts involve modelling of polarity generation in biological systems and understanding the role of feedback effects in particular physiological processes, in collaboration with experimentalists.





Chemical Manufacturing Systems

Application Domains 1

Research in the CPSE aimed at serving chemical manufacturing systems can be found in each of the three competence areas of Modelling & Model Solution Tools; Operations & Control; and Product & Process Design. The industries served can be broadly classified as continuous chemical processes including petrochemicals and oil & gas; polymers; the particulates industry and specialty chemicals.

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

Biomass conversion for liquid fuels:

Biomass can be used not only for direct energy production, such as through gasification, but also for the production of liquid fuels. Two such prevalent fuels are ethanol, often used in conjunction with gasoline for automotive applications, and diesel.

Three projects are currently in progress in this area. The first, in collaboration with Universidad Nacional de Colombia, Manizales, concerns the design and implementation of new models for process design for use with the Jacaranda system for automated design. The models are detailed and provide sufficient information for the evaluation of both economic and environmental criteria within a multi-objective optimisation framework. The second project, in collaboration with the Centre for CO₂ Technology at UCL extends the boundaries over which biomass conversion processes are assessed through the use of life cycle assessment techniques to evaluate and to optimise alternative process designs for sustainable production of these fuels. The third project, recently started, is looking at the processing requirements for waste streams, both for the feed to biomass conversion processes, such as for the conversion of lignocellulosic biomass waste products, and for the streams generated by the conversion processes.

Automated and interactive tools for process heat integration with stream splitting:

A targeted optimisation procedure is being developed for the design of heat exchanger networks for process integration, including the generation of stream splits. The aim, mostly achieved at this point, is the implementation of an easy-to-use tool which generates, automatically, good solutions to the problem but also presents these solutions visually with cues for better understanding of the complexities in the design, as shown in Figure 1.

Dynamic modelling and control of multistage flash desalination plant:

Desalination of salt water is becoming a major industrial activity across the globe. The industry provides a sustainable source of fresh water for various urban and industrial applications. Dynamic modelling of such units remains a significant challenge. The project aims to do a detailed steady state and dynamic model and control for a multi stage flashing desalination unit for two types of desalination units: once through and brine circulation.

Modelling of reaction/adsorption systems:

This project is developing a multiscale model for reaction/adsorption systems. Time synchronization is a major characteristic of pressure swing adsorption (PSA) units. The pressurization and depressurization steps occur at similar intervals. Feed introduction (adsorption) and purge (desorption) steps also occur at similar time intervals, but the latter steps take more time than the former. A new control strategy that breaks time synchronization of the adsorption and desorption steps has been developed using the model.

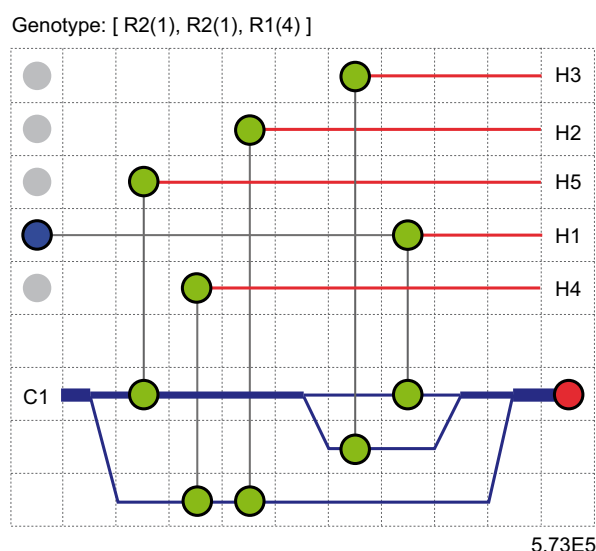


Figure 1. Heat exchanger network structure for a five hot stream, one cold stream integration problem with two stream splits, using visual cues to show relative energy flows in the network.

Continued overleaf

Chemical Manufacturing Systems

Application Domains 1

Hydrate prediction in oil-and-gas flows:

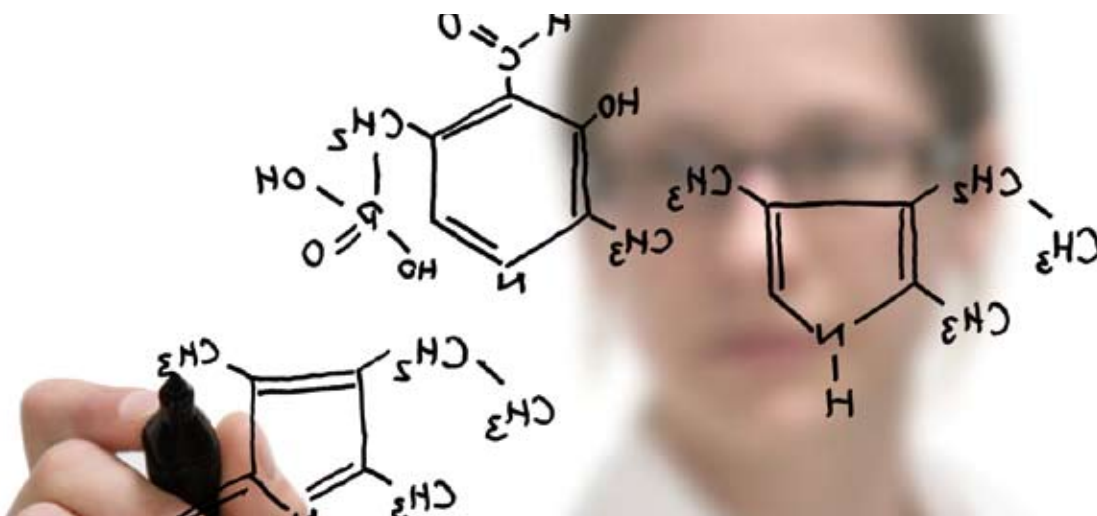
In parallel with efforts in the energy sector, a project is carried out on the development of efficient model-based state-estimation tools for oil-field applications towards effective flow assurance. The particular focus is to avoid hydrate formation in gas-liquid flows through pipelines. A dynamic model is developed to predict the possibility of hydrate formation. This model is linked with the available on-line measurements of key variables in state estimation algorithms to enhance the accuracy of the prediction of the open-loop model. The state estimation algorithms considered are the moving horizon estimation algorithm and the particle filtering algorithm.

Other activities:

Other projects within the Chemical Manufacturing Systems application area include bio-product purification, separation of carbon-dioxide and hydrogen from gaseous streams and emulsion polymerisation. There are more details of these projects in the reports on the Product and Process Design and Process Operation and Control competence areas.

Molecular Systems Engineering

Application Domains 2



In June 2007, the EPSRC and collaborating companies established a £4.6M research programme in Molecular Systems Engineering at Imperial College London to tackle process and product design problems where molecular-level information plays a pivotal role. It will combine fundamental physical understanding, mathematical models and numerical methods into new techniques and tools for the design of better products and processes. The emphasis is on integration of models across different scales so that molecular-level models can be used at the larger scale of products and processes.

Functional molecules (such as surfactants, ionic liquids and solvents) and structured phases (such as crystalline materials, micelles and liquid crystals) are of industrial importance in areas ranging from the chemical and petrochemical sectors to the personal care, pharmaceutical, agrochemical and biotechnology sectors. Molecular interactions are a fundamental consideration in the design of products and processes using functional molecules and structured phases. Structure can be related to physical properties through quantum mechanics, molecular mechanics, molecular and mesoscale simulations, group contribution methods, and equations of state. At the other end of the spectrum, modelling and optimal design of manufacturing processes is based on mechanistic descriptions of bulk kinetics and heat and mass transfer phenomena. Multiscale models combining

Molecular Systems Engineering

Application Domains 2

process models and computational fluid dynamics are used to model effects at smaller scales, such as mixing.

Computer-aided product and process design is currently based first on an analysis of molecular interactions, exploring the choice of materials at the molecular scale, followed by transfer of this information to the macroscale through simplified thermodynamic models. This sequential nature approach overlooks trade-offs between decisions at the molecular and process scales and the final design is therefore likely to be far from optimal. A large gap in information between the molecular scale and the macroscale has so far prevented the application of a more integrated design approach to optimise decisions at all scales. Recent attempts to bridge the gap have focused on the integrated design of solvents and separation processes. Further progress requires the incorporation of more general and predictive thermodynamic models in macroscale models. The Molecular Systems Engineering application area will develop reliable techniques which work across the whole spectrum of scales.

The research programme is structured around 2 drivers:

- 1) a set of molecular-based challenges faced by industry;
- 2) a set of generic challenges which provide a basis for long-term solutions.

Industrially-relevant challenges

Design of solvents for maximum selectivity and yield:

When designing a new process in the pharmaceutical or agrochemical industries, the choice of reaction medium (organic or “green” solvent) greatly affects key performance measures such as selectivity and yield. Unfortunately, the choice of reaction medium is often limited due to the cost of experimentation and lack of reliable predictive methods. Our objective is to develop predictive methods, and to incorporate them in design tools which can guide the choice of an optimal reaction medium.

Links have been established with experimental groups at Imperial and Warwick University for collaborations to generate data and test the approach.

Design of functional polymers, block co-polymer and blends:

Productivity in polymerisation reactors is closely linked to thermodynamics and phase equilibria, but thermodynamic models are currently restricted to a small set of materials. For further applications, it is critical to model the

thermodynamics of block co-polymers and other complex molecular structures. We are developing new molecular scale thermodynamic models and solution algorithms which will allow the design of complex polymers, block co-polymers and blends with a tailored structure and functionality.

Work within the SAFT framework has led to new models for surfactants which account for effects resulting from micelle formation. Water-surfactant phase diagrams have been calculated for a wide range of surfactant molecules.

Design of organic crystals for enhanced bioavailability:

The prediction of the crystal structures of complex organic molecules and their bioavailability is crucial for the pharmaceutical industry. Recent outcomes of the research include mathematical techniques that can reliably identify all polymorphs for rigid molecules and for a class of flexible molecules, and a predictive approach to encompass a wider class of flexible molecules and to consider polymorphism in salts and co-crystals of active pharmaceutical ingredients (API). Both approaches provide ways of controlling bioavailability without affecting the intrinsic biological action of the API. We are also working on the elimination of predicted polymorphs that are unlikely to appear in practice. Finally, via multiscale modelling and coarse dynamics, we will attempt to provide a quantitative assessment of the rate of dissolution of a given polymorph in a given solvent.

Design of microemulsions and liquid crystal mixtures:

The ability to tailor the properties of lyotropic materials (surfactants, colloidal suspensions, and liquid crystals) finds applications in the cosmetics, food, and oil industries. The key issue is the control of the formation of aggregated structures in the fluids. We are developing coarse-grained methods and equations of state to model these structures. We will then design novel liquid crystalline and nano-materials with optimal properties (in terms of their structure, templating, and optical characteristics) by taking advantage of their mixture properties.

A test case was chosen comprising a T-shaped bolamphiphile liquid crystal with grafted flexible side chains. This test molecule has been seen experimentally to have liquid crystal phases, lamellar phases and unique self-assembling behaviour. A coarse grained model of the molecule was developed, based on a repulsive liquid crystal core decorated with attraction sites to mimic the hydrogen bonding and flexible weakly attracting chains to mimic the grafted polymers. The work has led to a global phase diagram of

Molecular Systems Engineering

Application Domains 2

the system and simulation of its columnar triangular, square, and hexagonal phases. Lamellar behaviour was also seen.

Generic modelling and design tools

Identification of transition states:

The identification of transition states is important in understanding many physical phenomena and pathways, such as the kinetics of reactions, the folding of proteins, the formation of different crystal structures, and diffusion and adsorption processes. Transition states are at saddle points on an energy surface and most methods available require a starting point very close to the solution to achieve convergence, and the transition states found thus depend very much on intuition. The goal of this area of research is to develop reliable methods for the identification of transition states, which can be applied to energy surfaces calculated from molecular mechanics and at the electronic level.

Prediction of phase behaviour:

The design of molecular systems requires the ability to predict, quickly and reliably, the thermodynamics of new molecules or mixtures, and especially their phase equilibria. If this can be done when little or no experimental data are available, the time and cost needed for product and process development can be reduced and innovation can be stimulated. The design of novel molecules of tailored functionality through the control of molecular characteristics is of special relevance to the design of block-copolymers. We focus on group-contribution methods based on statistical mechanical approaches such as SAFT to give a clear physical link between the microscopic molecular features and the macroscopic properties.

Modelling of solute/solvent systems with coarse-grained models:

The modelling of macroscopic properties using statistical mechanics treatments to describe matter at the molecular level has become a powerful tool. Where the complexity of a given system is such that experimental studies are difficult and/or theory is lacking, it is through molecular simulation that a myriad of important details can be gathered from the careful study and observation of the molecular behaviour of bulk and confined fluids. Many interesting problems are very far from being within the realm of the computer power available, however. The molecular system engineering approach is ideally suited for modelling systems composed of large solutes dissolved in solvent systems, as exemplified by a colloid suspended in a polymer solutions, asphaltenes



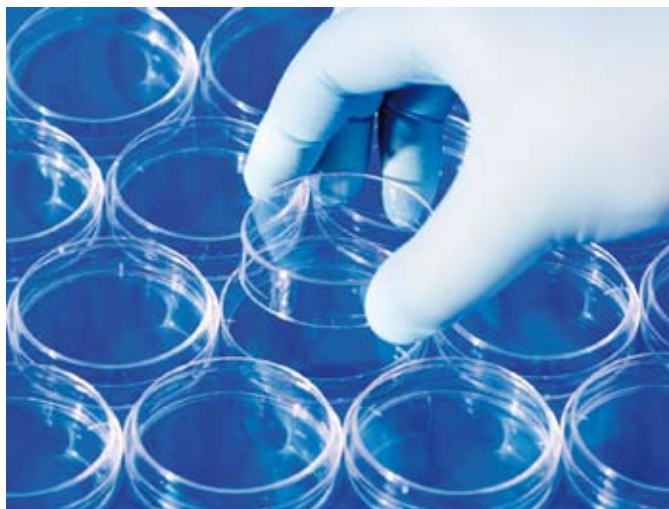
in crude oils, biomolecular and pharmaceutical products in supercritical CO₂, or micellar structures in liquid systems. In all these cases, differences in size, complexity and time scales preclude a direct atomistic simulation. Coarse-grained models and numerical methods to use these models are being developed in a systematic way to obtain practical tools without undue loss of the physics of the problem.

Minimisation of free energy functionals:

For important classes of systems such as liquid crystals, microemulsions, or micellar solutions, the molecules are not distributed in a spatially and/or orientationally uniform manner, and the thermodynamics properties such as free energy have to be expressed as functionals of the positional and orientational space. The determination of the equilibrium state is therefore much more mathematically demanding than in the simpler case of a uniform and isotropic fluid. The goal of this area of research is to develop a unified platform for the solution of free energy functionals, which can be applied to determine the properties of vapour-liquid/liquid-liquid interfaces, liquid crystal and micro-phase separated structures, and to solve the phase equilibria in polydisperse systems.

Biological Systems Engineering

Application Domains 3



The Biological Systems Engineering application area is developing engineering design and analysis approaches to the modelling of biological systems across multiple levels from cell signalling networks, gene, protein and metabolic networks and cellular systems, through to physiological systems. The research challenge in Systems Biology is to gain system-wide understanding in these areas.

The need for systems thinkers in life sciences research, in the pharmaceutical industry and in clinical services is widely acknowledged. The systems approach is instilled in process systems engineers and a second target is to train a new type of engineering biologist able to tackle multiple scale problems in manufacturing processes from the molecular scale through unit operations to plant-wide and enterprise wide systems.

Work of the Biological Systems Engineering application area falls into two themes: high value bioprocessing and systems biology.

High-value bioprocessing

Mammalian cell bioprocessing:

Animal cell culture produces a wide range of high-value products including vaccines, recombinant proteins, drugs for cardiovascular, respiratory and immune diseases, and monoclonal antibodies (MAB). MABs are one of the most important products in the biopharmaceutical industry because of their diagnostic and clinical applications but the production of industrial scale quantities of MAB is expensive and challenging. Complications that make it difficult to ensure that the culture is growing under controlled and optimal conditions at all times include the use of complex growth

media, lack of on-line measurements, limited experimental data and the extremely complex underlying reaction system.

Models of animal cell culture systems have a wide range of potential uses, such as analysis and prediction of experimental results, optimisation of culture conditions for prolonged viability, and the investigation of fundamental metabolic processes. Our research programme will integrate modelling, experiment design and validation, and control and optimisation into a single framework that would lead to increased productivity, regulated product quality, and reduced costs for mammalian cell culture systems.

Research on the area of recombinant protein and MAB production has focused on a framework for predictive mathematical modelling of protein-producing mammalian cell cultures. This was achieved through coupling of systems engineering tools such as global sensitivity analysis and design of experiments, with cell culture and molecular biology techniques. A collaboration with the Bioprocessing Technology Institute, A*STAR, in Singapore has led to the formulation and validation of models of amino acid metabolism for human embryonic kidney (HEK-293) and Chinese hamster ovary (CHO-IFN γ) cell lines.

Stem cell bioprocessing:

In order to harness the immense potential of stem cells (SCS) in terms of their plasticity and expansion capabilities, the physiological activity in relation to the culture parameters (local) such as pH, dissolved oxygen, nutrients/metabolite concentrations and growth factor concentrations needs to be recorded quantitatively and evaluated in a biologically meaningful manner. The project combines the expertise of cell biologists, engineers, scientists, and clinicians to develop a novel monitoring modality. The target is the systematic development of clinically relevant culture systems and methodologies which control and regulate stem cell self-renewal, expansion, differentiation, and death. A breakthrough in this area will lead to the engineering of reproducible, well-characterised, regenerated designer tissues and organs that meet strict regulatory criteria for clinical applications.

Peptide tags for improving downstream protein processing:

The development of more efficient downstream processes for therapeutic proteins is a time- and material-intensive as well as costly procedure. Consequently, it would benefit significantly from a predictive framework for identifying optimal purification strategies and for identifying peptide tags that would provide optimal recovery from desired purification sequences. The ability to identify peptide tags tailored to

Biological Systems Engineering

Application Domains 3

optimise the recovery of each new therapeutic protein with cost effective ion-exchange and hydrophobic-interaction chromatography steps would provide a highly desirable option. This project aims to develop optimisation-based models to integrate the selection of optimal peptide purification tags or protein mutants with the synthesis of protein purification processes.

Integrated modeling tools:

The goal for integrated modelling tools is a model library for commercially significant cell lines and a variety of processing units. There will be an emphasis on modelling and experimentation in the field of post-translational protein modification, especially glycosylation, as well as on the study of stress responses that represent a bottleneck in high-yielding manufacturing processes and how to overcome them. A collaboration with Lonza Biologics involves both fundamental biological research and the model-based control and optimisation of mammalian cell cultures.

Systems Biology

Analysis of biochemical and biological networks:

Insights into complex biochemical and biological networks and other biological systems can be gained from the structure of the network. Linear programming has been applied to the study of unweighted networks consisting of nodes (metabolites, enzymes) and edges (interactions between pairs of nodes) to calculate shortest path, average path lengths among nodes and the network diameter as measures of functionality. The algorithm deals effectively with edge directionality and circularity (e.g., cycles within metabolic pathways) proven to be a valuable analysis tool for complex biological networks.

Modular structures are usually found in networks where nodes are naturally divided into subgroups with dense within-module connections. Detection of such structures can be vitally beneficial to the study of various complex biological systems since nodes within the same module may share similar functional properties and novel patterns or functions can be deduced through the analysis of the interacting modules.

The algorithms have been successfully applied to metabolic networks, the p53 protein-protein interaction network in the mammalian cell cycle, and to DNA repair and apoptosis.

Modelling physiological systems – the liver:

The DTI funded Beacon project within CoMPLEX (Centre for Mathematics and Physics in the Life Sciences and Experimental Biology) at UCL, called 'Vertical Integration of Biological Scales', has just finished. It has delivered software

which integrates models developed using different modeling systems and its demonstrated with a working model of glucose homeostasis in hepatocyte cells. The principal input to the model is the time-course of glucose demand or supply by the body external to the model, which may represent feeding or the administration of intravenous glucose. The model's principal output is the resulting time-course of blood glucose. The model shows hyperglycemia in response to liver insulin resistance and ultradian oscillations in the case of high insulin sensitivity.

An application is to assess interventions in in vivo systems for beneficial or potentially harmful effects. Interventions can be environmental, through the introduction of chemical agents, pharmacological, through clinical interventions, or genetic. Engineering design techniques will be needed to make reliable system-wide predictions of the effects of interventions and to clarify the range of uncertainty that can be tolerated in the proposed environmental or clinical action. A new proposal to take this forward has been submitted.

Modelling Endothelial Cells:

A collaboration with CoMPLEX and Kings College London is developing a multiscale model of the effects of blood flow on the function of endothelial cells. In response to fluid flow endothelial cells stretch out and polarize in the direction of flow. A 3D model of an endothelial cell has been constructed and the force that the fluid flow exerts on the cell at a particular point has been calculated via a boundary integral method. Its purpose is to test hypotheses regarding the nature of the process.

Modelling biological regulatory processes:

Work on modelling the sub-processes involved in directed cell migration interacts with several activities and is reported in more detail in the Operations and Control and Modelling and Model Solution Tools competence areas. The goal is to develop a systems-based modelling framework to understand the directional sensing problem.

Mathematical Modelling of Glutamate in the Human Body:

Glial cells in the brain are responsible for neurotransmission through glial uptake of glutamate and the extra-cellular glutamate concentration must be controlled. This is achieved through a complex metabolic interaction between the glial and neuronal parts of the brain. The aim of this project is to model, analyze and understand the sensitivity of glutamate concentration and its possible link to development of neurological disorders such as Alzheimer's, Parkinson's and Schizophrenia. This analysis could then assist in development of drugs for treatment of neurological disorders.

Supply Chains of the Future

Application Domains 4



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

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.

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.

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.

Energy and materials from biomass:

A good example of the holistic approach is the production of energy and materials from biomass. This is often analysed in a piecemeal way, considering one or two sample pathways (e.g. producing biodiesel from palm oil). There is a much more fundamental problem of deciding on land use (what crops to go where), energy pathways and locations and scales of conversion technologies end use of energy products. Research at CPSE is focussing on a whole-systems approach to bioenergy via multi-scale modelling to address questions such as these.

Optimized hydrogen infrastructure:

Long-term infrastructure planning must also account for improvements in technology and processes. A good example of this is hydrogen. There is a lot of renewed interest in hydrogen as a carbon-free energy vector. Amongst the questions we are considering at CPSE is "What could a cost-optimised hydrogen infrastructure for the UK look like?". We develop a model of geographically-distributed demand which increases over time, together with the existing resources that can be used for hydrogen production, and determine locations of conversion technologies and the hydrogen transmission and distribution system. The components of the hydrogen infrastructure are shown in figure 1 (overleaf).

The optimised infrastructure then develops over time. It was found that an infrastructure based on liquid hydrogen would be cost-optimal, and that the total lifecycle cost to the consumer, in terms of £/km would be marginally less than that of taxed gasoline.

Closed loop supply chain:

In the future, it will be important for supply chains to have a closed-loop characteristic. In other words, rather than a linear flow from raw materials to basic materials to components to products to disposal, supply chains will have to be engineered to collect and re-use in some way products at the end of their life. Again, ideally this should be designed in a holistic way, so that the product, processes and chain are optimised for a closed loop system, rather than the current approach to bolting-on recycling processes. We are working on fundamental techniques for closed loop supply chain design and applying them to diverse applications, including fluorescent lamps (see figure 2, overleaf).

In summary, the supply chains of the future will have to be much more resource-efficient and responsive, and supply chain design should be considered along with basic science and process development and design.

Supply Chains of the Future

Application Domains 4

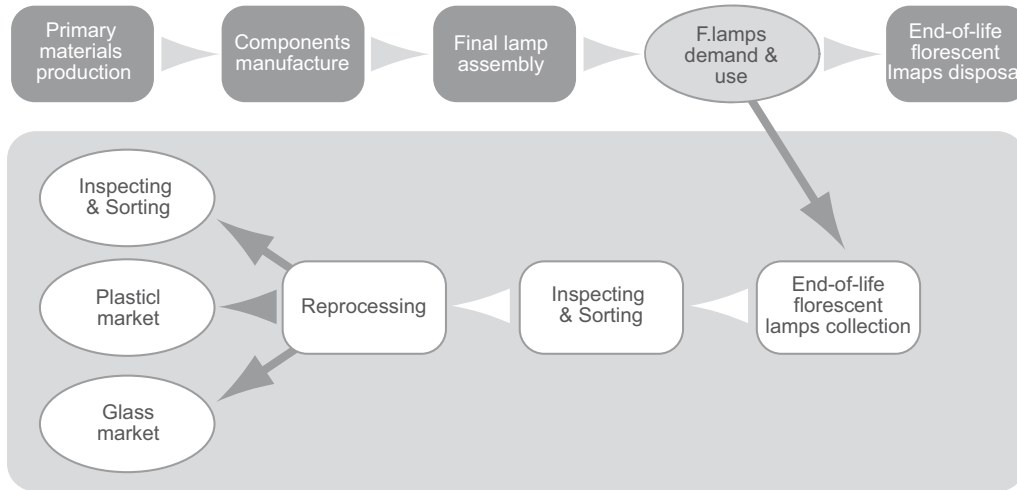


Figure 1. Components of hydrogen supply chain

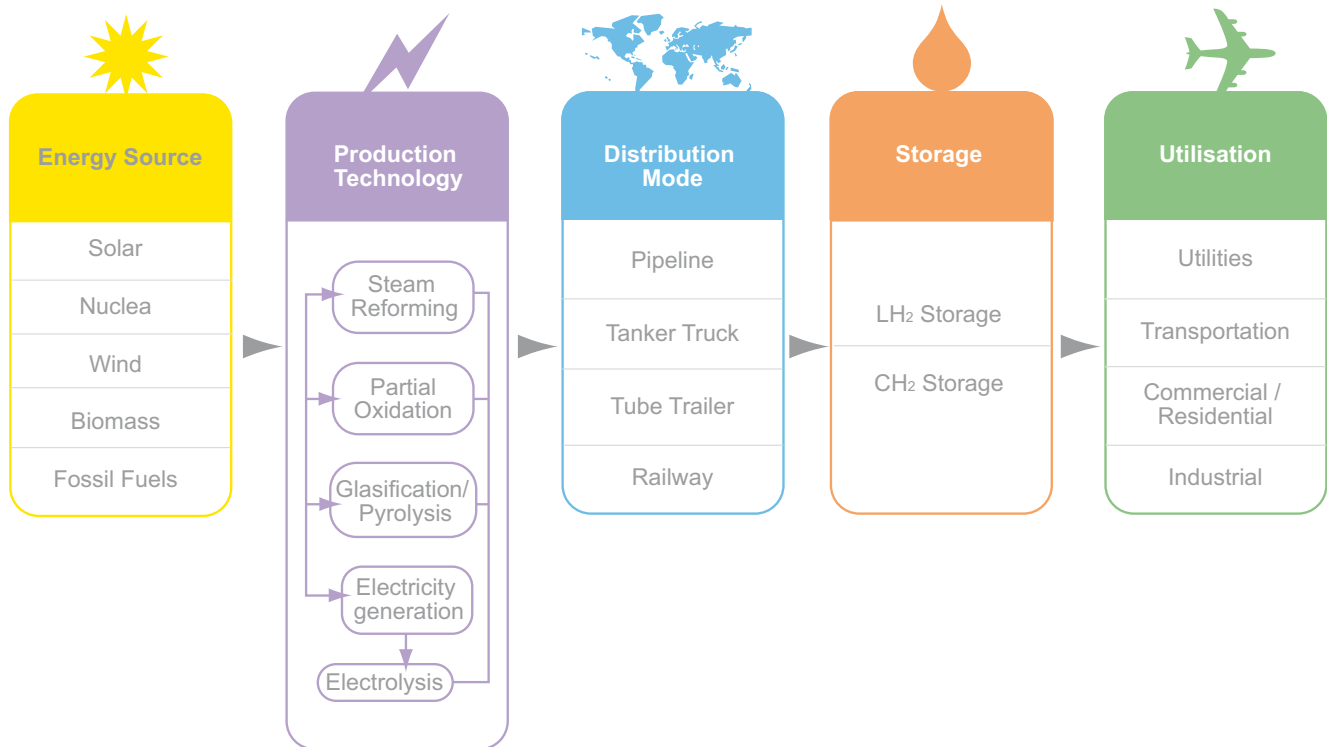


Figure 2. Fluorescent lamp recycling chain and process

Energy Systems Engineering

Application Domains 5



Energy systems encompass everything from the primary energy source to the final energy service. Whilst many technical options exist for developing a future sustainable and less environmentally damaging energy supply they are often treated separately driven by their own technical and political lobbies. The Energy Systems Engineering application area in CPSE finds realistic integrated solutions to such problems by adopting a systems approach.

Energy-related activities at Imperial College span several departments and centres including the Energy Futures Laboratory which coordinates college-wide initiatives in this area, the Centre for Transport Studies, the Innovation Studies Centre, the Centre for Environmental Policy, the Control and Power group in E&E Engineering, the Departments of Earth Sciences and Engineering, Civil Engineering and Chemical Engineering. CPSE personnel contribute to a new interdepartmental MSc in Sustainable Energy Futures, run by the Faculty of Engineering on behalf of Imperial College. Energy systems research within the CPSE relates to oil and gas production, clean routes to fossil fuel production, electric grids, fuel cells, and energy-integrated cities.

Oil and gas production – Separation of CO₂ from natural gas and from flue gas:

A joint activity with the Molecular Systems Engineering application area is directing an integrated approach to the design of new solvents and processes for the capture of CO₂ from natural gas. This system is very important in the oil and gas industry, where gas streams with a more than 50% CO₂ content are not uncommon. It is difficult to

separate such quantities of CO₂. Advanced thermodynamic model, process modelling and optimisation tools have led to a design for a high-pressure absorption process using a novel alkane solvent by means of simultaneously optimising the flowsheet structure, solvent molecular structure and operating conditions. Among the challenges that had to be overcome were the reliable representation of high-pressure high-temperature phase behaviour as a function of solvent structure and the optimisation of a complex integrated flowsheet with a large number of structural degrees of freedom and operating variables.

Other studies include the coupling of CO₂ with enhanced oil recovery and the development of processes for post combustion capture of CO₂ with amine solvents. The first phase of this latter project, which is funded by the British Coal Utilisation Research Association, has focussed on the development of models of the underlying physical phenomena, and this is now proceeding to the development of a system model.

Clean production of fossil fuels:

Over the next few decades coal, oil and gas will continue to supply a large fraction of the world's growing energy needs. Imperial College envisages radical changes towards new methods of production that aim to produce at the surface only what is required – low or zero carbon fuels, heat and power, and chemical building blocks for materials and chemical products. Much of the fossil fuel processing currently carried out on the surface (eg synthesis gas production, coal or gas-to-liquids) will be relocated in the sub-surface, exploiting the high temperature and high pressure environment and transforming the subterranean well network from a passive fluids transportation conduit to an active, continuous processing plant. A large part of the carbon will remain underground, either as low-value residues

Energy Systems Engineering

Application Domains 5

or CO₂ produced, captured and stored in the reservoirs without release. The energy efficiency of fossil fuel recovery will be enhanced and its environmental impact dramatically reduced. The responsibility for reducing carbon emissions will be transferred in large part from the user to the primary producer.

The Energy Systems Engineering application area is participating in the Shell-Imperial Grand Challenge on Clean Fossil Fuels, an Energy Futures Lab project also involving the Department of Earth Sciences and Engineering. Shell has committed £3M of funding over an initial five year period. The programme is directed by Professor Geoffrey Maitland.

Two main themes will be studied over this period. One is on CO₂ lifecycle engineering in the reservoir. The project is led by Earth Sciences and Engineering and will give a comprehensive understanding of the behaviour of CO₂ under reservoir conditions, its interaction with other fluids and with rocks/minerals, leading to the optimisation of its use for enhanced oil and gas recovery (EOR) and also its capture and sequestration within reservoirs (CCS). The second project will focus on low energy, low environmental impact processes for the recovery of non-conventional hydrocarbons, such as oil shales and tar sands. The Energy Systems Engineering application area of the CPSE offers a systems engineering approach to EOR, CCS and fossil fuel recovery and integration of the new approaches being explored with other emerging energy technologies such as biofuels.

Electric grids – Electric power transmission enhancement:

This project takes a measurement-based approach to the better understanding, early detection and diagnosis of instabilities in a.c. electrical power transmission systems and avoidance of situations leading to large scale power blackouts. More detail of this project can be found in the report on the Operations and Control competence area.

Microstructural modelling of solid oxide fuel cell (SOFC) electrodes:

The design and manufacture of electrodes for use in SOFCs is one of the greatest challenges to commercialization of fuel cell technology. A fundamental understanding of the quantitative effects of microstructure is crucial; the electrode performance is directly dependent on the abundance of triple phase boundaries and the transport properties of the three phases.

Electrode models commonly neglect heterogeneity and assume effective values for key parameters. By contrast, our

models use a virtual heterogeneous electrode, simulated as a packed bed of overlapping spheres. The porous structure obtained allows an analysis of the porosity and percolation of the various phases and the amount of triple phase boundary and its percolation throughout the electrode. Furthermore, the transport and redox phenomena are also modeled to determine the potential, current and chemical distribution throughout the different phases. It is then possible to predict electrode performance based on fundamental properties of the underlying microstructure. These results are used to relate microstructural properties to electrode performance. The microstructural properties can include porosity, particle radii and radius ratio, and the effect of graded electrodes.

Urban energy systems:

The BP-Imperial Urban Energy Systems project will identify the benefits of a systematic, integrated approach to the design and operation of urban energy systems, with a view to at least halving the energy intensity of cities. It involves several centres and departments at Imperial College. Professor Nilay Shah is one of the directors, and the Energy Systems Engineering application area of CPSE contributes a systems approach to modelling, optimization and design of urban energy systems.

The project is predicated on the assumption that while individual urban energy systems may have been optimised there has been no attempt to cross-optimize over the total energy consumption of a city. Such system-wide optimisation has improved efficiency by up to 40 or 50% in other systems such as refineries and petrochemical complexes. The research challenge is that cities are more than an order of magnitude more complex, they involve diverse energy vectors and are confounded by the daily decisions of millions of agents and so a new modelling framework will be required.

The first phase will give an estimate of the potential benefits to different classes of cities, and will identify the means and business models required to achieve these objectives.

Later phases will address detailed design issues and implementation. **The overall programme for phase 1 is divided into five activities as follows:**

- i) Review and appraisal of the state-of-the art relating to urban energy systems analysis, modelling and implementation.
- ii) Characterisation and modelling of urban energy systems over a wide range of systems and networks.

Energy Systems Engineering

Application Domains 5

- iii) Characterisation of the interplay between urban infrastructures, people and communities (and their needs), and business and service providers.
- iv) Modelling of real example cities or sub-cities using results from i) to iii), as well as representative cities based on synthesised, sampled data.
- v) Performing urban systems optimisation studies, in particular identifying a hierarchy of steps that will improve the economic performance, energy efficiency and environmental impact of urban energy systems.

Recent developments include the formulation of a hierarchical modelling strategy that captures the different facets of the urban system.

Dongtan, a new city in Shanghai China, will be three quarters the size of Manhattan and will be the world's first sustainable eco-city. The Chinese government's plans for Dongtan include a zero-greenhouse-emission transit system and self-sufficiency in water and energy. Imperial College is a member of the EPSRC's Dongtan Sustainable City Networks whose purpose is research for eco-city design. The Dongtan project gives an immediate holistic case study focusing on a greenfield city.

Research in existing cities includes a study on the thermodynamics of London.

For further information, see: <http://www.bp.com/genericarticle.do?categoryId=2012018&contentId=7018337>

www.imperial.ac.uk/urbanenergysystems



Personal Profiles

Portraits



Dr Claire Adjiman
p.29



Professor Roger
Benson p.30



Professor David
Bogle p.30



Professor Nigel
Brandon p.30



Dr Vivek Dua
p.31



Professor Eric Fraga
p.31



Dr Amparo Galindo
p.32



Dr Michael
C. Georgiadis p.32



Dr Charles
D. Immanuel p.33



Professor George
Jackson p.33



Dr Cleo Kontoravdi
p.34



Dr J. Krishnan
p.34



Dr Daniel Kuhn
p.35



Professor Geoffrey
Maitland p.35



Dr Athanasios
Mantalaris p.36



Professor Costas
C. Pantelides p.37



Dr Lazaros
Papageorgiou p.37



Professor Efstratios
N Pistikopoulos p.37



Professor
Berc Rustem p.38



Professor
Paul Rutter p.38



Professor Roger
W. H. Sargent p.39



Professor Nilay
Shah p.39



Dr Eva Sørensen
p.40



Professor Nina
Thornhill p.40



Professor Richard
B. Vinter p.41

Personal Profiles

Overview

Claire S Adjiman

Reader in Chemical Engineering, Department of Chemical Engineering, Imperial College London. Visiting Professor, Department of Chemistry, Warwick University

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Qualifications

MEng in Chemical Engineering (Imperial College London)
PhD in Chemical Engineering (Princeton University)

Awards and Distinctions

Royal Academy of Engineering ICI Fellowship, 1998-2003
Porter Ogden Jacobus Honorific Fellowship, Princeton University

Secondments

Process Systems Enterprise Ltd, September 06-August 07.

Research Interests

Development and use of mathematical models and optimisation techniques to address product and process design problems (e.g. solvent design for reactions or CO₂ capture, risk management). Model-based assessment of design of energy conversion systems. 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 or global sensitivity analysis.

Advances in the understanding and modelling of the behaviour of matter have opened the way for the development of systematic methodologies for the computer-aided design of materials. We focus on the selection of optimal processing materials such as solvents and the design of high-performance products such as polymers. In these problems, the molecular structure of the material and its interaction with the process are of importance in determining its performance. The methodologies being developed in my research group follow an integrated approach to the problem which recognises the need for reliable and efficient relationships between molecular structure, physical and mechanical properties, process and performance. This is achieved by exploring methods for the combination of optimisation tools and advanced property modelling tools. Current research themes thus include the use of advanced equations of state, molecular mechanics and quantum mechanics in molecular and process design, the integration of modelling tools at different time and length-scales and the simultaneous design of solvents and batch distillation columns. This work is complemented by the development of fundamental techniques for the global optimisation of

dynamic problems and the rigorous analysis of process operating spaces.

Modelling and optimisation techniques are applied to the design of energy systems at different scales. The dynamic behaviour of solid oxide fuel cell stacks has been studied, together with the overall system's performance. We are currently focussing on fuel cell components, by considering the impact of the microstructure of the anode on cell performance, in collaboration with Nigel Brandon (Earth Science and Engineering). This programme is closely tied with an experimental investigation of the anode properties. At the unit operation scale, we consider the modelling and design of biomass gasifiers, based on targeted experiments at several scales. Finally, on a larger scale, we optimise the gas production from deepwater fields under transient conditions, and we consider the optimal infrastructure for biofuel production in the UK.

Other Activities

AIChE: Technical area co-chair/chair for CAST10a, 2006-2008
IChemE: Committee Member, Fluid Separations Subject Group. EPSRC: Member of Peer Review College. Member of scientific committee for ESCAPE 18

Reviewer for

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

Academic Collaborations

Facultés Universitaires de Notre Dame de la Paix, Namur, Belgium, Theoretical Chemistry, Warwick University, Department of Chemistry, University of Western Macedonia, Kozani, Greece

Industrial Collaborations

Britest, BASF, P&G, BMS, Ineos, PSE Ltd, Schlumberger, Syngenta

Personal Profiles

2007

Roger Benson

Visiting Professor, Department of Chemical Engineering, Imperial College London. Visiting Professor, Department of Chemical Engineering, Newcastle University. Visiting Professor, Department of Chemical Engineering, Teesside University

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Industrial Positions prior to semi retirement

Chief Engineer – Technology: ICI. Global Technology Manager: Control and process Analysis: ABB

Industrial positions

Chairman – Perceptive Engineering Limited. Non Executive Director – Industrial Tomography Systems

Qualifications

BSc in Chemical Engineering (Swansea University). MSc in Control Systems (Manchester University). PhD in Chemical Engineering (Manchester University)

Awards and Distinctions

Fellow Royal Academy of Engineering. Fellow of the IChemE. Fellow of the IET

Other activities

Author – Benchmarking Process Manufacturing (I Chem E Publication). Member of RAE2008 Panel 26: Chemical Engineering. Judge for Britain's Best Factory Awards. Honorary President – CPACT. Member – CIKTN Academic Advisory Board 2007 Judge: Queen's Anniversary Prizes for Higher Education

Academic Collaborations

Industrial Advisor to the ZEAL Project for improving the performance of Industrial Cleaning

I David L Bogle

Professor of Chemical Engineering, Department of Chemical Engineering, UCL. Deputy Director CPSE

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Qualifications

BSc (Eng) Hons MSc PhD DIC CEng

Awards and Distinctions

FREng FICHEM. 2006 IChemE Council Medal.

Research Interests

Numerical global optimisation techniques for process design. Controllability analysis of nonlinear systems. Process modelling of PSA and desalination units. Systems Biology.

Other Activities

Head of the UCL Graduate School. Member of Council of the Institution of Chemical Engineers. Chairman 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 Board of Engineering Council UK. Member of International Federation of Automatic Control (IFAC) Technical Committees on Chemical Process Control and on Control of Environmental Systems. Member of Natural Sciences Committee of the U.K.'s National Commission for UNESCO. Member of College of Engineering for the Engineering & Physical Sciences Research Council (EPSRC). Member of BBSRC Integration and Systems Biology Strategy Panel.

Nigel Brandon

Shell Professor of Sustainable Development in Energy, Imperial College London

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Qualifications

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

Awards and Distinctions

Fellow of the Institute of Materials, Minerals and Mining. Fellow of the Energy Institute. 2007 Silver Medal Royal Academy of Engineering

Research Interests

Fuel cell science, engineering and technology. Energy systems analysis.

Nigel Brandon's research involves the quantitative analysis of energy systems, with a particular focus on the design, characterisation, modelling, control and optimisation of fuel cells. His present research work encompasses high temperature Solid Oxide Fuel Cells (SOFCs), metal supported Intermediate Temperature-SOFCs, and lower temperature

Personal Profiles

2007

Polmyer Fuel Cells. He collaborates extensively with industry in this field, as well with other research centres and universities around the world. He leads the EPSRC 'Supergen' Fuel Cell consortia, and the fuel cell topic within the UK Energy Research Centre.

Other Activities

Executive Director, Imperial College Energy Futures Lab. Senior Research Fellow to the Research Councils Energy programme. Co-founder and Chief Scientist, Ceres Power. Grove Fuel Cell steering committee member. Editorial Board member of the IET Journal of Renewable Power Generation.

Vivek Dua

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

Awards and Distinctions

National Award for the Best MTech Thesis in Chemical Engineering - Given by the Indian Society for Technical Education and the Indian Petrochemicals Corporation Ltd. (1995) Engineers India Ltd. Fellowship (1995), University Grant Commission Scholarship (1994-1995), Vice Chancellor's Open Merit Scholarship (1992)

Research Interests

Optimal configuration of artificial neural networks, Stability analysis of nonlinear model based controllers, Controlled release of active agents, Control and optimization of process and biological systems

Other Activities

Associate Member of the Institution of Chemical Engineers, Senior Member of the American Institute of Chemical Engineers, Co-founder of Parametric Optimization Solutions Ltd., London, Member of Society for Biological Engineering. Member of Drug Delivery Network.

Reviewer for:

AIChE Journal, Computers and Chemical Engineering, Chemical Engineering and Processing, Journal of Global

Optimization, IEEE Transactions on Automatic Control Systems and Control Letters

Co-editor of Wiley-VCH Book Series on Process Systems Engineering, Acted as session chair of the session on Biological Systems at the 16th European Symposium of Computer Aided Process Engineering and 9th International Symposium on Process Systems Engineering (2006), Garmisch- Partenkirchen.

Academic Collaborations

Eastman Dental Institute, UCL. Institute of Child health, UCL

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 visualization and knowledge discovery methods for 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. External examiner for the undergraduate programme in Information Technology, University of Kingston. Member of the ACDMnet (Adaptive Computing in Design and Manufacture) network. Reviewer for a number of journals and funding agencies, covering the interfaces between computer science, mathematics and engineering.

Academic Collaborations

Vytautas Magnus University, Lithuania. Universidad Nacional de Colombia, Manizales, Colombia. University of Dundee, UK University of Edinburgh, UK.

Personal Profiles

2007

Amparo Galindo

Reader in Physical Chemistry, Department of Chemical Engineering, Imperial College London.

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Qualifications

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

Awards and Distinctions

ExxonMobil Teaching Fellow (2005-2009)
ExxonMobil - Royal Academy of Engineering, 2005
Award for Excellence in Teaching (2007)

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.
Member of the peer review college of the Engineering and Physical Sciences Research Council (EPSRC).

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 Physics. Journal of Physical Chemistry B
Molecular Physics

Michael C Georgiadis

Associate Professor of Process Optimization, Department of Engineering Informatics and Telecommunications, University of Western Macedonia, Kozani, Greece.

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Qualifications

Diploma of Chemical Engineering (Aristotle University of Thessaloniki, Greece), M.Sc. in Advanced Chemical Engineering (Imperial College), Ph.D. (Imperial College)

Awards and Distinctions

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

Research Interests

Optimization of energy systems, Dynamic process modeling and simulation, Production scheduling, Advanced process control, Energy planning

Other Activities

European Commission: Evaluator of Collaborative research proposals under Research Framework 7. Member of the Scientific Committee of the European Congress of Chemical Engineering, Copenhagen 10-14 September 2007. Member of the Scientific Committee of PRES2006 CHISA 2006 Conferences, 27-31 August 2006, Prague, Czech Republic

Reviewer for:

AIChE Journal. Chemical Engineering Processing. Chemical Engineering Research and Design. Chemical Engineering Science. Computers & Chemical Engineering. Computers and Operational Research. European Journal of Operational Research. Industrial and Engineering Chemistry Research

Academic Collaborations

University College London. Josef Stefan Institute, Slovenia
Technical University of Denmark

Industrial Collaboration

MITOL S.A. Slovenia., ESTIA Consulting .KOTHALI.

Personal Profiles

2007

Charles D Immanuel

*Lecturer, Department of Chemical Engineering,
Imperial College London*

Qualifications

B.Tech. in Chemical Engineering (Anna University, Madras, India), M.Tech. in Chemical Engineering (Indian Institute of Technology, Kanpur, India), PhD in Chemical Engineering (University of Delaware, USA)

Research Interests

Population balance modelling of particulate and distributed parameter systems, Control of distributions in particulate processes, Sensitivity and reachability analyses.

My research deals with process modelling, dynamic optimisation and control. of the models attempt to incorporate information at the micro- and meso-scales of the processes, for processes such crystallisation and polymerisation, and thereby attempt to be commensurate with the current status of process knowledge, the state-of-the-art in instrumentation capabilities, and the computational resources. Several of the processes studied in my group employ the population balance concepts for model development. This enables the optimisation and control of various distributed variables (such as the crystal size distribution), which find strong correlations with the end-use properties, and thereby improve the quality of the end-products to a substantially better level than is feasible with lumped parameter models. The research themes addressed by the group include fundamental model development and efficient numerical solution techniques, process sensitivity analysis, and robust optimal feedback control. Experimental validation constitutes an integral part of the research.

Other Activities

Member of IChemE., Member of AIChE., Committee Member of the IChemE Computer-Aided Process Engineering Subject Group., Organiser of invited conference sessions on special themes for the American Control Conference 2005., Organiser of CPSE Seminar Series., Consultancy activity for TMF3 (EPSRC-Industry Joint Project headed by Imperial College) on review of slug control status in oil extraction., Member/reviewer for programming committees of international conferences

Reviewer for

Chemical Engineering Science. AIChE Journal. Industrial & Engineering Chemistry Research. Computers & Chemical Engineering. Journal Applied Polymer Science.

Journal Chemical Technology & Biotechnology. International Journal of Systems Sciences. Chemical Engineering Research & Development. Transactions of Institute of Measurement & Control. Polymer International

Academic Collaborations

University of California Santa Barbara, USA. University of Queensland, Australia. Purdue University, USA. Georgia Institute of Technology, USA

Industrial Collaboration

ICI, BASF

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

Personal Profiles

2007

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); Bristec 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).

Cleo Kontoravdi

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

Qualifications

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

Awards and Distinctions

Lonza/RCUK Academic Fellowship (2007-2012)
Alexander S. Onassis Public Benefit Foundation Scholarship (2003-2006)

Research Interests

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

Other Activity

Reviewer for Biotechnology and Applied Biochemistry

Industrial Collaboration

Lonza Biologics, U.K.

Academic Collaboration

Bioprocessing Technology Institute, A*STAR, Singapore

J Krishnan

Lecturer, Department of Chemical Engineering, Imperial College London.

Qualifications

PhD, Princeton University, 2000
B.Tech, Chemical Engineering, Indian Institute of Technology, Madras (Chennai), 1994.

Awards and Distinctions

Excellence in Teaching, Engineering Council, School of Engineering and Applied Science, Princeton University, 1997.
Patel Fellowship, Dept. of Chemical Engineering, Princeton University, 1994-96.

Research Interests

Mathematical and computational modelling of cellular processes including chemotaxis and cell migration, polarity generation and genetic processes. Systems biology. Non-linear dynamics and pattern formation in physico-chemical and biological systems.

Personal Profiles

2007

Other Activities

Reviewer for:

IEEE Transactions in Automatic Control. Interface Journal of the Royal Society. Journal of Theoretical Biology.

Academic Collaborations

School of Medical Sciences, University of Aberdeen

Daniel Kuhn

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

Stochastic optimization (development of approximation schemes and solution algorithms). Computational finance (derivatives pricing, portfolio optimization). Energy market modeling (power system operation and scheduling, risk management)

Other Activities

Member of Mathematical Programming Society

Reviewer for:

Automatica. Computational Finance. Computers and Operations Research. European Journal of Operational Research. Journal of Global Optimization. Kybernetika Mathematical Reviews. SIAM Journal on Optimization

Academic Collaborations

University of St. Gallen, Switzerland. Stanford University, USA
University of Vienna, Austria.

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

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, 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.

Existing research projects include

- Integrated monitoring, modeling and control of oilfield processes
- Carbon capture and sequestration

Other Activities

Institut Francais du Petrole: Member of Scientific Council.
EPSRC: Member of Peer Review College.

Personal Profiles

2007

Soft Matter Journal: Founder Member of Editorial Board. Member US National Petroleum Council Technology Task Group on Carbon Capture and Storage. Sheffield Hallam University: Chairman, Materials and Engineering Research Institute Scientific Advisory and Policy Boards. 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, International Advisory Board, SoftComp EU Network.

Reviewer for

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

Industrial Collaboration

Schlumberger and Shell

Athanasios Mantalaris

Reader in Biological Systems Engineering, Department of Chemical Engineering, Imperial College London.

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Qualifications

HBSc in Biochemistry (University of Western Ontario). MEng in Chemical Engineering (University of Rochester). PhD in Chemical Engineering (University of Rochester)

Awards and Distinctions

Special University Scholarship, The University of Western Ontario. Alexandros S. Onassis Foundation Scholarship Governor's Lecturer, Imperial College London. Best poster award, Tissue Engineering Society International, Florida, USA. Junior Moulton Award by the Institute of Chemical Engineers for best paper published in Food & Bioproducts Processing. Young Investigator Award for best paper presented in the 7th International Conference on Cellular Engineering, Seoul, Korea. Rector's Award for Research Excellence, Imperial College London. Live demo award at ISCAS

Secondments

Visiting Professor, The Parker H. Petit Institute for Bioengineering & Biosciences, Georgia Institute of Technology, 2008.

Research Interests

My research interests cover 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. They integrate experimentation with modelling from molecules into cell populations and to link the in silico with the in vitro through:

- a) The rationalisation and systematisation of the wide range of experimental data leading to advanced therapeutics and strategies, with the ultimate goal of delivering personalised health care.
- b) The horizontal and vertical integration of experimentalists, clinicians, engineers, and modellers.

Mammalian cell bioprocessing

Commercial synthesis of monoclonal antibodies (MAB) represents one of the most important products in the biopharmaceutical industry because of their diagnostic and clinical applications. However, the production of industrial scale quantities of MAB is an expensive and challenging task. Complications arising in these systems include the requirement to grow cultures in complex media, the lack of on-line measurements for many of the key substrates, metabolites, and products, the limited and noisy nature of much of the available experimental data and the extremely complex underlying reaction system. Our research programme sets out to integrate modelling, experiment design and validation, and control and optimisation into a single framework that would lead to increased productivity, regulated product quality, and reduced costs for mammalian cell culture systems.

Stem cell bioprocessing

To harness the immense potential of stem cells (SCS) in terms of their plasticity and expansion capabilities, the physiological activity in relation to the culture parameters (local) such as pH, dissolved oxygen, nutrients/metabolite concentrations and growth factor concentrations needs to be recorded quantitatively with the needed level of accuracy and subsequently evaluated in a biologically meaningful manner. We are seeking to develop a novel monitoring modality that allows the systematic development of clinically relevant culture systems and methodologies, which control and regulate stem cell self-renewal, expansion, differentiation, and death.

Personal Profiles

2007

Other Activities

UK-China Partnership Launch Meeting, TERMIS, London, September 2007. Monitoring in Tissue Engineering, TERMIS, London, September 2007. Keynote Speaker in TERMIS Europe Meeting, "Integrating ESC Bioprocessing: Examples for bone & cartilage tissue engineering", London, UK, September 2007.

Reviewer for

Biochemical Engineering Journal. Biomaterials. Biotechnology & Bioengineering. Biotechnology & Applied Biochemistry. Blood Cells, Molecules & Diseases. Food & Bioproducts Processing. Tissue Engineering

Academic Collaborations

Departments of Haematology, Bioengineering and the Institute of Biomedical Engineering, Imperial College London. Bioprocess Technology Institute, A-star, Singapore. Department of Biomedical Engineering, Rice University. The Parker H. Petit Institute for Bioengineering & Biosciences, Georgia Institute of Technology.

Industrial Collaborations

NovaThera

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

Beilby Medal from the SCI, RSC and IoM for contributions to process systems engineering. Esso Centenary Education Award. British Commonwealth Scholarship.

Research Interests

Computational chemistry. Design methodologies for continuous and batch processes. Design and operation of supply-chain networks. Design and implementation of software tools for process modelling, simulation and optimisation. Numerical methods for optimisation of hybrid

dynamic systems. Global optimisation techniques.

Other Activities

Reviewer for

Chemical Engineering Research and Design. Chemical Engineering Science. Computers and Chemical Engineering AIChE Journal. Industrial and Engineering Chemistry Research. Technology Director, Process Systems Enterprise Ltd. Member of the committee for the establishment of the new University of Applied Sciences and Arts, Cyprus

Lazaros Papageorgiou

Senior Lecturer 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

Production planning and scheduling. Production and cleaning scheduling. Maintenance planning and design. Process plant layout. Supply chain optimisation. Optimisation of biochemical systems. Computer aided process engineering

Other Activities

Member of IChemE CAPE Subject Group Committee

Reviewer for

AIChE Journal. Applied Thermal Engineering. Chemical Engineering Communications. Chemical Engineering Research and Design. Chemical Engineering Science Computers and Chemical Engineering. Industrial and Engineering Chemistry Research.

Efstathios N Pistikopoulos

PhD CEng FIChemE. Professor of Chemical Engineering CPSE Director.

Qualifications

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

Personal Profiles

2007

Awards and Distinctions

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

Co-Editor, Book Series in Process Systems Engineering, Wiley-VCH. Editorial Board, Computers and Chemical Engineering, Elsevier. Editorial Board, Journal of Global Optimization, Kluwer. Editorial Board, Computational Management Science, Springer. Co-Founder and Senior Consultant, PSE Ltd. Founder and Director, PAROS Ltd Co-organiser, Global Optimization Workshop, December 2007, Imperial College London. Plenary Lectures – ESCAPE-17 (Bucharest, Romania), ECCE-6 (Copenhagen, Denmark). International Programme Committee member – ESCAPE-17, PRES'07, ECCE-6. Invited Presentations – University of Manchester, National University of Singapore, University of Pannonia, University of Coimbra, Tsinghua University. External Examiner - DTU, UPC Reviewer – AIChE J, IECR, CCE, JOGO, CMS, IEEE Transactions, Process Control J, OR. Invited Member, Computer Aided Process Engineering (CAPE) Working Party, European Federation of Chemical Engineers. Member of the Advisory Scientific Committee, European Enterprise Institute (EPPED Association). Involved in 14 ongoing projects – 4 EPSRC-funded (two as PI), 1 BBSRC-funded, 2 BP-funded, 1 BASF-funded, 5 EU-funded (1 as Coordinator), Systems Engineering Initiative (Imperial, Faculty of Engineering).

Academic Collaborations

Tsinghua University (China), Cranfield University, DTU (Denmark), UPC (Spain), University of Coimbra (Portugal), University of Patras (Greece), University of Western Macedonia (Greece), University of Manchester, University of Birmingham, University of Porto (Portugal), University of Dortmund (Germany), Aachen University (Germany), Princeton University (USA).

Industrial Collaborations

BP, BASF, Air Products, Schlumberger, HyGear, CTI, IPCOS, HyStore, Biomedal.

Berc Rustem

Professor, Department of Computing, Imperial College London.

Qualifications

B.S. MSc PhD. FIMA, CMath.

Awards and Distinctions

President of Society of Computational Economics, 2002-04

Research Interests

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

Other Activities

Editor of: Automatica; Computational Management Science. Senior Editor of Journal of Economic Dynamica & Control. Associate Editor of: Journal of Global Optimisation; Computational Economics; Operations Research Letters

Academic Collaborations

J. Beasley (Brunel); P. Fryer (Birmingham); V. Wieland (Frankfurt).

Industrial Collaborations

Ericsson; Lehman Brothers; JP Morgan.

Paul Rutter

*Visiting Professor, Imperial College London
Marketing Manager, Centre for Process Systems Engineering.*

Qualifications

BSc, PhD, Chartered Engineer, Member IMM, Chartered Chemist Member RSC

Research Interests

The impact of Climate Change on industrial infrastructure. The development of urban energy systems. Energy economics: My principal interest is the reason why countries move from one system of energy supply to another e.g. the change from gas to electricity for lighting in the UK and whether parallels can be drawn for new energy systems like

Personal Profiles

2007

wind and hydrogen. Climate Change: Interest in the impact of climate change to industrial operations and infrastructures. Environmental engineering: General interest in applying environmental principles to engineering without losing economic competitiveness.

Other Activities

Member of Royal Society of Chemistry Energy Policy working group. Evaluation Panel member for the EU 6th Framework Programme Thematic call for Sustainable development, global change and ecosystems. Advisory panel member for the PIU cabinet Office project on Resource Productivity and Renewable Energy (2001), US National Centre for Clean Air Research Advisory Board (2000-2002). Member of the EPSRC User panel (1996-1999), EPSRC Engineering referee college (1995 -2000), IChemE Research Committee, WBC Sustainable Development technology and innovation member (1997-1999), IEA GHG R & D programme executive committee member (1998 -2002). Secretary of European Production Engineering Association (1996,1997). Chair of IChemE Sustainability Think Tank (1998-1999).

Research team leader in Unilever 1974-1980; Senior Research Fellow at London Hospital Medical School 1980-1981; BP Project Manager Particle Technology (10 staff) 1985-89; Manager, BP Minerals Processing Branch (32 staff) 1989-1992, Manager BP Exploration Production Operations branch (58 staff,) 1992-96; BP Group Environment technology manager 1996-02.

Industrial supervisor for PhD students at Bristol University, University of Surrey and Imperial College.

Roger W H Sargent

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

Qualifications

DSc(Eng) (University of London). BSc(Eng) in Chemical Engineering (Imperial College London). PhD in Chemical Engineering (Imperial College London)

Awards and Distinctions

Royal Academy of Engineering-Founder Fellow,1976. Honorary Fellowship of the City and Guilds of London Institute,1977. Docteur honoris causa, Institut National Polytechnique de Lorraine,1987. Fellow of the Royal Society of Arts,1989. AIChE CAST Division "Computing in Chemical

Engineering Award", 1990. Foreign Associate of the United States National Academy of Engineering, 1993

Honorary DSc(Edinburgh), 1993. Fellowship of Imperial College London, 1994. Docteur honoris causa, Universite de Liege, 1995.

Research Interests

Process model generation from physical description. Solution of variational inequality problems. Integration of differential-algebraic systems. Algorithms for optimal control. Robust on-line optimal control. Process scheduling

Other Activities

Associate Editor of Journal of Optimization Theory and Applications.

Reviewer for

Computers and Chemical Engineering. Journal of Optimization Theory and Applications. Operations Research Transactions of the IChemE.

Nilay Shah

Professor of Process Systems Engineering, 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. RSC/SCI/IOM Beilby Medal 2005. ICI/RAE 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. Director of Ashe Morris Ltd. Director of Britest Ltd. Defra panel member

Personal Profiles

2007

EPSRC college member. 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, CFACT Georgia Institute of Technology, iCPSE. Tsinghua University, Clean Energy Centre. National University of Singapore.

Industrial Collaborations

Ashe Morris (Novel reactor modeling and experimentation) BP (Urban Energy Systems Project). ICI (Supply chain management under uncertainty). Ineos (Supply chain study) Shell (H₂-CO₂ project). Syngenta (Supply chain network design).

Eva Sørensen

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

Qualifications

MSc Chemical Engineering, NTNU, Norway. PhD Chemical Engineering, NTNU, Norway

Awards and Distinctions

University Scholarship, NTNU, Norway (1990). Research Scholarship, Norwegian Research Foundation, Norway (1993) Postdoctoral Research Scholarship, Norwegian Research Foundation, Norway (1995). Faculty Teaching Award for Outstanding Achievements in Teaching, Faculty of Engineering, University College London, UK (2001) Royal Academy of Engineering Secondment Award for industrial secondment to BP Refining Technology, UK (2005).

Research Interests

Detailed dynamic modelling and simulation of fluid separation processes, in particular, distillation, membrane separation, chromatography and hybrids thereof. Optimal separation process selection. Optimal process design, operation and control.

Other Activities

Fellow of Institution of Chemical Engineers (FIChemE). Member of IChemE's Fluid Separations Subject Group Committee. Chair of European Federation of Chemical Engineers (EFCE) Working Party on Fluid Separations. Member of EFCE Section on Separation Technology. Member of American Institute of Chemical Engineers (AIChE). Member of The Society of Chemical Industry (SCI). Subject Editor of Chemical Engineering Research and Design. Editorial Board Member of Chemical Engineering & Technology. Regular journal reviewer for numerous international journals and conferences. Member of EFSRC Peer Review College. Chair of Organising Committee for Distillation & Absorption Conference, 2006.

Academic Collaboration

University College London, Department of Biochemical Engineering.

Industrial Collaboration

BP, UK.

Nina F Thornhill

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

Qualifications

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

Awards and Distinctions

Holder of the ABB/Royal Academy of Engineering Research Chair in Process Automation. 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 Society Industry Fellowship with BP International, 1992-5.

Research Interests

Industrial data analysis using time series analysis and signal processing. Plant-wide performance assessment.

Personal Profiles

2007

Applications in oil and gas, chemicals, bioprocesses and electricity supply.

Other Activities

IChemE: 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. Industrial and Engineering Chemistry Research. International Journal of Adaptive Control and Signal Processing. ISA Transactions Journal of Process Control

Academic Collaborations

University of Alberta, Department of Chemical and Materials Engineering. University of Cardiff Business School.

Industrial Collaborations

ABB Corporate Research, ABB Oil and Gas
BP Refining Technology, Eastman Chemical Company,
National Grid.

Richard B Vinter

Professor of Control Theory, Department of Electrical and Electronic Engineering, Imperial College London.

Qualifications

BSc in Engineering Science (Oxford University). PhD in Electrical Engineering (Cambridge University). ScD in Mathematics (Cambridge University)

Awards and Distinctions

Fellow of the IEE, 2001. Fellow, Institute of Electrical and Electronic Engineers, 2005. Fellow, Royal Academy of Engineering, 2007

Research Interests

Optimal control theory and new methods of nonlinear analysis related to the solution of variational problems. Robust nonlinear control design methods (optimisation

based methods in particular). Optimisation and control of hybrid systems. Applications of control design and optimisation techniques to process, mechanical, electrical power, medical systems, resource economics and mathematical finance.

Other Activities

Associate Editor, Computational and Applied Mathematics. Associate Editor, Optimal Control Applications and Methods. Associate Editor, European Series in Applied and Industrial Mathematics (Control, Optimization and Calculus of Variations). Associate Editor, Set Valued Analysis. Chair of Science and Technology Board and Project Manager, Data and Information Fusion Defence Technology Centre. External Examiner for Engineering Tripos Part II(A), Cambridge University Engineering Department, Board of Examiners. Committee Member, Defence Scientific Advisory Committee (DSAC).



CPSE Academics

2007

Imperial College London

Department of Chemical Engineering

Claire Adjiman
Amparo Galindo
Michael Georgiadis
Charles Immanuel
George Jackson
Cleo Kontoravdi
J Krishnan
Geoff Maitland
Sakis Mantalaris
Costas Pantelides
Stratos Pistikopoulos
Roger Sargent
Nilay Shah
Nina Thornhill

Department of Electrical Engineering

Richard Vinter

Department of Computing

Daniel Kuhn
Berc Rustem

Department of Earth Science & Engineering

Nigel Brandon

Visiting Professors

Roger Benson
John Perkins
Paul Rutter

University College London

Department of Chemical Engineering

David Bogle
Vivek Dua
Eric Fraga
Lazaros Papageorgiou
Eva Sørensen

Publications

2007

Claire S. Adjiman

Book chapters

B. Pereira Lo, A.J. Haslam, C. S. Adjiman, M. Laso, **A method for the systematic estimation of parameters for a stochastic reptation model**, MULTISCALE MODELLING OF POLYMER PROPERTIES, M. Laso and E.A. Perpète (Eds), Elsevier Science, Amsterdam, 2006.

A.J. Haslam, Ø. Moen, C.S. Adjiman, A. Galindo, G. Jackson, **Design of polyolefin reactor mixtures**, MULTISCALE MODELLING OF POLYMER PROPERTIES, M. Laso and E.A. Perpète (Eds), Elsevier Science, Amsterdam, 2006.

T.J. Sheldon, B. Giner, C.S. Adjiman, A. Galindo, G. Jackson, D. Jacquemin, V. Wathélet, E.A. Perpète, **The derivation of size parameters for the SAFT-VR equation of state from quantum mechanical calculations**, MULTISCALE MODELLING OF POLYMER PROPERTIES, M. Laso and E.A. Perpète (Eds), Elsevier Science, Amsterdam, 2006.

C.S. Adjiman, **Optimal solvent design approaches**, INVITED CONTRIBUTION TO ENCYCLOPEDIA OF OPTIMIZATION, Second Edition, 2007.

R.F.M. Oulton and C.S. Adjiman, **Global optimization for planar multilayered dielectric structures**, INVITED CONTRIBUTION TO ENCYCLOPEDIA OF OPTIMIZATION, Second Edition, 2007.

F.E. Pereira, E. Keskes, A. Galindo, G. Jackson, C.S. Adjiman, **Integrated design of CO₂ capture processes from natural gas**, ENERGY SYSTEMS ENGINEERING, M. C. Georgiadis, E. S. Kikkinides, E. N. Pistikopoulos, Wiley-VCH, 2008.

Journal Articles

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B. Pereira-Ló, A.J. Haslam, C.S. Adjiman, **An algorithm for parameter estimation of stochastic differential equations**, CHEMICAL ENGINEERING SCIENCE (2007) DOI: 10.1016/j.ces.2007.06.041.

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E.N. Pistikopoulos, N.P. Faisca, M.C. Georgiadis. **Advanced optimization techniques in the supply chain management of manufacturing industries**. Presented in the PulpPaper 2007 conference, 5-7 June 2007, Helsinki, Finland.

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Charles D. Immanuel

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2006 7th UK Particle Technology Forum, Imperial College, September 2006. Invited Keynote Lecture: **Challenges for Particle Technology in Oilfield Process Engineering**.

2006 IOP Conference on The Future of Conference Fuels, 26th October 2006. Invited Keynote Lecture, **Whither Oil and Gas?**

2006 Shell International Technical Symposium on Upgrading of Heavy Crudes, November 1st-3rd 2006, The Hague. Invited Lecture: **Challenges in in situ Upgrading**.

Athanasios Mantalaris

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Lazaros Papageorgiou

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Conference Papers

Sakizlis V, Kouramas KI, Faisca NP, et al. **Towards the design of parametric model predictive controllers for non-linear constrained systems**, International Workshop on Assessment and Future Directions of Nonlinear Model Predictive Control, AUG 26-30, 2005 ASSESSMENT AND FUTURE DIRECTIONS OF NONLINEAR MODEL PREDICTIVE CONTROL : 193-205, 2007

Faisca NP, Dua V, Rustem B, Pistikopoulos EN, **Parametric global optimisation for bilevel programming**, INTERNATIONAL WORKSHOP ON MULTILEVEL OPTIMIZATION - Algorithms and Applications, 2007, Pages: 609 – 623

Liu P, Gerogiorgis D and Pistikopoulos EN, **Modelling, Investment Planning and Optimisation for the Design of a Poly-generation Energy System**, PROCEEDING OF THE 17TH EUROPEAN SYMPOSIUM ON COMPUTER-AIDED PROCESS ENGINEERING (ESCAPE17), Rumania, May, 2007.

Pistikopoulos, E.N., Georgiadis, M.C., Dua, V. (2007) **Parametric programming & control: from theory to practice**, PROCEEDINGS OF 17TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING, Bucharest, V. Pleşu and P.S. Agachi (Editors), p.569-574, Elsevier, Amsterdam.

Dua, P., Dua, V., Pistikopoulos, E.N. (2006) **Optimal delivery of chemotherapeutic agents in cancer**, PROCEEDINGS OF 16TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING AND 9TH INTERNATIONAL SYMPOSIUM ON PROCESS SYSTEMS ENGINEERING, W. Marquardt and C. Pantelides (Editors), p.1643- 1648, Elsevier, Amsterdam.

Faisca, N.P., Dua, V., Saraiva, P.M., Rustem, B., Pistikopoulos, E.N. (2006) **A global parametric programming optimisation strategy for multilevel problems**, PROCEEDINGS OF 16TH EUROPEAN SYMPOSIUM ON COMPUTER AIDED PROCESS ENGINEERING AND 9TH INTERNATIONAL SYMPOSIUM ON PROCESS SYSTEMS ENGINEERING, W. Marquardt and C. Pantelides (Editors), p.215-220, Elsevier, Amsterdam

Publications

2007

D.I. Gerogiorgis, K.I. Kouramas, N. Bozinis, E.N. Pistikopoulos, **Design and Performance Evaluation of an Explicit Parametric Controller for a Solid Oxide Fuel Cell (SOFC) System: A Comparative Study**, in: PROCEEDINGS OF ECCE-6 (editor: R. Gani), Copenhagen, Denmark (2007).

C.O. Akinlabi, D.I. Gerogiorgis, E.N. Pistikopoulos, **Modelling, Design and Optimization of a Hybrid PSA- Membrane Gas Separation Process**, in: PROCEEDINGS, ESCAPE-17 (editors: V. Plesu, P.S. Agachi): 363-370, Bucharest, Rumania (2007).

Conference Presentations

Amaro B, Immanuel CD, Pistikopoulos EN and Hungenberg KD, **Modelling of Entire Molecular Weight Distribution for Free-Radical Semi-Batch Solution Polymerisation**, AIChE Annual Meeting 2006, San Francisco CA, USA (12 - 17 November 2006)

Amaro B, Immanuel CD, Pistikopoulos EN, Daiss A, Mussig S and Hungenberg KD, **Molecular Weight Distribution in Free-Radical Polymerization – Model Development, Reachability Studies and Process Optimisation, Modelling, Monitoring and Control of Polymer Properties**, Lyon, France (1 – 5 December 2007)

Folic M, Adjiman CS, Pistikopoulos EN, **Selection of solvents for reactions: A computer-aided methodology with robust design criteria**, AIChE Annual Meeting 2006, San Francisco CA, USA (12 - 17 November 2006)

Folic M, Adjiman CS, Pistikopoulos EN, **Computer-Aided Solvent Selection for increased Reaction Rate**, presented at ECCE-6, Copenhagen, Denmark (September 2007)

Narciso D, Pistikopoulos EN, **MPC via Novel Multi-Parametric Nonlinear Programming Techniques**, AIChE Annual Meeting 2006, San Francisco CA, USA (12 - 17 November 2006)

Lam CM, Wong DCF, Yap MGS, Pistikopoulos EN, A. Mantalaris A, **Dynamic Optimisation of a CHO-IFN β Fed-Batch Cell Culture Time-Profile**, in Proceedings of the 20th European Society for Cell Animal Technology Meeting. Dresden, Germany (2007)

Carolyn M. C. Lam, Danny C. F. Wong, Miranda G. S. Yap, Efstratios N. Pistikopoulos, and Athanasios Mantalaris. (2006) **Model-Based Optimisation of Mammalian Cell Cultures: a Case Study for Optimising Glucose and Glutamine Fed-Batch Profiles for CHO-IFN β Cell Line**, AIChE Annual Meeting 2006, San Francisco CA, USA (12 - 17 November 2006)

Gerogiorgis DI, Kouramas KI, Pistikopoulos EN, **Parametric Control of Solid Oxide Fuel Cell (SOFC) Systems**,

presented at the Tenth Grove Fuel Cell Symposium, Queen Elizabeth II Conference Centre, London, UK (09/2007).

Gerogiorgis DI, Kouramas KI, Bozinis N, Pistikopoulos EN, **Design and Performance Evaluation of an Explicit Parametric Controller for a Solid Oxide Fuel Cell (SOFC) System: A Comparative Study**, presented at the European Congress of Chemical Engineering (ECCE-6), Copenhagen, Denmark (09/2007).

Gani R, Gerogiorgis DI, Pistikopoulos EN, **Innovation in Integrated Chemical Product-Process Design – A Systems Approach**, invited presentation at the 1st International Symposium on Sustainable Chemical Product-Process Engineering/SSCPPE 2007 (Keynote Lecture), Guangzhou, China (09/2007)

Dua, V., Pistikopoulos, E.N. (2007) **Global Optimization issues in Parametric Programming & Control**, Workshop on Global Optimization: Methods and Applications, Fields Institute

Faísca, N. P., O. Exler, J. R. Banga and E. N. Pistikopoulos. **A multiparametric programming approach for dynamic programming & robust control**, In: EUROPEAN CONGRESS OF CHEMICAL ENGINEERING - 6, September 16-21, Bella Centre. Copenhagen, Denmark: European Federation of Chemical Engineering, (2007)

Exler, O., N. P. Faísca, L. T. Antelo, A. A. Alonso, J. R. Banga and E.N. Pistikopoulos. **A Tabu search-based algorithm for the integrated process and control system design**, In: EUROPEAN CONGRESS OF CHEMICAL ENGINEERING - 6, September 16-21, Bella Centre. Copenhagen, Denmark: European Federation of Chemical Engineering, (2007)

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Publications

2007

Berc Rustem

Book Chapters

Parpas P, Rustem B, **Global optimization of the scenario generation and portfolio selection problems**, LECTURE NOTES IN COMPUTER SCIENCE, Springer-Verlag, 2006(publication)

Journal Articles

N. Gulpinar, B. Rustem, **Optimal Decisions and Robust Methods for Forecast Errors**, COMPUTATIONAL STATISTICS & DATA ANALYSIS, 51, 7, 3595-3611, 2007.

N. Gulpinar, P. Harrison, B. Rustem, L. F. Pau, T. Field, U. Harder, **Performance Optimization of a Tandem M/GI/1 Router Network with Batch Arrivals**, JOURNAL OF CLUSTER COMPUTING, 10, 203-216, 2007.

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N. Gulpinar, B. Rustem, **Optimal Decisions and Robust Methods for Forecast Errors**, COMPUTATIONAL STATISTICS & DATA ANALYSIS, 51, Issue 7, 1 April 2007, p. 3595-3611.

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Conference Contributions

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Nilay Shah

Journal Articles

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Publications

2007

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Conference Contributions

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Eva Sørensen

Journal Articles

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Chan, S., N. Titchener-Hooker and E. Sørensen (2007), **Optimal economic design and operation of single and multi-column chromatographic processes**, to appear in BIOTECHNOLOGY PROGRESS. (in press)

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Nina F Thornhill

Book Chapter

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2007

Thornhill, NF, Melbo, H, Wiik, J, **Multidimensional visualization and clustering of historical process data**, IND ENG CHEM RES, 2006, Vol: 45, Pages: 5971 - 5985, ISSN: 0888-5885

Thornhill, NF, Naim, MM, **An exploratory study to identify rogue seasonality in a steel company's supply network using spectral principal component analysis**, EUR J OPER RES, 2006, Vol: 172, Pages: 146 - 162, ISSN: 0377-2217

Huang, B, Ding, SX, Thornhill, N, **Alternative solutions to multi-variate control performance assessment problems**, J PROCESS CONTR, 2006, Vol: 16, Pages: 457 - 471, ISSN: 0959-1524

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Thambirajah, J., Benabbas, L., Bauer, M., and Thornhill, N.F., 2007, **Cause and effect analysis in chemical processes utilizing plant connectivity information**, IEEE Advanced Process Control Applications for Industry Workshop 2007, May 14-16, Vancouver.

Edwards-Parton, S., Bracewell, D., Thornhill, N.F., Liddell, J.M., and Titchener-Hooker, N.J., 2007, **Application of partial least squares to sparse data sets for early stage design of chromatographic separations**, ABIO08 Conference on Accelerating Biopharmaceutical Development, March 19-22 2007, Coronado Island, California.

Richard B Vinter

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J M C Clark and R B Vinter, **A New Class of Moment Matching Filters for Nonlinear Tracking and Estimation Problems**, Proc. IEEE Nonlinear Statistical Signal Processing Workshop, Cambridge, 2006

P.E. Caines, F.H. Clarke, X.Liu and R.B.Vinter, **A Maximum Principle for Hybrid Optimal Control Problems with Pathwise State Constraints**, Proc. 45th Conference on Decision and Control, San Diego, 2006

Academic Staff

2007

Academic Staff

Dr C S Adjiman	c.adjiman@imperial.ac.uk
Prof R Benson	roger.s.benson@btinternet.com
Prof I D L Bogle	d.bogle@ucl.ac.uk
Prof N Brandon	n.brandon@imperial.ac.uk
Dr V Dua	v.dua@ucl.ac.uk
Prof E S Fraga	e.fraga@ucl.ac.uk
Dr A Galindo	a.galindo@imperial.ac.uk
Dr M C Georgiadis	m.georgiadis@imperial.ac.uk
Dr C D Immanuel	c.immanuel@imperial.ac.uk
Prof G Jackson	g.jackson@imperial.ac.uk
Dr C Kontoravdi	cleo.kontoravdi98@imperial.ac.uk
Dr J Krishnan	j.krishnan@imperial.ac.uk
Dr D Kuhn	d.kuhn@imperial.ac.uk
Prof G C Maitland	g.maitland@imperial.ac.uk
Dr A Mantalaris	a.mantalaris@imperial.ac.uk
Prof C C Pantelides	c.pantelides@imperial.ac.uk
Dr L Papageorgiou	l.papageorgiou@ucl.ac.uk
Prof E N Pistikopoulos	e.pistikopoulos@imperial.ac.uk
Prof B Rustem	b.rustem@imperial.ac.uk
Prof P Rutter	p.rutter@imperial.ac.uk
Prof R W H Sargent	r.w.h.sargent@imperial.ac.uk
Prof N Shah	n.shah@imperial.ac.uk
Dr Eva Sørensen	e.sorensen@ucl.ac.uk
Prof N F Thornhill	n.thornhill@imperial.ac.uk
Prof R B Vinter	rbv@imperial.ac.uk

Support Staff

Ms C Romano	c.romano@imperial.ac.uk
Ms S Selassie	s.selassie@imperial.ac.uk
Mr G Stuart	g.stuart@imperial.ac.uk
Ms J Thomson	j.thomson@imperial.ac.uk

Research Project List

2007

Name: **Mr Allen, Richard**

Supervisor: Prof D Bogle
Title: Modelling Endothelial Cells
Starting Date: Sep-05
Finishing Date: Sep-08

Name: **Mr Amaro, Bruno**

Supervisors: Dr C Immanuel & Prof EN Pistikopoulos
Title: Modelling and Optimisation of Molecular Weight Distribution for Free-Radical Solution Polymerisation in Batch Reactors
Starting Date: Dec-05
Finishing Date: Dec-08

Name: **Mr Balendra, Sujan**

Supervisor: Prof D Bogle
Title: Global Optimisation of Modular Systems
Starting Date: Oct-01
Finishing Date: Jun-07

Name: **Mr Bianco, Nicola**

Supervisor: Dr C Immanuel
Title: Control of Particle Size Distribution in Emulsion Polymerisation
Starting Date: Oct-04
Finishing Date: Mar-08

Name: **Mr Brumby, Paul**

Supervisor: Prof G Jackson
Title: Characterisation of the Link Between Molecular Chirality and Bulk Phase Chirality in Systems of Liquid Crystals
Starting Date: Oct-05
Finishing Date: Oct-08

Name: **Mr Chang, Le**

Supervisors: Prof N Shah & Prof EN Pistikopoulos
Title: Modelling and Optimization of China Hydrogen Infrastructure
Starting Date: Oct-06
Finishing Date: Jan-07

Name: **Mr Cheung, Kwok Yuen**

Supervisors: Prof N Shah & Prof CC Pantelides
Title: Site-wide and Supply Chain Optimisation for Continuous Chemical Processes
Starting Date: Oct-04
Finishing Date: Sep-07

Name: **Mr Clark, Gary**

Supervisors: Dr A Galindo & Prof G Jackson
Title: Phase Behaviour of Water-soluble Polymers Using the SAFT Equation of State
Starting Date: Oct-04
Finishing Date: Sep-07

Name: **Mr Crane, Andrew**

Supervisors: Dr E Muller & Prof G Jackson
Title: Molecular Systems Engineering
Starting Date: Jul-07
Finishing Date: Jul-11

Name: **Mr Dominguez, Luis**

Supervisor: Prof EN Pistikopoulos
Title: Multiparametric Mixed Integer Dynamic Optimization of Process Systems
Starting Date: Jul-07
Finishing Date: Jul-10

Name: **Mr Dunnett, Alexander**

Supervisors: Prof N Shah & Dr C Adjiman
Title: Biofuel Supply Chain
Starting Date: Oct-05
Finishing Date: Oct-08

Name: **Mr Faisca, Nuno**

Supervisors: Prof EN Pistikopoulos & Dr V Dua
Title: Parametric Programming and Control
Starting Date: Oct-04
Finishing Date: April 2008

Name: **Miss Fiandaca, Giovanna**

Supervisors: Prof E Fraga & Prof S Brandani (University of Edinburgh)
Title: Optimal Design of Pressure Swing Adsorption for CO₂ Capture
Starting Date: Apr-06
Finishing Date: Mar-09

Name: **Mr Gang, Xu**

Supervisors: Dr LG Papageorgiou
Title: Optimisation-based Analysis of Biochemical Systems
Starting Date: Oct-04
Finishing Date: Oct-07

Name: **Ms Hala, AlFulajj**

Supervisor: Prof D Bogle
Title: Modelling of Desalination Processes
Starting Date: Apr-07
Finishing Date: Apr-12

Name: **Mr Harish, Khajuria**

Supervisor: Prof EN Pistikopoulos
Title: Advanced Control and Optimization of PSA Hybrid System
Starting Date: Oct-07
Finishing Date: Jan-11

Name: **Mr Hosseini, Seyed Ali**

Supervisor: Prof N Shah
Title: Multiscale modelling of Bio
Starting Date: Sep-07
Finishing Date: Sep-10

Name: **Mr Iyun, Oluwatope Ebenezer**

Supervisor: Prof NF Thornhill
Title: Plant-wide Fault Diagnosis: Cause-and-Effect Analysis Using Process Connectivity
Starting Date: Dec-07
Finishing Date: Dec-10

Research Project List

2007

Name: **Mr Kazantsev, Andrei**

Supervisors: Dr C Adjiman & Prof C Pantelides

Title: Design of Organic Crystals for Enhanced Bioavailability

Starting Date: Oct-07

Finishing Date: Oct-10

Name: **Mr Kiparissides, Alexandros**

Supervisor: Prof EN Pistikopoulos & Dr S Mantalaris

Title: Development of a Combined Mathematical and Experimental Framework for the Control and Optimisation of Mammalian Cell Cultures

Starting Date: Jan-07

Finishing Date: Jan-10

Name: **Mr Konda, Naga**

Supervisor: Prof N Shah

Title: H₂-CO₂ Infrastructure Design

Starting Date: Aug-06

Finishing Date: Jul-09

Name: **Mr Konstantinidis, Spyridon**

Supervisors: Dr C Adjiman & Prof D Blackmond

Title: Design of Solvents for Complex Organic Reactions

Starting Date: Oct-07

Finishing Date: Jul-10

Name: **Mr Laakso, Gunilla**

Supervisor: Dr LG Papageorgiou

Title: Supply Chain Management for the Paper Industry

Starting Date: Feb-04

Finishing Date: Feb-07

Name: **Miss Lam, Ming-Chi (Carolyn)**

Supervisors: Dr S Mantalaris & Prof EN Pistikopoulos

Title: Creating a Predictive in Silico Model of Mammalian Cell Cultures

Starting Date: Oct-04

Finishing Date: Apr-08

Name: **Mr Lee, Chang-Gun Colin**

Supervisor: Prof N Shah

Title: Optimisation of Closed-Loop Supply Chain

Starting Date: Jun-07

Finishing Date: Jun-10

Name: **Mr Liu, Cong**

Supervisors: Dr J Krishnan

Title: Mathematical Modelling of Drug Delivery in Cancer Tumors

Starting Date: Jan-08

Finishing Date: Jun-11

Name: **Mr Lovell, L Felix**

Supervisor: Prof G Jackson

Title: Study of Interfacial Properties of Mixtures of CO₂, Water and Hydrocarbons Using DFT and Simulations

Starting Date: Dec-07

Finishing Date: Dec-10

Name: **Mr Dominguez, Luis**

Supervisor: Prof EN Pistikopoulos

Title: Multiparametric Dynamic Optimization

Starting Date: Jul-07

Finishing Date: Jul-10

Name: **Mr Lymperiadis, Alexandros**

Supervisors: Dr A Galindo, Prof G Jackson & Dr C Adjiman

Title: A New Group Contribution Method for Solvent Design

Starting Date: Apr-04

Finishing Date: Apr-07

Name: **Mr MacDowell, Niall**

Supervisors: Prof G Jackson, Dr C Adjiman & Dr A Galindo

Title: Improvements in Amine Based Absorption Systems for Post Combustion CO₂ Capture

Starting Date: Oct-06

Finishing Date: Oct-09

Name: **Mr Meepetchdee, Yongyut**

Supervisor: Prof N Shah

Title: Supply Chain Optimisation

Starting Date: Oct-04

Finishing Date: Sep-07

Name: **Miss Mortera-Blanco, Teresa**

Supervisor: Dr S Mantalaris

Title: Development of an Ex-vivo Leukaemic 3-D Culture System

Starting Date: Oct-04

Finishing Date: Sep-07

Name: **Mr Palma Rosillo, Javier**

Supervisors: Prof N Shah & Prof EN Pistikopoulos

Title: Model Predictive Control of Supply Chain Systems

Starting Date: Oct-06

Finishing Date: Oct-09

Name: **Mr Paopo, Idtisak**

Supervisors: Dr S Mantalaris & Dr Xu

Title: Design and Modelling of 3D Perfusion Bioreactor for Stem Cell Bioprocessing

Starting Date: Oct-07

Finishing Date: Feb-11

Name: **Mr Patel, Mayank**

Supervisor: Prof N Shah

Title: Design, Operation & Control of the Next Generation Flexible Process Plant

Starting Date: Jun-07

Finishing Date: Jun-10

Name: **Miss Pereira, Frances**

Supervisors: Prof G Jackson, Dr C Adjiman, Dr A Galindo

Title: From CO₂ Capture to Advanced Oil Recovery

Starting Date: Oct-06

Finishing Date: Oct-09

Research Project List

2007

Name: **Mr Pereira, Gabriela**
 Supervisor: Prof N Shah
 Title: Supply Chain Modelling
 Starting Date: Oct-05
 Finishing Date: Sep-08

Name: **Mr Perera, Chamila**
 Supervisor: Dr E Sørensen
 Title: Optimal Design and Operation of Essential Oil and Oleoresin Separation Processes
 Starting Date: Jan-06
 Finishing Date: Jan-09

Name: **Mr Pinto, Mark**
 Supervisor: Dr C Immanuel
 Title: Modelling and Control of Biological Systems
 Starting Date: Oct-04
 Finishing Date: Mar-08

Name: **Miss Pollock, Michaela**
 Supervisors: Dr A Galindo, Prof G Jackson & Dr C Adjiman
 Title: Predictive Thermodynamic Models for Replacement Refrigerants and Blends
 Starting Date: Oct-04
 Finishing Date: Oct-07

Name: **Mr Poon, Jonathon**
 Supervisors: Dr C Immanuel
 Title: Modelling and Control of Granulation Processes Employing Population Balances
 Starting Date: Oct-04
 Finishing Date: Mar-08

Name: **Mr Ramachandran, Rohit**
 Supervisors: Dr C Immanuel & Dr Stepanek
 Title: Control of Distributed Parameter Systems
 Starting Date: Oct-05
 Finishing Date: Sep-08

Name: **Mr Rodriguez Perez, Javier**
 Supervisors: Dr C Immanuel & Dr C Adjiman
 Title: Optimal Sensor Location
 Starting Date: Jan-06
 Finishing Date: Jan-09

Name: **Mr Safinia, Laleh**
 Supervisor: Dr S Mantalaris
 Title: Preparation and Surface Characterization of Polymer Constructs for Tissue Engineering Applications
 Starting Date: Oct-04
 Finishing Date: Sep-07

Name: **Mr Samaraweera, Milinda Sanjeewa**
 Supervisors: Prof N Shah & Prof EN Pistikopoulos
 Title: Modelling and Optimisation of Urban Energy Systems
 Starting Date: Oct-06
 Finishing Date: Oct-09

Name: **Mr Sampayo-Hernandez, Jose Guillermo**
 Supervisor: Prof G Jackson

Title: Theory and Simulation of Interfacial Systems
 Starting Date: Oct-05
 Finishing Date: Sep-08

Name: **Mr Schreckenberg, Jens**
 Supervisors: Prof G Jackson, Dr C Adjiman & Dr A Galindo
 Title: Modelling Aqueous Polymers Microemulsions and Micelles
 Starting Date: Jul-07
 Finishing Date: Jun-11

Name: **Mr Seyed, Ali Hosseini**
 Supervisor: Prof N Shah
 Title: Multiscale Modelling of Biorefineries
 Starting Date: Oct-07
 Finishing Date: Oct-10

Name: **Mr Soh, Boon Seng**
 Supervisors: Dr S Mantalaris, Dr A E Bishop & Dr L Bing (Genome Institute of Singapore)
 Title: Directed Differentiation of Human Embryonic Stem Cells to Lung Bronchioalveolar Stem Cell
 Starting Date: Apr-06
 Finishing Date: Apr-09

Name: **Mr Strubing, Heiko**
 Supervisors: Dr C Adjiman, Prof EN Pistikopoulos, Dr A Galindo
 Title: Design of Solvents for Organic Reactions
 Starting Date: Nov-07
 Finishing Date: Nov-10

Name: **Mr Suwanapal, Panthot**
 Supervisor: Prof N Shah
 Title: Energy Systems with Application to Thailand
 Starting Date: Oct-05
 Finishing Date: Sep-08

Name: **Mr Suwanapal Pasant**
 Supervisor: Prof N Shah
 Title: Chemical Complex Supply Chain
 Starting Date: Oct-05
 Finishing Date: Sep-08

Name: **Mr Sweetman, Stephen**
 Supervisor: Dr C Immanuel
 Title: Population Balance Modelling of Emulsion Polymerisation Systems
 Starting Date: Nov-04
 Finishing Date: Nov-07

Name: **Mr Tangviriyasirikul, Supacharn**
 Supervisor: Dr S Mantalaris
 Title: Development of a Perfusion Bioreactor with Mechanical Stimulation for Bone or Cartilage Tissue Engineering
 Starting Date: Oct-07
 Finishing Date: Oct-10

Research Project List

2007

Name: **Mr Thambirajah, Jegatheeswaran**

Supervisor: Prof NF Thornhill

Title: A Wide-Area System for Power Transmission Security
Enhancement Using a Process Systems Approach

Starting Date: Jul-07

Finishing Date: Jul-10

Name: **Mr Sumner, Tom**

Supervisor: Prof D Bogle

Title: Computational Modelling of Liver Glucose Homeostasis

Starting Date: Oct-06

Finishing Date: Oct-09

Name: **Miss Voelker, Anna**

Supervisor: Prof EN Pistikopoulos

Title: Control of MUAVs

Starting Date: Oct-07

Finishing Date: Oct-10



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