Centre for
Process
Systems
Engineering

Annual Report 2006

| The Centre for Process Systems Engineering (CPSE) |

Imperial College London | UCL

Annual Report 2006

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| CPSE Annual Report 2006 – Contents |

"..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 |

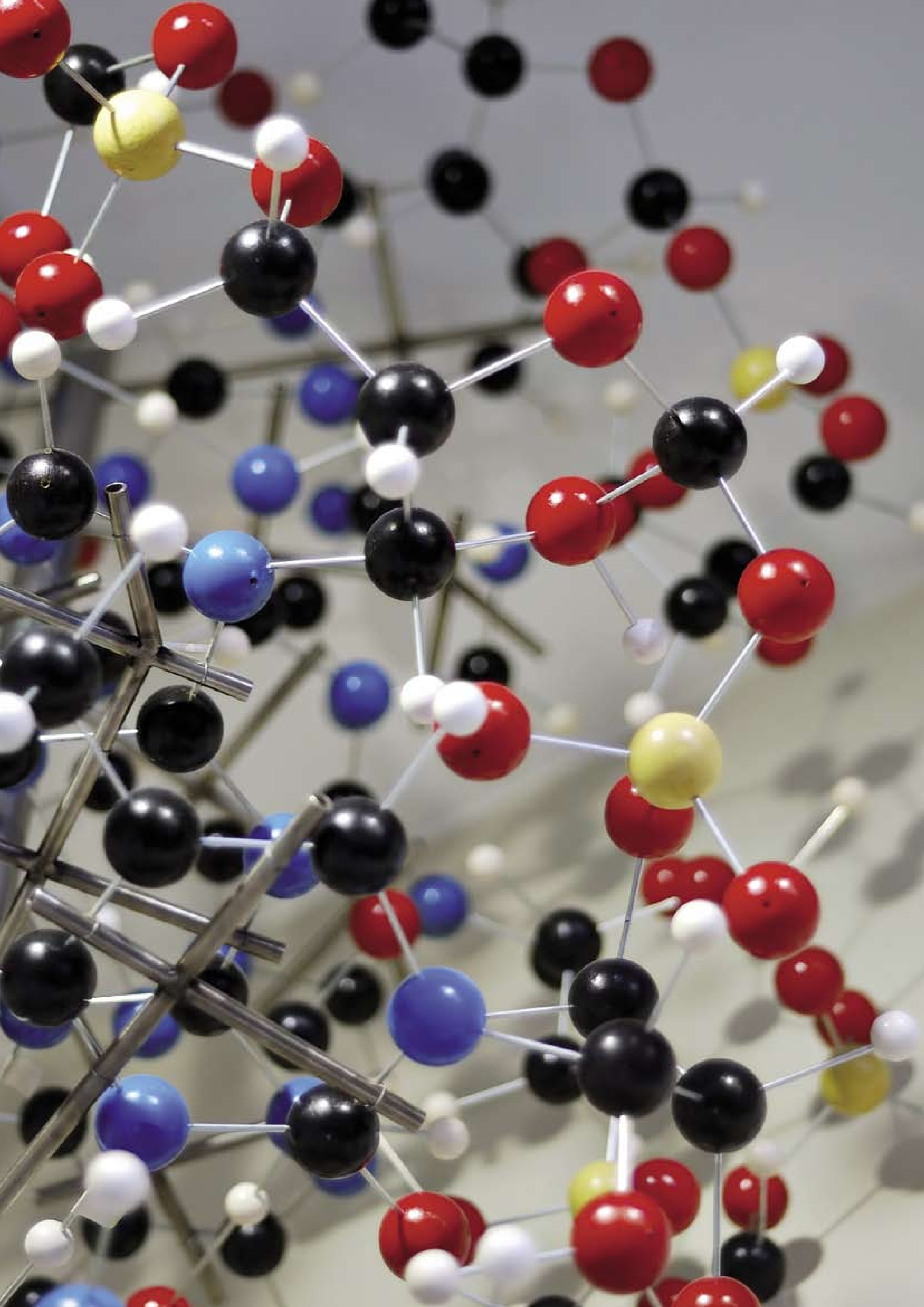
The Centre for Process Systems Engineering (CPSE) is a multi-institutional research centre inaugurated in August 1989. It involves Imperial College London and University College London, and is based at the Imperial College London South Kensington campus.

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



| Review of the Year |

I have been CPSE Director for 2006 while Stratos Pistikopoulos was taking a sabbatical – not in sunny academic environments (although there were brief periods of this) but to launch his start-up company PAROS. It has been a valuable experience as the first Centre Director from UCL and fortunately I know both institutions pretty well. It is some years since CPSE produced a printed Annual Report but I felt that people needed to have an overview of our activities on a reasonably regular basis.

A few years ago we decided to widen the scope of the application domains in which we work. Process Systems Engineering techniques are very widely applicable to complex systems involving molecular change. This embraces systems from molecular scale product design to global sustainability, particularly in energy.

We have approached this by restructuring the Research Programme as three 'Competence Areas' bringing together work in our areas of core competence: Process and Product Design, Operations and Control, and Modelling and Model Solution Methods; and five 'Application Domains' where these competence areas are focussed: Chemical Manufacturing Systems, Molecular Systems Engineering, Biological Systems Engineering, Supply Chains of the Future, and Energy Systems Engineering. These Domains will ebb and flow in the intensity of work, new ones may be launched, and some may be stopped if we feel our priority needs be directed elsewhere.

Our expertise is in Process Systems Engineering and we cannot have deep levels of expertise in all these Application Domains as well. We have therefore recruited to the Centre some new members who have expertise in these areas and are also fully signed up to working within the framework of Systems Engineering i.e. they are systems thinkers. George Jackson and Amparo Galindo have huge expertise in thermodynamics and are working with Claire Adjiman on Molecular Systems Engineering. Geoff Maitland and Nigel Brandon (of the Dept of Earth Science and Engineering) similarly have much experience with energy systems. Sakis Mantalaris works in biological systems with a significant experimental effort on mammalian cell systems. We have much in house experience in chemical manufacturing systems and in supply chain work. As well as this we work with many collaborators at molecular level, with computational expertise, with physiological expertise, and so on across both Imperial College and UCL and with other institutions. In particular we are working closely with the Energy Futures Laboratory at Imperial on Energy Systems Engineering and with CoMPLEX (the Centre for Mathematics and Physics in the Life Sciences and Experimental Biology) at UCL on Systems Biology. In this way we can continue to lead in developing Process Systems tools and techniques while anchoring our work in important concrete problems.

Two new companies have joined our Industrial Consortium, GlaxoSmithKline and Petrobras. While member companies have wide interests, we have a number of companies with particular interests in the Oil and Gas business: Shell, BP and Petrobras; in pharmaceutical manufacture: Bristol Myers Squibb, GlaxoSmithKline, and Bayer, in chemicals and polymers manufacture: Dow, Ineos-Fluor, BASF, Air Products, Bayer and ICI, on consumer products: Procter and Gamble, and on automation of many of these areas: ABB. We will seek to explore these synergies in the future.

The Centre involves 22 academic staff from Imperial College and UCL, and we currently have 65 PhD students and 13 Research fellows and associates. Since 2002 we have been managing a portfolio of grants worth £5.9 million. Of this 43% of the awards are from industry, 14% from the European Commission, 36% from the Research Councils and the remaining 7% from DTI and charities.

The U.K. Government is becoming increasingly interested in promoting Knowledge Transfer which we have always seen as part of our mission. We do this through our Industrial Consortium, through the PhD graduates and postdoctoral researchers who continue to move to excellent positions in both industry and academia, through the spinoffs and licencing, as well as the traditional routes of conference presentation and journal publication. Our spin-off companies PSEnterprise and Britest continue to grow strongly, and Paros has recently been launched.

We have strengthened our links with Georgia Tech this last year. The Spring Consortium was held in Atlanta and next years spring Consortium meeting will again be joint and will be held back in London. We have active projects with Georgia Tech in polymers and in supply chain research.

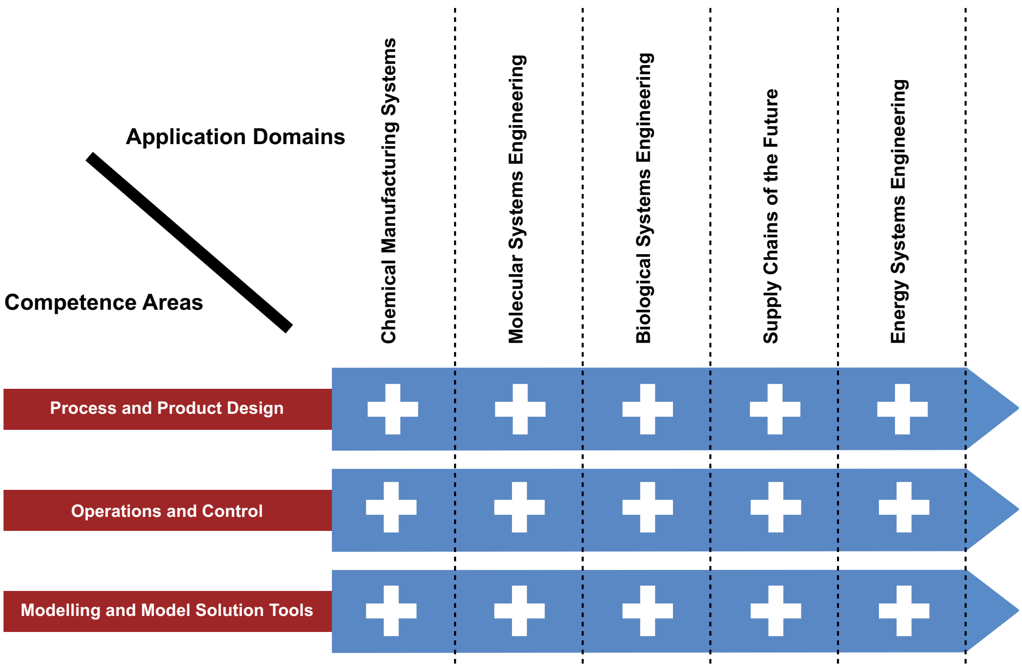
We work with many academic institutions around the world. We are working more closely with CPACT at Newcastle University in the UK who have complementary expertise in data analysis research.

Concerning staff news from the Centre, Eva Sorensen and Amparo Galindo were promoted to Reader and Geoff Maitland, who has recently joined the Centre, was elected a Fellow of the Royal Academy of Engineering. Harris Makatsoris, our Industrial Marketing Manager, left recently to take up a lecturing post at Brunel University.

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

Prof David Bogle FREng
Director, Centre for Process Systems Engineering

| CPSE Research Programme |



| 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

| International Centre Launch |

iCPSE - Imperial College, UCL and Georgia Institute of Technology launch International Centre For Process Engineering

On 17 March 2005, Imperial College, University College London and the Georgia Institute of Technology collaborated to launch the International Centre for Process Systems Engineering (iCPSE). The iCPSE aims to tackle many issues that face the process industry. There are many universal problems best tackled by an international alliance which can make a significant impact for the process industry, which operates globally, and the particular focus initially will be on managing risk and uncertainty. The London and Atlanta partnership are working together to create novel engineering solutions for industry and to promote the transfer of leading edge research into industrial practice. It will focus on international research and educational activities spanning a whole range of length scales seen in chemical process industries, from molecular phenomena to enterprise-wide optimisation and control. Joint projects have been established in polymer process modelling and in supply chains.

Our training objective is to educate graduate students to the highest international level in Process Systems Engineering principles ensuring rigour and creativity, in ensuring they gain a practical approach, and that they think as researchers in a truly international context. We aim to prepare our students for international entrepreneurial research careers in business or academia through joint supervision, exchange, and cross Atlantic student activities on top of their normal institutional research program. To do this we aim to ensure that many of our students spend some time in both hemispheres. This requires common projects with students spending time in both countries to create truly international researchers. It will also be developed through short courses taken in the UK and the USA by common cohorts of graduate students and industrial collaborators.

The Spring Consortium meeting was held in Atlanta as the second of the iCPSE joint Consortium meetings. Alongside two technology sessions, we held a session on industrial perspectives on industry-academic collaborations, and one on the education of research students. A poster session with the students stimulated much discussion on a range of PSE topics. All the presentations and posters can be found on the CPSE website.

> "..to educate graduate students to the highest international level in Process Systems Engineering principles ensuring rigour and creativity.."

"...This wide-ranging activity engages on average 20 researchers along four main themes..."

| Product and Process Design |

Overview

Our work on the development of systematic model-based methodologies for the rational design of processes 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. We thus consider not only economic aspects, but also environmental, safety and health factors. This is exemplified both in our theoretical work and in our technology development projects. Part of our 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. This 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 CO_2 capture from natural gas. This wide-ranging activity engages on average 20 researchers along four main themes:

- **Materials design for process synthesis:**

  The design of products and processing materials is tackled from the development of property prediction techniques, to their use in the design of environmentally benign, yet functional systems.

- **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.

- **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:

Process synthesis and the environment: Strategies for process integration and pollution prevention strategies are developed for the design and operation of plant-wide sustainable processes. Novel process synthesis modelling concepts are explored together with life-cycle and environmental impact assessment aspects, leading to new designs which feature step-change improvements in energy efficiency, waste minimization and process sustainability.

Systematic methodologies for modelling and optimisation of separation processes: Strategies for the development of systematic approaches to modelling of separation processes are developed which assist in determining which model parameters are most important and will have the highest impact on the final design, how these model parameters should be estimated from experimental data and which level of modelling detail is required for different applications. The approaches are applied to different separation processes such as the investigation of hybrid distillation/pervaporation processes, membrane processes and chromatographic separation in both single and multiple column arrangements.

Systematic methodologies for computer-aided design of materials: Advances in the understanding and modelling of the behaviour of matter have opened the way for the development of systematic methodologies for 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 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.

| Product and Process Design |

Overview (cont'd)

Design of bioprocesses for the production of ethanol: Renewable energy can and should play an important role for solving the problems arising as a consequence of the enormous demand of fossil fuels required by the global economy. One of the most relevant renewable resources is lignocellulosic biomass, mainly agricultural and forestry residues or agro-industrial wastes. Lignocellulosic biomass is an abundant and cheap feedstock that can be utilized for energy production. For instance, it can be converted into renewable liquid biofuels such as ethanol.

Our work investigates the use of the Jacaranda framework for process design and optimisation for bioethanol production from lignocellulosic biomass. The conversion of lignocellulosic biomass is a complex process. The system considered comprises the step of biological transformation of the pretreated feedstock through different technological options (separate hydrolysis and fermentation, simultaneous saccharification and fermentation, and simultaneous saccharification and co-fermentation), and the step of ethanol dehydration using distillation. Early results demonstrate that Jacaranda handles the complexity of the design problem robustly with respect to the numerical difficulties that arise from the complex models used.

Design and operation of essential oil separations: Essential oils are extracts of plants which constitute various volatile aromatic compounds. Before use, the essential oils are enriched in certain aromatic compounds, although in some cases, a single aromatic compound must be completely isolated. The separation of essential oils is usually performed in batch columns. Recently, however, other separation methods, such as spinning band distillation columns, have emerged as promising alternatives to the more traditional batch columns. Spinning band distillation creates intimate contact between vapour and liquid using a helix rotating at high speeds inside the column and is very efficient with a low hold-up.
In this work, a methodology is developed for the generation of mathematical models of separation processes where little or no data is available. Optimal design and operation for the rectification of essential oils using traditional batch distillation is explored using the models and is compared to the novel alternatives. Examples from different industries such as the rectification of orange oil and peppermint oil, the two largest produced essential oils, and the fractionation of Eucalyptus oil to isolate Citrinellal, are used to demonstrate the developed modelling and optimisation methodology.

Product and Process Design - Highlighted project

Optimal Synthesis, Design and Operation of Hybrid Separation Processes

Distillation is the most commonly used technique for separating liquid mixtures within the chemical industries despite being an energy and capital intensive process. Many mixtures commonly encountered in the fine chemical and pharmaceutical industries are, however, difficult or impossible to separate by normal distillation due to azeotropic behaviour, tangent pinch or low relative volatilities. Pervaporation has been hailed as an alternative to distillation for such mixtures as the separation mechanism is different, relying on differences in solubility and diffusivity between the components in the mixture, and not vapour-liquid equilibrium as in distillation. Recently, hybrid systems have been proposed where a distillation column unit and a pervaporation unit are integrated into one process. In such a process, the shortcomings of one method are outweighed by the benefits of the other, allowing for significant savings in terms of energy consumption and cost. The distillation column and pervaporation membrane units can be integrated in different ways; the pervaporation unit can be positioned before the distillation column, after the column, or fully integrated. Depending on the particular separation task, the configuration, design and operation of a hybrid should be optimised to achieve the most suitable performance in terms of maximum revenue and minimum energy consumption.

The project considers the simultaneous optimisation of configuration, design and operation of hybrid batch distillation/ pervaporation processes by considering all possible process structures. The overall problem is formulated as a mixed integer dynamic optimisation (MIDO) problem. The optimisation strategy comprises of an overall economics index that encompasses capital investment, operating costs and production revenues. Furthermore, rigorous dynamic models developed from first principles for distillation and pervaporation are used. Based on the optimisation results, it is shown that a significant increase in overall profitability can be achieved when hybrid configuration is used instead of conventional distillation or pervaporation processes.

The first part of the project deals with the application of the simultaneous optimisation methodology mentioned above, to continuous hybrid distillation/pervaporation processes. It is again demonstrated that a hybrid process can increase overall profitability when compared to distillation alone. Furthermore, the annualised operating costs are found to be significantly reduced for the hybrid.
The second part of the project considers simultaneous multi-objective optimisation of design and operation of batch hybrid distillation/pervaporation processes. The performance of these processes depends on a number of different criteria that are often conflicting (e.g. revenue versus cost), therefore an effective optimisation of such systems requires the consideration of multi-criteria approaches to effectively evaluate and optimise the performance, whilst meeting the desired separation requirements. The overall problem is formulated as a multi-objective mixed integer dynamic optimisation (MO-MIDO) problem. The optimisation strategy comprises of economics indices that reflect capital investment, operating costs and production revenues. A novel genetic algorithm based multi-objective framework that can be applied to multi-dimensional engineering problems is proposed. The proposed algorithm is found to successfully handle the multi-objective nature of the simultaneous design and operation of batch hybrid distillation/ pervaporation processes.

| Operations and Control |

Overview

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

Process Measurement and Control covers the theory and practice of advanced automation and control with an emphasis on application to the process industries. The research continues to support activity from the most fundamental control theory, for instance the reduction of the complexity of large dynamic models for model-based control, through to technology transfer, for instance in signal analysis methods for plant-wide disturbance diagnosis. A special feature of the programme is the ability to move new theory rapidly towards practical realisation and thus to help the process control sector take early advantage of developments.:

Activities and noteworthy achievements in the past year include:

- **Optimal operation and control:** Optimal operations can achieve significant improvements in a wide range of complex processes particularly in fine chemicals and polymer manufacture. Projects involve extensive modelling and in many cases have links to experimental programmes. Our highlighted project this year concerns granulation and emulsion polymerization using population balance modelling within dynamic optimization in batch operation. This has led to methods for control over variables such as particle size distribution and the ability to directly improve end-product quality.

  Kriging metamodelling is being used in real-time optimization to find promising regions in the search space by functional interpolation between points evaluated using a rigorous model. The method has obtained accurate solutions with fewer then 30% of the simulation runs required by optimization with the rigorous model.

  Optimal control is moving towards control at multiple scales to be sure that profitability and environmental objectives are met, with an application in reaction adsorption systems. A new methodology is being investigated that correlates phenomena at different scales, aims to establish stability conditions and to investigate why nonlinear interaction induces dissipative structures.

  Other projects also look at methods to support company-wide decision making for plant operations, for planning the future product portfolio and development of long-term capacity and investment plans.

- **Control theory:** Theoretical work is centred on robust and optimal control design, nonlinear systems, system identification and model reduction. Efficient model reduction techniques can reduce large first principles dynamic models into a form suitable for real-time model-based control. The big challenge is to extend that knowledge to non-linear systems all too frequent in industry.
  Progress is being also being made on stability analysis for nonlinear model predictive control using the Centre's strengths in mixed-integer nonlinear programming. The key step is the representation of time periods by binary (0-1) variables, and the stability criterion is that the state and control variables reach target values at the end of the time period.
  Research in robust and optimal control design is leading to practical approaches to the design of feedback controllers of nonlinear systems based on the theory of differential games. Robust Control is linked to Differential Games because disturbances and model changes can be interpreted as strategies of an antagonistic player. The Differential Games approach provides controllers that deal with disturbances on a worst case basis.

- **Integration of process design and operation:** Research into the integration of operability objectives in process design and operation has centered on simultaneous assessment of the flexibility, controllability, robustness, reliability and availability of complex process manufacturing systems. The aim is to provide decision support and scenario analysis. A project involving a reactive distillation system optimized the design and control decisions simultaneously optimized representing a 17% savings over the original design. Other studies are covering chromatographic separation, batch distillation and food processes. A particular challenge is the optimisation of non-linear dynamic systems under uncertainty and for this purpose non-linear expected value optimisation is being explored as well as optimisation of higher order moments to cover nonlinearities in uncertain variables. The main tools and methodologies used for this purpose are deterministic, local, global and stochastic optimisation, parametric programming and minimax optimization.

- **Supply chain management and integrated batch processing**: 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 **(continued oveleaf on page 14).**

| Operations and Control |

Overview (cont'd)

Supply chain management and integrated batch processing (cont'd)

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.
Batch processing work is, in many respects, a microcosm of supply chain work and includes short- and medium-term planning and scheduling planning. Decision tools are coming from these approaches that address regulatory pressures and capacity constraints in biopharmaceutical manufacture.

- **Biomedical modelling and healthcare systems:** Biomedical modelling has included compartmental models for delivery of drugs under anaesthesia and the determination of the optimal regime for delivery of drugs in chemotherapy. Parametric control is a relatively new concept in model predictive control which transforms on-line model predictive control and optimization into an off-line problem which is solved just once. On-line optimization is achieved by implementing the solution as a function look-up and evaluation table in a microchip. Parametric control has been combined with detailed first principles modelling for real-time insulin delivery for Type I diabetes.

- **Plant-wide root cause analysis:** Technology transfer of our measurement-based methods for plant-wide disturbance detection and diagnosis has been completed in a project with ABB. It is a measurement-based analysis tool that analyzes simultaneously multiple loops, detects common behaviours and identifies possible root causes.
Isolation and diagnosis of root causes is further enhanced when process connectivity is considered. A prototype software has been designed and implemented which, when given an electronic process schematic of a plant and results from a data-driven analysis, allows the user to pose queries about the plant and to find root causes of plant-wide disturbances. The plant topology information is written in XML according to the Computer Aided Engineering Exchange (CAEX) schema. Uses for CAEX in other applications such as HAZOP analysis and alarm management are also being explored.

Operations and Control - Highlighted project

Control of Particle Size Distribution in Semi-batch Emulsion Polymerisation

Emulsion polymerisation is characterised by a distribution of polymer particles in water. The particle size distribution (PSD) is a key determinant of the end-use properties including rheology, adhesion, optical properties and film-forming.

Typical end-use applications necessitate a non-Gaussian and multi-model PSD, thereby warranting control of the shape of the distribution. Also, typical operation of the emulsion polymerisation process is in the batch/semi-batch mode. Although measurements of PSD can be obtained on-line, these are usually delayed by a sampling time of about 10 minutes. Further, the first reliable PSD measurement is not available until about 20 minutes into operation, but the first mode of particles in the target multi-modal PSD is nucleated and partly grown by this time. Both nucleation and growth being irreversible processes, it is likely that the shape of the PSD may be irreversibly altered by this time. Therefore, a batch-to-batch feedback control holds promise for this process, in place of the more common in-batch feedback control. The philosophy is that although there is little feedback correction that could be done within any given batch, feedback measurements obtained from the batch can be used to improve the subsequent batch. The aim of this study is to develop one such iterative batch-to-batch control for semi-batch emulsion polymerisation towards the attainment of multimodal PSD.
As the first step, a dynamic optimisation problem is solved for batch operation, to determine the feed policy of the monomer and surfactant to attain the target distribution.

$$\frac{\partial F(r,t)}{\partial t}+\frac{\partial}{\partial r}\left(F(r,t)\Re_{growth}(r)\right)=\Re_{nuc}\delta\left(r-r_{nuc}\right)+\Re_{coag}(r)$$

The equation shows how *F(r,t)*, the shape of the particle density distribution with respect to the radius *r*, changes with time. $\Re_{nuc}$ is the rate of nucleation which is restricted to the smallest end of the size distribution r_{nuc} (as picked out by the use of the delta function), $\Re_{growth}$ is the growth rate of the individual particles, and $\Re_{coag}$ is the rate of inter-particle coagulation.
The aim is to control the final PSD by finding the best feed profiles of surfactant and monomer through the use of this population balance model. The solution leads to multi-scale process considerations that are currently a major focus of work in the Centre, combining macroscopic population-level behaviour and the PSD with meso/micro-scopic particle-level behaviour such as nucleation, growth, aggregation and breakage. The emulsion polymerisation process is modestly multi-scale because the surface conditions and behaviour of individual particles influence the population PSD. Important factors are depicted in Figure 1a. The multi-scale character is also exploited in the controller formulation in which the feed profiles are determined subject to limitations in the actuator, the process and the measurements. Figure 1b indicates the concept, it shows an explicit link between the inputs and outputs through the particle-level phenomena.

The highlight of the work has been an optimization approach that takes explicit account of the multi-scale process based on targets for the particle rate processes (nucleation and growth)

| Operations and Control |

Operations and Control - Highlighted project (cont'd)

in addition to the PSD. Figures 2 a-c indicate the achievements in a simulation of the match of the three targets. In the plots, "Target" refers to the PSD and the nucleation and growth rates aimed for, and "Optimal" refers to the actual PSD and the nucleation and growth rates obtained by the optimisation. Figure 3 is a surface plot of , The shape of the particle density distribution with respect to radius and time. It shows how nuclei seeded at the start of the batch grow in size to about 200nm (the right hand ridge), while more nuclei are initiated under controlled conditions (left hand ridge), leading to the desired bimodal distribution by the time the batch ends at 150 minutes. The next step in the project is a laboratory implementation of the recipe obtained from the dynamic optimiser. The data from these experiments will provide the feedback correction to the next batch in a batch-to-batch control framework.

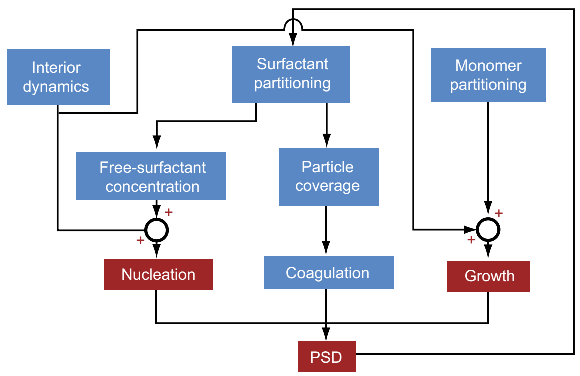


Fig 1a: Depiction of the modestly multi-scale character of the emulsion polymerisation process.

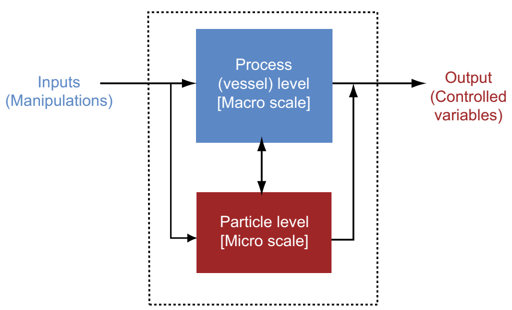


Fig 1b: Explicit accounting of the multi-scale process physics in controller formulation for enhanced performance

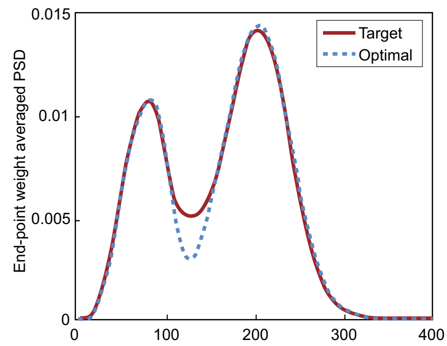


Fig 2a: PSD match with target.

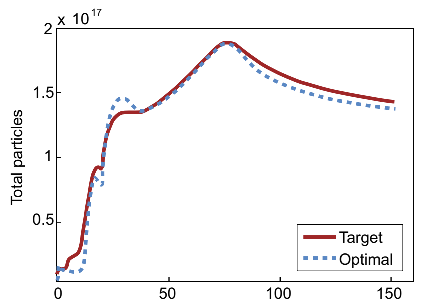


Fig 2b: Match of nucleation trajectory target.

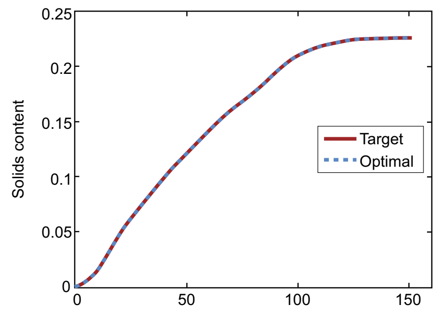


Fig 2c: Match of growth trajectory target.

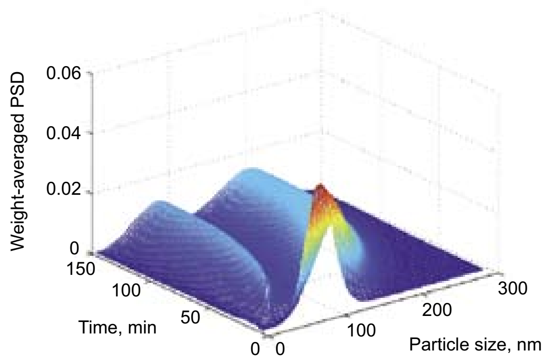


Fig 3: Evolution of the bimodal PSD

| Modelling and Model Solution Tools |

Overview

Underpinning all the application areas in the Centre is the development of new modelling and model solution tools. New models and associated tools are allowing us to tackle new types of problems as well as more traditional problems with greater complexity, minimising the assumptions required and leading to greater insight into the behaviour of processes and the properties of products.

In the past year, new modelling techniques and models have been developed for emulsion polymerisation, granulation processes and for bioreactors. Emulsion polymerisation is a heterogeneous polymerisation method in which the polymer radicals are compartmentalised within particles. A detailed model for this process has been formulated and solved, accounting for particle size distribution (PSD) and molecular weight distribution (MWD). The PSD is incorporated through a population balance framework that accounts for particle rate phenomena of nucleation, growth and coagulation. An identification of potential manipulated variables for control of PSD and MWD is done through sensitivity analysis. Experimental work is currently being undertaken in a laboratory scale reactor for validating the models. Also for polymerisation, another project has addressed the development of a model for the entire molecular weight distribution in free-radical solution polymerisation under batch non-isothermal conditions. A technique has been developed for the solution of the entire distribution model. This technique deals with the incorporation of the phenomena of termination by combination that is important in polymerisation kinetics. This model will be used for product design and process control.

The aim of another project in modelling is to incorporate mechanistic models for particle rate phenomena (such as agglomeration and nucleation) within a population balance framework. This will allow us to predict the PSD of granules in batch, semi-batch and continuous operation of the granulators. A framework based on transition state kinetic theory has been identified as being effective in accounting for both agglomeration and nucleation phenomena. Validation of the agglomeration kernel is also being considered, using both experimental data and discrete element simulations of the aggregation processes.

Several biological processes exhibit preferential behaviour such as preferential substrate utilisation and preferential product formation that is not captured by the well-known Monod kinetics. A cybernetic modelling framework has been proposed to incorporate such preferential behaviour. This new framework is being used to model the production of a biopolymer, poly-ß-hydroxybutyrate, that involves several such preferential traits. The aim is to use the model for dynamic analysis and control. Recent developments in solution tools have addressed population balances, configuration of artificial neural networks and data analysis with visualisation for robust nonlinear optimisation.

The new models for granulation and bioreactors, for example, require solution methods for working with multi-dimensional population balance models. A novel technique has been developed based on a hierarchical decomposition algorithm that considers the various particle rate phenomena of aggregation, nucleation, growth and breakage in an independent (sequential) manner. This decomposition strategy enables considerable pre-processing, thereby aiding computation. The specific contributions include the development of the technique to handle breakage/division phenomena in population balances and the demonstration of the feasibility of the technique to handle modestly multi-dimensional population balance models that mainly become important in processes such as granulation and bioreactors. The breakage technique has been demonstrated on one-dimensional, three-dimensional and six-dimensional population balance models. In each case, the results are found to be qualitatively consistent with theory. The computational times are also found to be conducive for the intended applications (dynamics & sensitivity analysis, and dynamic optimisation & control).

Artificial neural networks can be used for system identification, model reduction, control of chemical processes and developing property prediction correlations. A key factor in the success of a neural network in any of these applications is the effectiveness of the training stage. Recently, a mixed-integer programming approach for training the network has been developed. This approach relies on modelling the existence or non-existence of nodes by introducing 0-1 binary variables. The interconnection between the nodes and the layers is also similarly modelled. This results in a mixed integer program where the objective is not only the minimization of the error but also the number of nodes. The key advantage of this approach is that a reduced number of nodes and a much simplified network are obtained.
Using many of the models required by the application areas typically results in the need to solve high-dimensional nonlinear optimisation problems, often with multiple criteria. One research project has concentrated on the use of data analysis and visualisation tools for developing targetted optimisation methods for these problems. This is described in more detail on page 17.

| Modelling and Model Solution Tools |

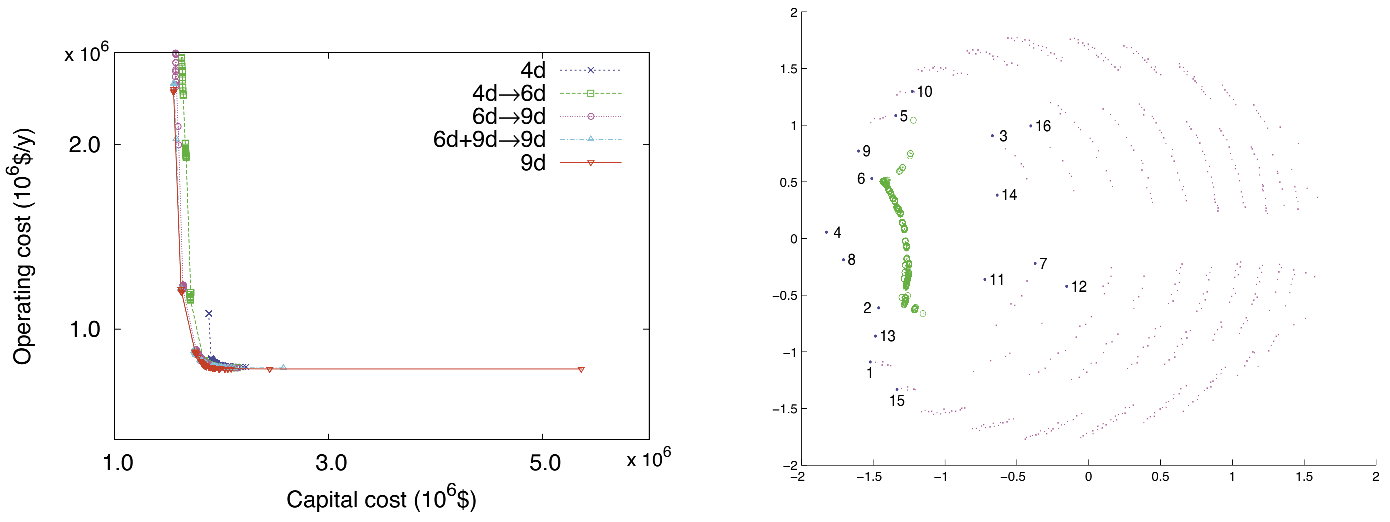
Overview

Modelling and Model Solution Tools - Highlighted Project:

Data analysis and visualisation for robust multi-criteria optimisation

The solution to a multi-criteria optimisation problem is often represented by a Pareto set which represents the trade-off between the different criteria. Generating such a Pareto set can be computationally intensive and often requires the development of targeted techniques. This highlighted project involves the use of multi-dimensional analysis and visualisation techniques to support an iterative procedure for generating a Pareto set for highly nonlinear and constrained problems. In particular, the technique addresses the problems that arise when the feasible region is small in comparison with the size of the domain defined by simple bounds on the decision variables.

The basis procedure is as follows. A number of points in the domain of the optimisation problem are generated randomly. Using this set of points, a multi-dimensional analysis is performed to identify the key contributing decision variables for the feasibility of the solution. This analysis allows us to define a lower dimension problem which can be solved more easily. Further analysis, using principal component analysis for instance, allows us to then identify a second set of decision variables, those which have some impact on feasibility but less than the key ones identified in the first stage. A higher dimension problem is defined using these variables and solutions obtained. This procedure repeats iteratively, increasing the dimension of the problem solved until the original problem is solved successfully. The figure below shows the evolution of the Pareto set, represented as a graph for a bi-criterial problem, for an optimisation problem with 9 decision variables.



The final Pareto set can be visualised in a number of ways. One useful visualisation is the use of multi-dimensional scaling to represent the high-dimension space in two dimensions. The figure above shows the Pareto set relative to the vertices in the domain of the problem.

| Chemical Manufacturing Systems |

Overview

Research in the CPSE aimed at serving the 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; polymer industry; particulate industry and specialty chemical industry.

Continuous Chemical Production Industry

Studies dealing with continuous chemical processes include the following: Integrated multi-scale model-based solvent and process design demonstrated for CO_2 removal from natural gas, and its optimal operation [Keskes, Adjiman and Jackson; Ogunbayo and Adjiman]; Management of technological risks in process design [Blanco-Gutierrez, Adjiman and Pantelides]; Multi-scale modelling for use in control, demonstrated on a reaction-adsorption system [Al-Soudani and Bogle]; Design of a non-linear robust control system, implemented on an exothermic reaction scheme [Luis, Kershenbaum and Astolfi]; Hybrid CLP and MIB approaches to production scheduling [Roe, Shah and Papageorgio]; Tools for root cause diagnosis for faults in chemical plants [Bauer and Thornhill]; Design of facility and process plant layout [Westerlund and Papageorgiou]. A generic study serving the chemical production processes is the optimal design of a hybrid separation process, comprising distillation and pervaporation operations, and its optimal operation [Bakarat and Sorensen].

A highlight of activities in the Centre that deal with the chemical industry is the work on the molecular thermodynamic modelling to predict macroscopic properties of solvents, catalysts and other chemicals. Two representative projects in this regard include predictive thermodynamic models for replacement refrigerants and blends [Pollock, Galindo, Jackson and Adjiman], and thermodynamics of mixed-solvent electrolyte solutions [Patel and Galindo].

There are a large number of activities that address the anticipated enhanced energy needs of the society, addressed in detail in a separate report. A few of the activities that are mentioned here deal with biofuel supply chain optimisation [Dunnett and Shah]; hydrogen gas distribution planning and scheduling [Al-Mansoori and Shah]; oil-and-gas production optimisation [Ali and Pistikopoulos]; and a project on the development of an integrated multi-scale model of oil reservoir, flow line and top-side separation facilities to be employed for optimal deployment of sensor for flow assurance (prevention of hydrates) [Rodriguez Perez, Adjiman, Pantelides and Immanuel].

Several of the above tools and algorithms are generic and are applicable to several continuous process industries. In addition, the Centre also has activities specific to the polymer industry, particulate and specialty chemical sector, and the biochemical sector. A brief outline of some such projects is presented next.

Polymer Industry

Projects dealing with polymers include: solvent selection for reaction employing multi-scale process models [Folic, Adjiman and Pistikopoulos]; modelling of molecular weight distribution for free-radical solution polymerisation in batch reactors for process and recipe optimisation [Amaro, Immanuel and Pistikopoulos]; parameter estimation for stochastic models of polymer rheology [Pereira Lo and Adjiman]; studies on emulsion polymerisation processes with an aim to develop detailed models based on population balances, accounting for the distributed character of the process, to be employed for model-based optimal control of underlying particle size distribution. The applications of emulsion polymerisation are in paints, adhesives, synthetic rubber, specialty products, and drug-delivery vehicles [Sweetman, Bianco and Immanuel].

Pharmaceutical and Specialty Chemical Industry

Activities that focus on the pharmaceutical industry include the following: multiscale planning and scheduling in the pharmaceutical industry [Stefansson and Shah]; population-balance based modelling of granulation processes to serve as a tool for technology transfer of the accrued scientific knowledge on granulation fundamentals via dynamic analysis and feedback control [Poon, Ramachandran and Immanuel]. Besides the pharmaceutical industry, the last project also targets the agricultural and food processing industry.

In addition to the above mentioned conventional chemical activities, there is a range of activities in the biochemical sector. These are addressed separately. Two projects to highlight in this regard are the work on creating a predictive in-silico model of mammalian cell cultures [Lam, Mantalaris, Pistikopoulos], and the studies on the production of monoclonal antibodies, aimed at the development of advanced models with experimental validation to be employed for optimal control [Kontoravdi, Pistikopoulos and Mantalaris].

Several works on the polymer and particulate sectors are with regard to batch operation. Another generic study on batch chemical manufacturing processes is on the optimal design and operation of batch distillation [Zahoor and Sorensen].

| Molecular Systems Engineering |

Overview

Molecular systems engineering focuses on the development of methods and tools for the design of better products and processes in applications where molecular interactions play a central role. By Molecular we refer to the development of predictive models that are built upon a fundamental understanding of the behaviour of functional materials, and which rely on physically meaningful parameters. The resulting models should incorporate the most up-to-date scientific knowledge and be accessible to non-experts. By Systems we refer to the development of techniques that are generic and can therefore be used to tackle problems in a range of applications. We place particular emphasis on the correct and efficient integration of models across different scales, so that molecular-level models can be used reliably at the larger scale of products and processes. By Engineering we refer to our focus on applications where the key issue is to achieve desired behaviour, be it optimal end-use properties for a product or optimal performance for a manufacturing process. We thus fully exploit the capabilities of our predictive models by using them not only to gain basic understanding but to solve industrially relevant problems. We have carried out some initial work in this area, such as the dynamic modelling of complex distillation columns using advanced thermodynamics, the design of solvents to enhance the solubility of complex organic molecules, and the design of optimal solvents and operating policies for batch separation in the agrochemicals industry.The combination of fundamental physical understanding, mathematical models, and numerical methods is the cornerstone of molecular systems engineering. It allows us to reduce our dependence on heuristics and rules-of-thumb which have traditionally been used to make models tractable but which have a limited validity and applicability. Furthermore, it allows us to obtain models which can be used for a wide range of scales and applications, ranging from hypothesis-testing to design. We have a coordinated research programme which involves the development of generic modelling and design tools, and the solution of key industrially relevant problems, using these generic tools.

Thus, the research programme is structured around two drivers:

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

The industrial problems are drawn from a wide range of sectors, including the polymer, pharmaceutical, agrochemicals and optoelectronics industries.

A major new project has recently been funded in which the team of investigators consists of three thermodynamicists, Amparo Galindo, George Jackson and Erich Müller, and three systems engineers, Claire Adjiman, Costas Pantelides and Stratos Pistikopoulos.

The investigators offer a unique integration of advanced thermodynamic techniques in process modelling and design. The team is well-versed in the terminology and methods used in diverse domains, and has developed a common vision. Functional molecules (such as surfactants, ionic liquids and solvents) and structured phases (such as crystalline materials, micelles and liquid crystals) are of immense industrial importance in areas ranging from the traditional chemical and petrochemical sectors to the personal care, pharmaceutical, agrochemical and biotechnology sectors. For example, surfactants are used in scale inhibitor squeeze treatments of oil fields, as well as in shampoo, pesticide and drug formulations. Whenever functional molecules and structured phases are involved, the consideration of molecular interactions becomes a fundamental element in the design of optimal products and processes. This has driven the molecular modelling and thermodynamics community to develop molecular models which relate structure to physical properties. These models are based on quantum mechanics, molecular mechanics, molecular and mesoscale simulations, group contribution methods, and equations of state. At the other end of the spectrum, there has been significant progress in the modelling and optimal design of manufacturing processes, based on mechanistic descriptions of bulk kinetics and heat and mass transfer phenomena.

Effects at smaller scales, such as mixing, can be taken into account through multiscale models that combine process models and computational fluid dynamics. The current best-practice for computer-aided product and process design builds on these advances. It is based first on an analysis of molecular interactions, exploring the choice of materials at the molecular scale, and second, on a transfer of this information to the macroscale through simplified thermodynamic models, which can be used to find the best process or product. Because of the sequential nature of this approach, the final design overlooks trade-offs between decisions at the molecular and process scales and is therefore very likely to be far from optimal. The large gap in information between the molecular scale and the macroscale has so far prevented the application of a more integrated design approach, which would optimise decisions at all scales based on a direct quantitative assessment of their effect on process or product performance. Recent attempts to bridge this 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. We will undertake a comprehensive effort to develop reliable techniques which work across the whole spectrum of scales, under the theme of Molecular Systems Engineering

| Biological Systems Engineering |

Overview

This area represents a multidisciplinary research group that has as its mission the advancement of an integrated systems engineering platform for the generation of solution strategies through the development of adaptive algorithms for the model-based design of experiments, prediction, control, and optimisation of complex biological and biomedical problems. Much of the work involves collaboration with Life Science groups at Imperial College and UCL. At UCL we collaborate with the Centre for Mathematics and Physics in the Life Sciences and Experimental Biology (CoMPLEX) on modelling physiological systems: on endothelial cells and in a DTI sponsored project entitled Vertical Integration of Biological Scales looking at multiscale approaches to modelling organs, in particular the liver.

The Biological Systems Engineering programme aims to enable the rationalisation and systematisation of the wide range of experimental data that is currently generated for specific biological and biomedical problems and will formulate models and solutions leading to advanced therapeutics and strategies with the ultimate goal of delivering personalised health care.

The research core consists of selected areas of specific biomedical and biopharmaceutical research and will be treated through the proposed integrative biological process systems approach. The following major areas of research are in progress with tangible clinical applications based on the scientific impact that this approach will have on the clinical deliverables:

Systems-assisted drug/gene therapy

Automated control applications in biomedicine have been in the limelight for a number of years. Automation of the drug delivery process can result in improved consistency of delivery and more effective therapy. The use of control engineering tools on biomedical drug delivery problems minimise the negative impact of side effects associated with the therapy while treating the disease.

Specific examples of the drug delivery systems include:

- insulin delivery to type 1 diabetic patients
- automatic regulation of haemodynamic variables
- delivery of chemotherapeutic agents in cancer
- modelling for cardiac assist devices

Model-based control and optimisation of mammalian cell cultures

A major challenge for the 21st century is the exploitation of biological expression systems for the production of valuable biopharmaceutical products, such as the production of monoclonal antibodies by mammalian cell cultures.

Currently, an exclusively experimental approach is employed and favoured by industry, which is largely empirical and relatively inefficient in terms of time and cost. Alternatively, predictive mathematical models could be applied, which, although they still come at a (fractional) cost in the form of validating experimentation, offer significant cost- and time-saving advantages, and can be implemented efficiently as part of a novel systematic approach to model development.

A new tightly integrated approach is being developed to handle the increasingly high throughput of biological information. This model development environment can be viewed as multiple computational interfaces linking the model validation data with the structural model building and experimental design, in an automated online, real-time fashion. By treating the process of model development as a systematic framework consisting of logical steps necessitating decision-making, it can be scrutinised and uncertainty controlled or ultimately removed. Ultimately this process can itself become subject to multi-objective optimisation; minimising some measure of development cost whilst simultaneously maximising the quality of the end product – the model.

Systems-assisted immune therapy optimal peptide tag design and synthesis of downstream protein processing

The overall aim of this project is to develop, and verify experimentally, a mathematical model based on mixed integer optimisation techniques for the design of peptide tags that optimise the purification steps for a target product protein. Physicochemical data such as net charge and hydrophobicity will be derived experimentally for each protein. Then a mathematical framework will be developed using the above data to determine the optimal peptide tag and sequence of chromatographic operations by applying a suitable performance criterion (eg. number of operations, purity, flowsheet cost). The applicability of the model will be demonstrated by constructing genetically the optimal peptide tags as fusions to the target protein, and then validate experimentally the effect on purification at each stage.

Modelling Endothelial cells

In conjunction with the Ludwig Institute for Cancer Research and the UCL Dept of Biochemistry this project aims to develop a multiscale model of the effects of blood flow on the function of endothelial cells. The model will embrace fluid flow, shape change of the cells causing a structural change in the cytoskeleton, which in turn affects the biochemical metabolism. Proteins are excreted which can cause arteriosclerosis.

| Biological Systems Engineering |

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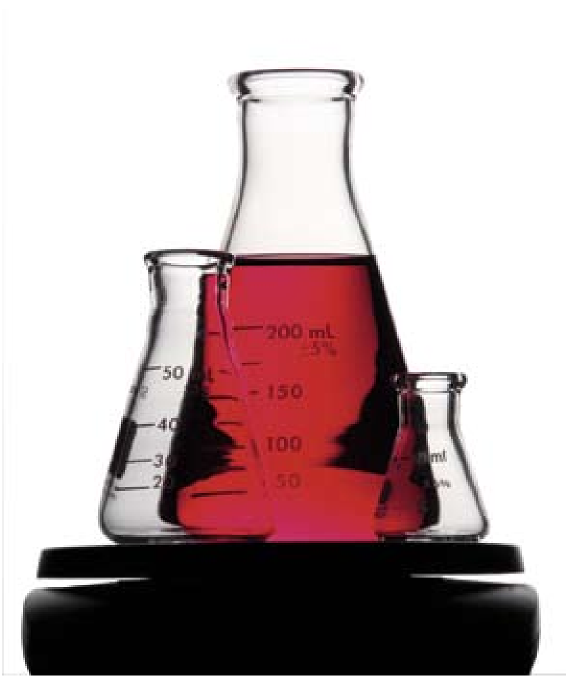
Vertical Integration of Biological Scales
(part of CoMPLEX at UCL)

David Bogle is a principal investigator with members of the Departments of Anatomy and Developmental Biology, Physiology, Computer Science, and Mathematics at UCL of this physiology modelling project, one of six DTI sponsored 'Beacon Projects' in their 'Harnessing Genomics' programme. The main aim of the UCL Beacon project is to build an in-silico model of the human liver. The aim of this work is three-fold:

- The construction of the model itself, which should allow the study of important liver diseases like diabetes.
- To study the effects of modelling across scales. The concept of scales refers to temporal scales: fast and slow processes, spatial scales: from cellular and sub-cellular processes up to the whole organ, and other heterogeneous processes such as the distinction between the hepatocytes that make up most of the liver and their interaction with blood and bile flow.
- To develop modelling tools and methodologies to tackle organ modelling projects.



| Supply Chains of the Future |

Overview

The activities in this area essentially address enterprise-wide and supply chain optimisation and management mainly for process industries. Supply chain problems can be organised into a three-level hierarchy:

- **Develop the right infrastructure** (assets and network) and set the right strategy – determine the best decision-making structure and associated parameters and targets (*strategic level*).
- **Plan optimally** – best resource allocation and inventory and capacity planning (*planning level*).
- **React quickly and appropriately** – scheduling and control (*operational level*). This also involves the design of effective control systems for localised, real-time management of the supply chain. Information modelling and information infrastructures are important here too.

Our approach is a model-based, systems one. This implies using abstraction and high-fidelity mathematical modelling together with powerful numerical methods appropriate to the class of problem to answer particular questions. The systems under investigation are very complex and there are many interactions and a large decision space. Decisions based on local logic or intuition are unlikely to be optimal, and systems approaches are best able to deal with the complexity of the issues involved. Our typical analysis of an existing or proposed new supply chain involves an overall, high level, supply chain-wide analysis initially to identify the main performance bottlenecks and then zooming in on the bottlenecks and identifying changes in operation or redesigns to alleviate them. From a modelling perspective, the optimal aggregation and segmentation of the supply chain is important – the objective being to ensure that relevant details are accounted for without burdening the models and algorithms with unnecessary detail.

There are two main types of supply chain model developed in our group: "analytical" and "simulation". Their application depends on the task in hand. Analytical models are used to optimise high-level decisions involving unknown configurations, taking an aggregate view of the dynamics and detail of operation (e.g. supply chain network design, medium term production and distribution planning). On the other hand, simulation models can be used to study the detailed dynamic operation of a fixed configuration under operational uncertainty, and can be used to evaluate expected performance measures for the fixed configuration to a high level of accuracy.

A special case of modelling is demand modelling. We have an ongoing activity in the development of mathematical models to describe product demands. These tend to perform much better than the standard techniques (e.g. exponential smoothing) that are available in most commercial software.

| Supply Chains of the Future |

(cont'd)

One of the key research challenges in developing a modelling framework (the abstraction and description of a physical entity using mathematical constructs) for supply chains is the need for a *hybrid* descriptive capability capturing both the "hard" physical aspects (e.g. manufacturing and logistics resources available, process recipes, etc.) and the "soft" business process aspects (e.g. how are replenishment decisions taken, by whom and using what logic?). In addition to models of systems, we also develop algorithmic machinery to manipulate the models, link the models to data, and obtain answers to questions.

In our case, these algorithmic techniques include:

- Statistical techniques to analyse supply chain data. Good examples are forecasting future product demands using historical data and extracting the important performance-influencing parameters for important assets in the supply chain.
- Advanced, low-discrepancy sampling techniques that allow us to predict the performance of a supply chain when some of its relevant data (e.g. future demands, distribution and processing times) are uncertain.
- Global sensitivity analysis of very complex systems. Global Sobol' analysis is a technique that can be used to rank different factors in a complex system in terms of their contribution to an overall performance measure (e.g. customer service level).
- Aggregation and decomposition techniques for large-scale optimisation under uncertainty. Whenever supply chain elements consider infrastructure investments, the lifetimes of the assets involved tend to exceed the life of the known data (e.g. product demands and prices).

An indicative list of recent projects is given below:

- **Hydrogen supply chains for the UK**
  Based on different future demand scenarios, a large-scale production-distribution model determines the type of production and storage facilities as well as transportation infrastructure. This project investigates in more detail whether centralised production and distribution of hydrogen is favoured over local production or in-situ reforming, and indeed what form the fuel should be distributed in.
- **Dynamic analysis of existing supply chains**
  This is important as it generates considerable insight about the relationship between policies/parameters and performance measures of the supply chain. Recently, a generic modelling approach has been developed, which captures physical and business processes. The above approach has successfully been applied to enhance the supply chain management for short-lifetime products.
- **Therapeutic product supply chains**
  This projects aims at improving the responsiveness these supply chains are notoriously slow processes and often need to deal with quickly changing demand scenarios. A three-stage procedure has been developed to devise an appropriate strategy and supporting infrastructure by developing potential scenarios, then devising a strategy that is robust against these and finally providing necessary infrastructure.
- **Capacity planning of global pharmaceutical networks**
  The problem under study is complicated by the high value-added nature of the products and varying tax regimes, which mean that simple regional manufacturing strategies are not necessarily optimal. A systematic optimisation-based framework has been developed to answer certain issues that supply chain managers usually face: allocation of the manufacturing of each product; production rates and inventory profiles in time; establishment of production distribution networks.
- **Supply chain planning for seasonal products**
  Paint products exhibit strongly seasonal demands. However, it is not economic to configure the supply chain for throughputs equivalent to peak demands. This places considerable strains on the supply chain while also providing opportunities to explore interesting trade-offs. This project will apply a holistic approach to paints supply chain optimisation. This includes the following steps: demand forecasting to support the prediction of annual product demands and seasonal dynamics, and production and inventory planning with batchsize optimisation. The supply chain plan is derived using forecast data, which is subject to some uncertainty. The robustness of the supply chain production plan may then be assessed using stochastic simulation/planning, and the plan may be updated if necessary.
- **Optimisation of vendor managed inventory systems**
  According to this new emerging class of supply chain policy, instead of having downstream nodes of the supply chain managing material stocks and issuing requests as necessary, a contract established between supply chain nodes with upstream nodes focussing on replenishment/manufacturing and downstream nodes concentrating on business/sales thus enhancing efficiency for both partners. Detailed and aggregate mathematical models have been developed for the distribution of products at various locations while an efficient rolling horizon solution algorithm has been developed, an important, emerging class of supply chain policy.

| Energy Systems Engineering |

Overview

Energy systems encompass everything from the primary energy source to the final energy service. For early humans this was a very simple system since the sun provided all our heat and light but once we discovered fire questions of fuel supply and quality rapidly became apparent. Since then our energy system has grown in complexity to include the many subsystems and components required to provide the basic energy services of heat, light, mechanical power and communication.
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. Our task in CPSE is to try and arrive at realistic integrated solutions to some of these problems by adopting a systems approach.

During 2006 CPSE has expanded its portfolio of energy systems related work by adding a number of projects oil and gas production, biofuels, fuel cells, electrical grids, and urban energy systems.

Oil and Gas Production: Separation of CO_2 from Natural Gas

Natural gas reserves containing large amounts of CO_2 (>50%) are not uncommon in the oil and gas industry and it is difficult to separate such quantities of CO_2 using conventional separation processes, such as amine-based absorption or membrane processes. By combining advanced thermodynamic models and advanced process modelling and optimisation tools, we have been able to propose a high-pressure absorption process using a novel alkane solvent. This involves simultaneously optimising the flowsheet structure, solvent molecular structure and operating conditions. Amongst the challenges that had to be overcome is 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. We are currently embarking on projects investigating how the CO_2 can be coupled with EOR in a general theme of using CO_2 as a reservoir fluid. On a related theme we have secured some funding from BCURA to investigate the process of post combustion capture of CO_2 with amine solvents.

Integrated clean production of Fossil Fuels: (part of the Energy Futures Lab at Imperial College London)

Oil, gas and coal will continue to provide a large fraction of our energy needs well into the middle of this century. Yet if fossil fuels are to play a full role in meeting the world's rapidly growing energy demands without continuing to produce high carbon emissions and the accompanying climate change impact, it is imperative that we develop radical new ways of producing and using these resources in a more sustainable manner. Most current solutions for reducing carbon emissions focus on the *use* of fossil fuels. Here we emphasise the huge potential impact of *cleaner production processes* and integrating into them much of the downstream processing. These new processes must be capable of upstream extraction of unwanted carbon, with minimal release of greenhouse gases, lead to step-increases in recovery factors from the current moderate values of 30-40% in clastic reservoirs and <20% in carbonates, greatly improve the overall utilization efficiency of the in situ energy source and exploit the benefits of integration of the entire processing chain, from latent energy source to the delivery of end use products, be these fuels, power, heat or petrochemicals. The broad vision and potential projects have been created during 2006 and industrial sponsorship has been secured to begin work on some aspects in October 2006. The initial theme focuses on CO_2 as a reservoir process fluid and involves the cradle to grave engineering of CO_2 from its generation and capture, through its use as a hydrocarbon recovery fluid, to its eventual geological sequestration.

Electric Grids: Signal analysis for power transmission systems

Following serious electrical power blackout incidents in 2003, policy makers in the European Union and the USA have highlighted (i) the need for improved a.c. transmission grid infrastructure and advanced control technologies, and (ii) the importance of emerging measurement-based technology towards achieving more secure operation. The aim is to create computational tools to exploit measurements from future high bandwidth fast SCADA and wide-area measurement systems, and to enhance situation awareness by converting the measurements into information about performance and operation. Recent work on measurement-based analyses for oil, gas and chemicals plants has pointed the way towards much better signal analysis for power transmission systems. A measurement-based approach will greatly extend the basic methods that are used at present and will lead to localization and real-time diagnosis of the root causes of threats to transmission system stability and actions to control the situation. A preliminary investigation has shown promising early results in this new project area.

Biofuels: The design and optimisation of bioprocesses for the production of bioethanol

New models and new solution techniques have been developed for the Jacaranda framework for automated design. This is work in progress and preliminary results were presented in Florence.

| Energy Systems Engineering |

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Fuel Cells: Systems Modelling, Analysis and Design of A ZEBRA Battery/Intermediate Temperature Solid Oxide Fuel Cell Hybrid for Automotive Applications

Electrical drive systems can be found in pure electric, hybrid electric and fuel cell (FC) vehicles. Their advantages include: zero emissions at point of use (for batteries or hydrogen fuelled FCs), fast acceleration, quiet operation, recuperation of regenerative energy from braking and high efficiency drive trains and energy conversion. However, battery-only vehicles are known to have limited range, slow recharge and lack of a recharging infrastructure. Hydrogen fuelled fuel cell vehicles also suffer from range and refuelling infrastructure limitations and from the need for a FC system that is large enough to hold the maximum power requirement, which may only be a small fraction of the drive cycle.
Models of the fuel cell and battery have been developed to simulate how each system performs in isolation, when exposed to vehicle operational conditions, as well as to inform on the best methods for operation of the hybrid system over a range of driving conditions and options for thermal integration.
A 1/10th scale 'bench top' system is currently being commissioned in order to demonstrate this hybrid strategy and for model validation.

Fuel Cells: Modelling and Analysis of Fuel Cells for Distributed Energy Systems

One of the characteristics of fuel cell systems is that their efficiency is nearly unaffected by size. This means that small, relatively high efficiency power plants can be developed, avoiding the high capital costs normally associated with large plants. Fuel cells are thus suited to distributed generation (DG), which is characterised by small, modular power systems that are sited at or close to the power demand source. However, while it is known that the operation of a Solid Oxide Fuel Cell (SOFC) system is normally subjected to frequent load changes due to variable power demand, its response and, in particular, its interaction with the distributed energy network, is not yet well known. Dynamic modelling is therefore essential for fuel cell systems design, as it allows the prediction of the cell response under transient conditions, and contributes to the definition of appropriate control strategies, not only necessary when load changes occur, but also during start-up or shutdown.

This interdisciplinary research project between the Fuel Cell Technology group and the CPSE in the Chemical Engineering Department, the Control & Power Group in the Electrical and Electronic Department, and the Environmental Policy & Management Group in the Environmental Science and Technology Department, has developed fuel cell models to be embedded in electrical distribution systems and enabling the assessment of their interaction with the electrical network as well as their environmental and economic impact in different system configurations and operational strategies.

Urban Energy Systems (part of the Energy Futures Lab at Imperial College London)

Urbanisation will characterise world population in the first half of this century. By 2030, the proportion of urban dwellers is expected to grow to around 80% in the most prosperous countries and to 60% globally. The pattern of future energy demand will be increasingly characterised by the network of the city, since solutions to the grave challenges faced by cities in a world of over 8 billion all have implications for urban energy systems. The resource flows inherited from 20th century cities are characteristically path-dependent and based on un-integrated discrete systems with many legacy technologies. Neither the data nor systems technology were available to realise the economies from process integration, two barriers now surmountable by cutting edge research and data handling technologies. As a consequence there is potential to deliver equivalent or better services in the world's cities at substantially reduced resource flows, with energy figures of merit certainly better than 20%, but may be as much as 50% or more.
2006 is the first year of an industrially funded project that focuses on systems and technologies across the whole field of engineering (civil, electrical, mechanical, materials and process engineering as well as communications and IT) appropriate to cities. In parallel it will look at business models for the realisation of innovative approaches in the urban context. It will combine systems analysis of the supply-side with detailed understanding of changes on the demand-side, including user-requirements and different patterns and cultures of consumption, thereby linking technological possibility with economic and social desirability in new business models. It will cover cities in all stages of development (mature, developing and new) but with special emphasis on those associated with large future energy consumption.

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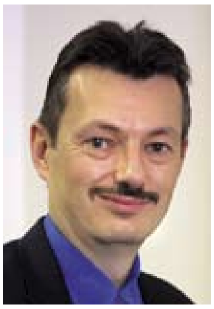

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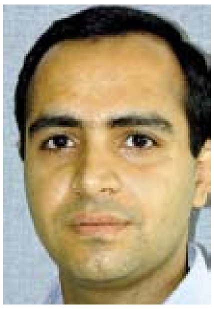

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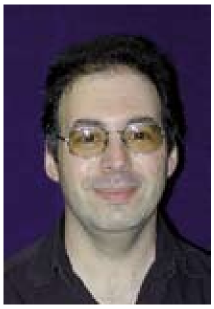

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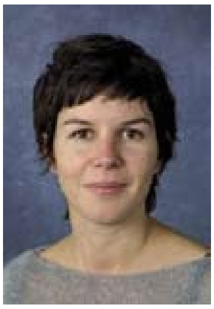

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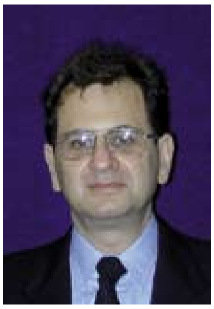

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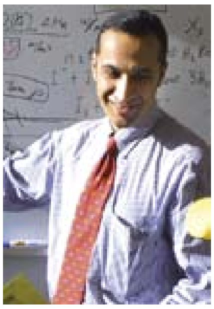

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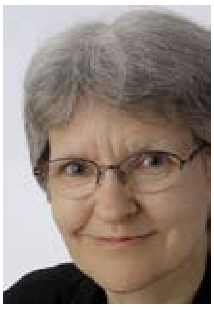

Professor N.F. Thornhill
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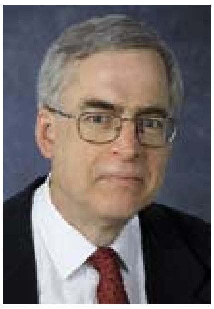


Professor Richard B Vinter
p.36

| CPSE Contributors 2006 |

| Personal Profiles |

Dr Claire S. Adjiman

Senior Lecturer in Chemical Engineering, Department of Chemical Engineering, Imperial College London.

Qualifications

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

Awards and Distinctions

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

Secondments

Process Systems Enterprise Ltd, September 2006-August 2007.

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 CO_2 capture, risk management). 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.

Other activities

AIChE: Technical area co-chair/chair for CAST10a, 2006-2007, IChemE: Treasurer of the Fluid Separations Subject Group, EPSRC: Member of Peer Review College. Member of organising committee for Distillation and Absorption 2006. Member of scientific committee for ESCAPE 16/PSE 2006.

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:

Denmark Technical University, IVC-SEP, Facultés Universitaires de Notre Dame de la Paix, Namur, Belgium, Theoretical Chemistry, Universidad Politecnica de Madrid, Department of Chemical Engineering, Warwick University, Department of Chemistry.

Industrial collaborations:

Britest, Ineos, PSE Ltd, Schlumberger, Syngenta

Professor Ian David Lockhart Bogle

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

Qualifications

BSc (Eng) Hons MSc PhD DIC

Awards and Distinctions

Fellow of the Royal Academy of Engineering, Fellow of the Institute of Chemical Engineers, 2006 IChemE Council Medal.

Research Interests

Numerical Global Optimisation Techniques for Process Design, Controllability Analysis, Nonlinear Systems, 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, Deputy Chair of European Federation of Chemical Engineers, Working Party on Computer Aided Process Engineering and UK representative, 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), Technical Programme Director 7th World Congress of Chemical Engineering July 2005, Member of International Programme Committee for16th European Symposia on Computer Aided Process Engineering (ESCAPE/PSE).

| Personal Profiles |

Professor Nigel Brandon

Shell Professor of Sustainable Development in Energy, Imperial College London.

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.

Research Interests

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

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, Associate Editor, ASME Journal of Fuel Cell Science and Technology, Grove Fuel Cell steering committee.

Dr Vivek Dua

Lecturer, Department of Chemical Engineering, University College London

Qualifications

PhD in Chemical Engineering, Imperial College London, MTech in Chemical Engineering, Indian Institute of Technology, Kanpur BE 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).

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, 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, IEEE Conference on Decision and Control (2004), European Control Conference (2005), European Symposium on Computer Aided Process Engineering and International Symposium on Process Systems Engineering (2006), Co-editor of Wiley-VCH Book Series on Process Systems Engineering, Acted as session chair of the session on Systems Biology at the 7th World Congress of Chemical Engineering (2005), Glasgow and 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.

Research Interests

Optimal Configuration of Artificial Neural Networks, Stability Analysis of Nonlinear Model Based Controllers, Controlled Release of Drugs, Drug Discovery.

Academic Collaborations

Eastman Dental Institute, UCL

| Personal Profiles |

Professor E. S. Fraga

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

Qualifications

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

Research interests

Nonlinear optimisation, Visualisation and data analysis, Engineer-computer interfaces, Distributed and parallel computing.

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.

Dr Amparo Galindo

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

Qualifications

PhD in Physical Chemistry, University of Sheffield. Thesis title: “Prediction of the phase equilibria of associating systems using the SAFT approach”, BSc Chemistry, Universidad Complutense de Madrid (Spain).

Awards and distinctions:

EPSRC Advanced Research Fellow (2000-2005), ExxonMobil Teaching Fellow (2005-2009).

Other activities:

Referee for Fluid Phase Equilibria, Molecular Physics, Industrial and Engineering Chemistry Research, Journal of Chemical Physics, Journal of Physical Chemistry B, AIChE Journal, Indian Journal of Pure and Applied Physics and Journal of Molecular Liquids. Member of the peer review college of the Engineering and Physical Sciences Research Council (EPSRC). Associate Member of the Royal Society of Chemistry.

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.

| Personal Profiles |

Dr. 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).

Awards and Distinctions

University of Delaware Competitive Fellowship (2001-2002), Robert L. Pigford Teaching Assistant Award from the University of Delaware (2001).

Research interests

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

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, Georgia Institute of Technology, USA.

Industrial collaboration

ICI (on-going joint project), BASF (on-going joint project).

Professor George Jackson

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

Qualifications

BSc DPhil FRSC CChem.

Awards

Chelsea Final Year Prize (1983), McGhie Prize (1982), Nicolet Instruments Prize (1981), BSc Chemistry, 1st Class Chelsea College, University of London. DPhil in Physical Chemistry, Exeter College, University of Oxford. Supervisor, Sir John S. Rowlinson FRS.

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: 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. We have recently formed the Molecular Systems Engineering (MSE) Group in which we are seeking to incorporate advanced thermodynamics modelling in process design and optimisation.

We also have an established international reputation 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.

| Personal Profiles |

Dr Imad M Jaimoukha

Senior Lecturer in Electrical Engineering, Imperial College London.

Qualifications

BSc, Electrical Engineering, University of Southampton,1983,
MSc, Control Engineering, Imperial College London,1986,
PhD, Control Systems, Imperial College London, 1990

Research Interests

Robust controller design for structured and unstructured uncertainties, Controller reduction, Model reduction for large-scale systems, Hierarchical optimization in robust controller design, Robust control design for power systems.

Other Activities

Reviewer for IEE Transactions on Automatic Control, European Journal of Control, International Journal of Control, Journal of Economic Dynamics and Control Automatica.

Dr J. Krishnan

Lecturer, Department of Chemical Engineering, Imperial College London.

Qualifications

PhD

Work Experience

Associate Research Scientist, Dept. of Electrical Engg, Johns Hopkins University, 2001-2005

Awards and Distinctions

Excellence in Teaching, Engg Council, School of Engineering and Applied Science, Princeton University, 1997.

Patel Fellowship, Dept. of Chemical Engg, Princeton University, 1994-96.

Research Interests

Mathematical and computational modelling of cellular processes Systems biology, Non-linear dynamics and pattern formation in physico-chemical and biological systems.

Other Activities

Reviewer: IEEE Transactions in Automatic Control,
Journal of Theoretical Biology.

| Personal Profiles |

Professor 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, 1998.

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.

Other activities

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

Dr Athanasios Mantalaris

Lecturer, Department of Chemical Engineering, Imperial College London.

Qualifications

PhD in Chemical Engineering, University of Rochester, U.S.A. BSc (Hons) Biochemistry, UWO, Canada.

Research Interests

My research interests lie in the areas of stem cell bioprocessing, tissue engineering and mammalian cell bioprocessing.

| Personal Profiles |

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

Dr Lazaros Papageorgiou

Reader, Department of Chemical Engineering, University College London.

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.

Other Activities

Reviewer for Industrial and Engineering Chemistry Research, Computers and Chemical Engineering, Chemical Engineering Research and Design, Chemical Engineering Science, Applied Thermal Engineering, Chemical Engineering Communications AIChE Journal, FOCAPO 2003, Member of IChemE CAPE Subject Group Committee.

| Personal Profiles |

Professor Efstratios N Pistikopoulos

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

Qualifications

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

Awards and Distinctions

ICI/Royal Academy of Engineering Fellowship, FIChemE.

Research Interests

(i) theory, algorithms and computational tools for continuous and integer parametric programming, (ii) advanced model based control and its biomedical and industrial applications and (iii) energy and the environment – sustainable process development.

Other activities

Co-Editor, Book Series in Process Systems Engineering, Wiley-VCH, 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, Invited Member, Computer Aided Process Engineering (CAPE) Working Party, European Federation of Chemical Engineers, Member of the Advisory Scientific Committee, European Enterprise Institute (EPP-ED Association).

Professor Berc Rustem

Professor, Department of Computing, Imperial College London.

Qualifications

FIMA, CMath.

Awards and Distinctions

President of Society of Computational Economics, 2002-04, Editor: Automatica, Computational Management Science.

Research Interests

Deterministic and Stochastic Optimisation and Algorithms; Worst-case design; Risk management.

| Personal Profiles |

Professor Paul Rutter

Industrial Relation Consultant, Department of Chemical Engineering, Imperial College London.

Qualifications

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

Industrial Experience

The Boots Company Oct.1971 – Mar. 1973, Unilever Research Mar.1973-Sept 1979., BP Jun 1980 – retired Dec 2002.

Research Interests

The impact of Climate Change on industrial infrastructure. The development of urban energy systems.

Committees etc.

Member of Royal Society of Chemistry Energy Policy working group, Evaluation Panel member for the EU 6th Framework Programme Thematic call "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), Institute of Chemical Engineering Research Committee, WBC Sustainable Development technology and innovation member (1997-1999), IEA GHG R & D programme executive committee member (1998 –2002), Secretary European Production Engineering Association (1996,1997), Chair I Chem. E Sustainability Think Tank (1998-1999).

Management

Research team leader in Unilever; 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.

Professor 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 Journal of Optimization Theory and Applications, Computers and Chemical Engineering, Trans. I Chem.E, Operations Research.

| Personal Profiles |

Professor 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, Supply chain and enterprise optimization, Planning and scheduling.

Other activities

Director of Process Systems Enterprise Ltd, Director of Ashe Morris Ltd, Director of Britest Ltd, Defra panel member, EPSRC college member, IChemE transactions editorial board member Scientific committee member for World Congress in Chemical Engineering.

Reviewer for:

AIChE Journal, Chemical Engineering Research and Design Computers & Chemical Engineering, Chemical Engineering Science, A-Star research council (Singapore).

Academic Collaborations

University College London, Department of Chemical Engineering Newcastle and Strathclyde Universities, CPACT, Georgia Institute of Technology, iCPSE, Tsinghua University, Clean Energy Centre.

Industrial collaboration

Ashe Morris (*Novel reactor modeling and experimentation*), BP (*Urban Energy Systems Project*), ICI (*Supply chain management under uncertainty*), Ineos (*Supply chain study*), Shell (*H2-CO_2 project*), Syngenta (Supply chain network design).

Dr Eva Sørensen

Reader in Chemical Engineering, Department of Chemical Engineering, University College London.

Qualifications

MSc in Chemical Engineering (NTNU, Norway), PhD in 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 separation processes, e.g. distillation, membrane separation, chromatography and hybrids thereof, Optimal separation process selection, Optimal process design, operation and control.

Other Activities

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

Academic collaboration

University College London, Department of Biochemical Engineering.

Industrial collaboration

BP, UK.

| Personal Profiles |

Professor N.F. Thornhill

Professor of Control Systems, Department of E&E Engineering, University College London.

Qualifications

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

Awards and Distinctions

Fellow of the IChemE, Fellow of the IEE, Honorary Professorial Research Fellow, Imperial College London Winner of the Journal of Process Control Best Paper Award in the category *methodology/ theory* for the period 2002 to 2005 for: Thornhill, N.F., Huang, B., and Zhang, H., 2003, Detection of multiple oscillations in control loops, *Journal of Process Control*, 13, 91-100.).

Secondments

Royal Academy of Engineering Global Research Award with ABB Corporate Research, Norway, April-Sept 2005. Project title: *Detection and diagnosis of distributed disturbances*.

Research interests

Process data analysis, Detection and diagnosis of plant-wide disturbances, Controller performance assessment.

Other activities

IEE: Executive Team Member for Control & Automation PN IChemE: Co-opted member of Process Management & Control Subject Group. EPSRC: Member of Peer Review College Technical Area Co-chair for Dycops-2004 Conference. Member of the International Editorial Board of the Journal of Process Control.

Reviewer for

AIChE Journal, Automatica, Canadian Journal of Chemical Engineering, Chemical Engineering Research and Design Chemometrics and Intelligent Laboratory Systems, Computers & Chemical Engineering, Control Engineering Practice (Designated editor), IEE Proceedings D, IEEE Transactions on Control Systems Technology, IEEE Transactions on Industrial Electronics Industrial and Engineering Chemistry Research, International Journal of Control, Journal of Adaptive Control and Signal Processing, Journal of Process Control.

Academic Collaborations

Imperial College London, Department of Electrical and Electronic Engineering, University of Alberta, Department of Chemical and Materials Engineering, University of Glasgow, Department of Mechanical Engineering, University of Cardiff Business School.

Industrial collaboration

ABB Corporate Research (*six month placement, sponsored research and co-authored papers*) Eastman Chemical Company (*co-authored papers*).

Professor Richard B Vinter

Professor of Control Theory, Department of Electrical 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.

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 of IMA Journal of Mathematical Control and Information, Associate Editor of Journal of Applied Mathematics and Computation, Associate Editor of Journal of Set Valued Analysis.

| CPSE Academics |

Imperial College London

Department of Chemical Engineering

Roger Sargent
Stratos Pistikopoulos
Nilay Shah
Costas Pantelides
Claire Adjiman
Charles Immanuel
George Jackson
Amparo Galindo
Sakis Mantalaris
J Krishnan
Geoff Maitland

Department of Electrical Engineering

Richard Vinter
Imad Jaimoukha
Martin Clark
John Allright

Department of Computing

Berc Rustem

Department of Earth Science & Engineering

Nigel Brandon

Visiting Professors

Paul Rutter
Roger Benson
John Perkins

University College London

Department of Chemical Engineering

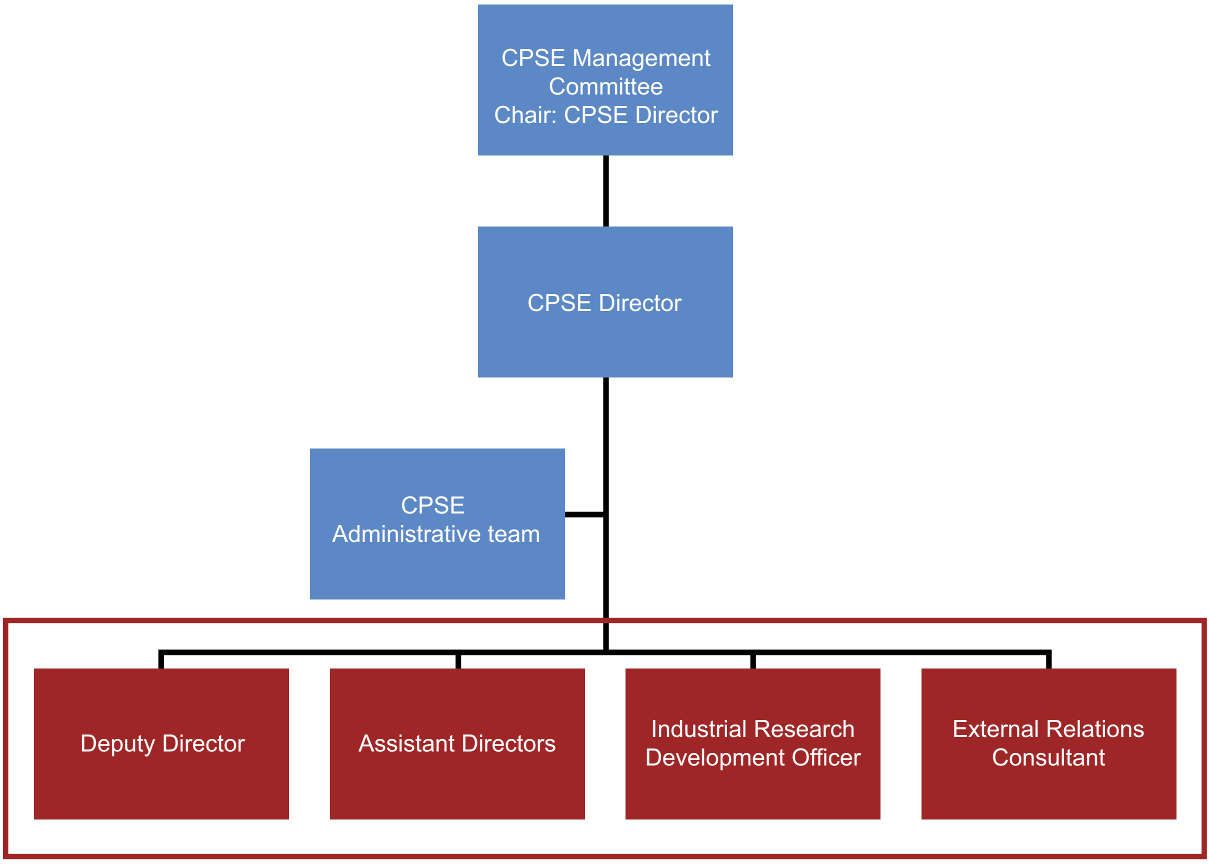
David Bogle
Eric Fraga
Lazaros Papageorgiou
Eva Sorensen
Vivek Dua

Department of Electrical Engineering

Nina Thornhill

| CPSE Management Structure Organisational Chart |

The following figure shows the management structure of CPSE. The Centre's director chairs the CPSE management Committee and also the CPSE management team meetings.



CPSE Management Team

| List of Publications |

Aguiar P, Adjiman CS, Brandon NP, **Anode-supported intermediate-temperature direct internal reforming solid oxide fuel cell - II. Model-based dynamic performance and control**, Journal of Power Sources, 2005, Vol: 147, Pages: 136 - 147, ISSN: 0378-7753

Algusane TY, Proios P, Georgiadis MC, et al , **A framework for the synthesis of reactive absorption columns**, Chemical Engineering and Processing, 2006, Vol: 45, Pages: 276 - 290, ISSN: 0255-2701

Allen R., Bogle I.D.L., and Ridley A. (2006) **Modelling morphological change in endothelial cells induced by shear stress**. In Proc. PSE2006, Garmisch-Partenkirchen ed. W.Marquardt and C.C. Pantelides, Elsevier.

Anaparthi K, Chaudhuri B, Thornhill NF and Pal B, **Coherency identification in power systems through principal component analysis**, IEEE Transactions on Power Systems, 2005, Vol: 20, Pages: 1658-1660, ISSN: 0090-6778

Barakat T, and Sørensen E, (2005), **Optimal synthesis and design of hybrid batch separation processes**, in *Proc. 7th World Congress of Chemical Engineering, Glasgow, 10-14 July*.

Barakat, T.M. and Sørensen E, (2005), **Optimal configuration, design and operation of hybrid batch distillation/ pervaporation processes**, presented at AIChE 2005 Annual meeting, Cincinnati, paper 445d.

Behzadi B, Ghotbi C, Galindo A, **Application of the simplex simulated annealing technique to nonlinear parameter optimization for the SAFT-VR equation of state**, Chemical Engineering Science, 2005, Vol: 60, Pages: 6607 - 6621, ISSN: 0009-2509

Behzadi B, Patel BH, Galindo A, et al , **Modeling electrolyte solutions with the SAFT-VR equation using Yukawa potentials and the mean-spherical approximation**, Fluid Phase Equilibria, 2005, Vol: 236, Pages: 241 - 255, ISSN: 0378-3812

Bezzo F, Macchietto S, Pantelides CC, **Computational issues in hybrid multizonal/computational fluid dynamics models**, AIChE Journal, 2005, Vol: 51, Pages: 1169 - 1177, ISSN: 0001-1541

Black L, Breen C, Yarwood J, Phipps J, and Maitland G, ***In situ* Raman analysis of hydrating C3A and C4AF pastes in presence and absence of sulphate**, Advances in Applied Ceramics, 105, 209-216 (2006)

Black L, Breen C, Yarwood J, Deng CS, Phipps J, and Maitland G, Mater J, **Hydration of tricalcium aluminate (C3A) in the presence and absence of gypsum – studied by Raman spectroscopy and X-ray diffraction**, Chem., 16, 1263-1272 (2006)

Bogle I.D.L. and Ydstie B.E. (2006) **Model based process equipment design**. In Computer Aided Process and Product Engineering. Ed. L. Puigjaner and G Heyen. Elsevier

Bogle IDL, Dunger R, Estaba R (2005) **A systems approach to identifying added value in oil supply chain companies**. In Proc 7th World Congress of Chemical Engineering Paper C12-003

Bogle IDL, Li L, Saffrey P, Hetherington J, Margoninski O, Wright RJ, Fernandez M, Finkelstein A, Callard R, Seymour R, Horton R, Warner A, (2005) **Addressing the challenges of multiscale model management in systems biology**. In Proc 7th World Congress of Chemical Engineering Paper P30-004

Bogle IDL, Cipollina A., Micale G. (2006) **Dynamic Modelling tools for solar powered desalination processes during transient operations**. In Proc NATO Advanced Workshop, Hammarmet Tunisia, 2006. ed. L. Rizzuti.

Cameron IT, Wang FY, Immanuel CD, et al , **Process systems modelling and applications in granulation: a review**, Chemical Engineering Science, 2005, Vol: 60, Pages: 3723 - 3750, ISSN: 0009-2509

Casas-Lisa J, Pinto JM and Papageorgiou LG, **“An MINLP Approach for the Cyclic Scheduling of Multiproduct Plants under Performance Decay”**, 7th World Congress of Chemical Engineering (accepted).

Casas-Lisa J, Pinto JM and Papageorgiou LG, **“Mixed Integer Optimization for Cyclic Scheduling of Multiproduct Plants under Exponential Performance Decay”**, Chem. Eng. Res. Des.(accepted).

Chan S, Sørensen E, and Titchener-Hooker N, (2005), **Modelling chromatographic processes – The good, the bad and the ugly**, in *Proc. 7th World Congress of Chemical Engineering*, Glasgow, 10-14 July.

Chan S, Sørensen E, Titchener-Hooker N, (2005), **Optimal economic design and operation of single and multi-column chromatographic processes**, presented at AIChE 2005 Annual meeting, Cincinnati, paper 79f.

Choudhury MAAS, Thornhill NF and Shah SL, **Modelling valve stiction**, Control Engineering Practice, 2005, Vol: 13, Pages: 641-658, ISSN: 0967-0661.

Colston S.L, Barnes P, Jupe A.C, Jacques S.D.M, Hall C, Lovesey P, Dransfield J, Meller N, and Maitland GC, **An in situ synchrotron enery-dispersive diffraction study of the hydration of oilwell cement systems under high temperature/autoclave conditions up to 130 oC**, Cement and Concrete Research, 35, 2223-2232 (2005)

Couillet I, Hughes TL, Maitland GC, Candau F, **Synergistic effects of aqueous solutions of mixed wormlike micelles and hydrophobically modified polymers**, Macromolecules, 38, 5271-5282 (2005)

| List of Publications |

Croce V, Cosgrove T, Dreiss CA, King S, Maitland GC, and Hughes TL, **Giant Micellar Worms Under Shear: A Rheological Study Using SANS**, Langmuir, 21, 6762-6768 (2005)

Dartnell L, Simeonidis E, Hubank M, Tsoka S, Bogle IDL and. Papageorgiou LG, **Robustness of the p53 network and biological hackers** • SHORT COMMUNICATION *FEBS Letters, Volume 579, Issue 14, 6 June 2005, Pages 3037-3042*

Dartnell L, Simeonidis E, Hubank M, Tsoka S, Bogle IDL, and L.G. Papageorgiou, **"Robustness of the p53 Network and Biological Hackers"**, *FEBS Letters,* 579, 3037-3042 (2005).

Day GM, Motherwell WDS, Ammon HL, et al , **A third blind test of crystal structure prediction, Acta Crystallographica Section** B-Structural Science, 2005, Vol: 61, Pages: 511 - 527, ISSN: 0108-7681

del Rio EM, Galindo A, de Miguel E, **Density functional theory and simulation of the columnar phase of a system of parallel hard ellipsoids with attractive interactions (Article no.051707)**, Physical Review E, 2005, Vol: 72, Pages: 1 - 12, ISSN: 1539-3755

Dua P, Pistikopoulos EN, **Modelling and control of drug delivery systems**, Computers & Chemical Engineering, 2005, Vol: 29, Pages: 2290 - 2296, ISSN: 0098-1354

Emanuelsson EAC, Baptista IIR, Mantalaris A, et al, **Strain stability in biological systems treating recalcitrant organic compounds**, Biotechnology and Bioengineering, 2005, Vol: 92, Pages: 843 - 849, ISSN: 0006-3592

Folic M, Adjiman CS, Pistikopoulos EN, **A computer-aided methodology for optimal solvent design for reactions with experimental verification**, European Symposium on Computer-Aided Process Engineering-15, Elsevier Science Bv, 2005, Pages: 1651 - 1656, ISBN: 0-4445-1987-4

Folic M, Adjiman CS, Pistikopoulos EN, **A computer-aided methodology for optimal solvent design for reactions with experimental verification**, European Symposium on Computer-Aided Process Engineering-15, Elsevier Science Bv, 2005, Pages: 1651 - 1656, ISBN: 0-4445-1987-4

Georgiadis MC, Levis AA, Tsiakis P, Sanidiotis I, Panteldies CC, and Papageorgiou LG, **"Optimisation-based Scheduling: A Discrete Manufacturing Case Study"**, *Comput. Ind. Eng.*, 49, 118-145 (2005).

Gjerdrum J, Samsatli NJ, Shah N, and Papageorgiou LG, **"Optimisation of Policy Parameters in Supply Chain Applications"**, *International Journal of Logistics: Research and Applications*, 8, 15-36 (2005).

Gloor GJ, Jackson G, Blas FJ, et al , **Test-area simulation method for the direct determination of the interfacial tension of systems with continuous or discontinuous potentials (Article no.134703)**, Journal of Chemical Physics, 2005, Vol: 123, Pages: 1 - 19, ISSN: 0021-9606

Hetherington J, Saffrey P, Margoninski O,.Bogle IDL, Li L, Rey MV, Yamaji S, Baigent S, Ashmore J, Page K, Seymour R, Finkelstein A, Warner A, (2006) **Addressing the challenges of multiscale model management in systems biology**. Comput chem. Engng in press

Huang B, Ding SX and Thornhill NF, **Alternative solutions to multivariate control performance assessment problems**, Journal of Process Control, 2006, Vol: 16, Pages: 457-471, ISSN: 0959-1524.

Huang B, Ding SX and Thornhill NF, **Practical solutions to multivariate feedback control performance assessment problem: reduced a-priori knowledge of interactor matrix**, Journal of Process Control, 2005, Vol: 15, Pages: 573-583, ISSN: 0959-1524.

Hugo A, Pistikopoulos S, **Long-range process planning under uncertainty via parametric programming**, European Symposium on Computer-Aided Process Engineering-15, Elsevier Science Bv, 2005, Pages: 127-132, ISBN: 0-4445-1987-4

Hugo A, Rutter P, Pistikopoulos S, et al , **Hydrogen infrastructure strategic planning using multi-objective optimization**, International Journal of Hydrogen Energy, 2005, Vol: 30, Pages: 1523 - 1534, ISSN: 0360-3199

Immanuel CD, Doyle FJ, **Solution technique for a multi-dimensional population balance model describing granulation processes**, Powder Technology, 2005, Vol: 156, Pages: 213 - 225, ISSN: 0032-5910

Iora P, Aguiar P, Adjiman CS, et al, **Comparison of two IT DIR-SOFC models: impact of variable thermodynamic, physical, and flow properties. Steady-state and dynamic analysis**, Chemical Engineering Science, 2005, Vol: 60, Pages: 2963 - 2975, ISSN: 0009-2509

Jaimoukha IM, El-Zobaidi H, Limebeer DJN, et al , **Controller reduction for linear parameter-varying systems with a priori bounds**, Automatica, 2005, Vol: 41, Pages: 273 - 279, ISSN: 0005-1098

Johnson DB, Bogle IDL (2006) **Handling Uncertainty in the Development and Design of Chemical Processes**, Reliable Computing, vol.12, issue 6, pp. 409-426.

| List of Publications |

Karamertzanis PG, Pantelides CC, **Ab initio crystal structure prediction - I. Rigid molecules**, Journal of Computational Chemistry, 2005, Vol: 26, Pages: 304 - 324, ISSN: 0192-8651

Kontoravdi C, Asprey SP, Pistikopoulos EN, et al , **Application of global sensitivity analysis to determine goals for design of experiments: An example study on antibody-producing cell cultures**, Biotechnology Progress, 2005, Vol: 21, Pages: 1128 - 1135, ISSN: 8756-7938

Kontoravdi C, Asprey SP, Pistikopoulos S, et al , **Dynamic model of MAb production and glycosylation for the purpose of product quality control**, European Symposium on Computer-Aided Process Engineering-15, Elsevier Science Bv, 2005, Pages: 307 - 312, ISBN: 0-4445-1987-4

Kosmidis VD, Perkins JD, Pistikopoulos EN, **A mixed integer optimization formulation for the well scheduling problem on petroleum fields**, Computers & Chemical Engineering, 2005, Vol: 29, Pages: 1523 - 1541, ISSN: 0098-1354

Koutinas M, Martin J, Peeva LG, et al , **An oil-absorber-bioscrubber system to stabilize biotreatment of pollutants present in waste gas. Fluctuating loads of 1,2-dichloroethane**, Environmental Science & Technology, 2006, Vol: 40, Pages: 595 - 602, ISSN: 0013-936X

Lakhdar K, Farid S, Savery J, Titchener-Hooker NJ, and Papageorgiou LG, **"Medium term planning of biopharmaceutical manufacture under uncertainty"**, PSE/ Escape-16 conference (submitted).

Lakhdar K, Zhou Y, Savery J, Titchener-Hooker NJ, and Papageorgiou LG, **"Medium Term Planning of Biopharmaceutical Manufacture using Mathematical Programming"**, *Biotechnology Progress*, 21, 1478-1480 (2005).

Lakhdar K, Zhou YH, Savery J, Titchener-Hooker NJ and Papageorgiou LG, **"Medium term production planning of biopharmaceutical manufacturing facilities"**, 7th World Congress of Chemical Engineering (accepted).

Levis AA, and Papageorgiou LG, **"Customer Demand Forecasting via Support Vector Regression Analysis"**, *Chem. Eng. Res. Des.*, 83, 1009-1018 (2005).

Low K.H. and Sørensen E, (2005), **Simultaneous optimal configuration, design and operation of batch distillation**, AIChE J., 51(6), 1700-1713.

Maitland GC, **Transforming 'formulation': systematic soft materials design**, Soft Matter, 1, 93-94 (2005)

Manthanwar AA, Sakizlis V, Pistikopoulos EN, **Robust parametric predictive control design for polytopically uncertain systems**, American control conference 2005 (ACC), 08-10 June 2005, Portland, New York, IEEE, 2005, Pages: 3994 - 3999, ISBN: 0-7803-9098-9

Oulton RF, Adjiman CS, Handa K, et al , **Enhancement of optical extraction from OLEDs using scattering layers**, In: Grote JG, Kaino T, Kajzar F, editor, Conference on organic photonic materials and devices VII, San Jose, CA, 24 - 26 January 2005, Bellingham, Spie-Int Society Optical Engineering, 2005, Pages: 191 - 201, ISBN: 0-8194-5698-5

Pagliarani A, Kenyon A J, Thornhill N F, Sirisena E, Lee K and Law VJ, **Process harmonic pulling in a RIE plasma-tool**, Electronics Letters, 2006, Vol: 42, Pages: 120-121, ISSN: 0013-5194.

Panoskaltsis N, Mantalaris A, Wu JHD, **Engineering a mimicry of bone marrow tissue *ex vivo***, Journal of Bioscience and Bioengineering, 2005, Vol: 100, Pages: 28 - 35, ISSN: 1389-1723

Papamichail I, Adjiman CS, **Proof of convergence for a global optimization algorithm for problems with ordinary differential equations**, Journal of Global Optimization, 2005, Vol: 33, Pages: 83 - 107, ISSN: 0925-5001

Patel B.H, Docherty H, Varga S, Galindo A, and Maitland GC, **Generalized equation of state for square-well potentials of variable range Molec**. Phys., 103(1), 129-139 (2005)

Patsiatzis DI, Xu G, and Papageorgiou LG, **"Layout Aspects of Pipeless Batch Plants"**, Ind. Eng. Chem. Res., 44, 5672-5679 (2005).

Peleties F, Trusler JPM, Goodwin ARH, and Maitland GC, **Circulating pump for high-pressure and high-temperature applications**, Rev. Scientific Instruments, 76, 1-3 (2005)

Pinto MA, Immanuel CD, **Model of population heterogeneity and metabolic regulation in bioreactors**, American control conference 2005 (ACC), 08-10 June 2005, Portland, OR, New York, IEEE, 2005, Pages: 931 - 936, ISBN: 0-7803-9098-9

Proios P, Goula NF, Pistikopoulos EN, **Generalized modular framework for the synthesis of heat integrated distillation column sequences**, Chemical Engineering Science, 2005, Vol: 60, Pages: 4678 - 4701, ISSN: 0009-2509

Proios P, Pistikopoulos EN, **Generalized modular framework for the representation and synthesis of complex distillation column sequences**, Industrial & Engineering Chemistry Research, 2005, Vol: 44, Pages: 4656 - 4675, ISSN: 0888-5885

| List of Publications |

Purdy KR, Varga S, Galindo A, et al , **Nematic phase transitions in mixtures of thin and thick colloidal rods (Article no. 057801)**, Physical Review Letters, 2005, Vol: 94, ISSN: 0031-9007

Repke, J.-U.; Klein, A.; Bogle, D.; Wozny, G. (2006) **"Pressure Swing Batch Distillation for Homogeneous Azeotropic Separation**, in Proc. Distillation and Absorption 2006, London, IChemE.

Roe B, Papageorgiou LG, and N. Shah, **"A Hybrid MILP/CLP Algorithm for Multipurpose Batch Process Scheduling"**, *Comput. Chem. Eng.*, 29, 1277-1291 (2005).

Roe B, Papageorgiou LG, Shah N, **A hybrid MILP/CLP algorithm for multipurpose batch process scheduling**, Computers & Chemical Engineering, 2005, Vol: 29, Pages: 1277 - 1291, ISSN: 0098-1354

Ryu JH, Pistikopoulos EN, **Design and operation of an enterprise-wide process network using operation policies. 1. Design**, Industrial & Engineering Chemistry Research, 2005, Vol: 44, Pages: 2174 - 2182, ISSN: 0888-5885

Safinia L, Blaker JJ, Maquet V, et al , **Characterisation of 'wet' polymer surfaces for tissue engineering applications: are flat surfaces a suitable model for complex structures? (Article no. 010)**, E-Polymers, 2005, ISSN: 1618-7229

Safinia L, Datan N, Hohse M, et al , **Towards a methodology for the effective surface modification of porous polymer scaffolds**, Biomaterials, 2005, Vol: 26, Pages: 7537 - 7547, ISSN: 0142-9612

Sakizlis V, Perkins JD, Pistikopoulos EN, **Explicit solutions to optimal control problems for constrained continuous-time linear systems**, Iee Proceedings-Control Theory and Applications, 2005, Vol: 152, Pages: 443 - 452, ISSN: 1350-2379

Shah N, **Process industry supply chains: advances and challenges**, Computers & Chemical Engineering, 2005, Vol: 29, Pages: 1225 - 1235, ISSN: 0098-1354

Sheldon TJ, Adjiman CS, Cordiner JL, **Pure component properties from group contribution: hydrogen-bond basicity, hydrogen-bond acidity, Hildebrand solubility parameter, macroscopic surface tension, dipole moment, refractive index and dielectric constant**, Fluid Phase Equilibria, 2005, Vol: 231, Pages: 27 - 37, ISSN: 0378-3812

Sheldon TJ, Folic M, Adjiman CS, **Solvent design using a quantum mechanical continuum solvation model**, Industrial & Engineering Chemistry Research, 2006, Vol: 45, Pages: 1128 - 1140, ISSN: 0888-5885

Sidoli FR, Mantalaris A, Asprey SP, **Toward global parametric estimability of a large-scale kinetic single-cell model for mammalian cell cultures**, Industrial & Engineering Chemistry Research, 2005, Vol: 44, Pages: 868 - 878, ISSN: 0888-5885

Simeonidis E, and Papageorgiou LG, **"A Mixed Integer Optimisation Approach to Lattice Protein Folding"**, PSE/ Escape-16 conference (submitted).

Simeonidis E, Dartnell L, Bogle IDL, and Papageorgiou LG, **"Analysis of Biochemical Networks using Linear Programming"**, 7th World Congress of Chemical Engineering (accepted).

Simeonidis E, Dartnell LR, Bogle IDL, Papageorgiou LG, (2005) **Analysis of biochemical networks using linear programming**. In Proc 7th World Congress of Chemical Engineering Paper P30-008

Simeonidis E, Pinto JM, and Papageorgiou LG, **"An MILP Model for the Optimal Design of Purification Tags and Synthesis of Downstream Protein Processing"**, ESCAPE-15 Conference, ESCAPE-15 Conference, L. Puigjaner and A. Espuna (editors), 1537-1542 (2005).

Simeonidis E, Pinto JM, Lienqueo ME, Tsoka S and Papageorgiou LG, **"MINLP Models for the Synthesis of Optimal Peptide Tags and Downstream Protein Processing"**, *Biotechnol. Prog.*, 21, 875-884 (2005).

Sousa RT, Shah N, and Papageorgiou LG, **"Global Supply Chain Network Optimization for Pharmaceuticals"**, ESCAPE-15 Conference, L. Puigjaner and A. Espuna (editors), 1189-1194 (2005).

Stefansson H, Shah N, **Multi-scale planning and scheduling in the pharmaceutical industry**, European Symposium on Computer-Aided Process Engineering-15, Elsevier Science Bv, 2005, Pages: 1003 - 1008, ISBN: 0-4445-1987-4

Sun NF, Immanuel CD, **Efficient solution of population balance models employing a hierarchical solution strategy based on a multi-level discretization**, Transactions of the Institute of Measurement and Control, 2005, Vol: 27, Pages: 347 - 366, ISSN: 1477-0369

Tsiakis P and Papageorgiou LG, **"Optimal Design of an Electrodialysis Brackish Water Desalination Plant"**, *Desalination*, 173, 173-186 (2005).

Tangirala AK, Shah SL and Thornhill N.F, 2005, PSCMAP: **A new measure for plant-wide oscillation detection**, Journal of Process Control, 2005, Vol: 15, Pages: 931-941, ISSN: 0959 1524.

| List of Publications |

Thornhill NF, 2005, **Finding the source of nonlinearity in a process with plant-wide oscillation**, IEEE Transactions on Control System Technology, 2005, Vol: 13, Pages: 434-443, ISSN: 1063-6536.

Thornhill NF and Naim MM, **An exploratory study on the use of spectral principal component analysis in supply networks to identify rogue seasonality**, European Journal of Operational Research, 2006, Vol: 172, Pages: 146-162, ISSN: 0377-2217.

Varga S, Purdy K, Galindo A, et al , **Nematic-nematic phase separation in binary mixtures of thick and thin hard rods: results from Onsager-like theories (Article no.051704)**, Physical Review E, 2005, Vol: 72, Pages: 1 - 19, ISSN: 1539-3755

Vladu CM, Hall C and Maitland GC, Colloid J, **Flow properties of freshly prepared ettringite suspensions in water at 25^{o}C**, Int Sci, 291, 466-472 (2006)

Wang M, Thornhill NF and Huang B, 2005, **Closed loop identification with a quantizer**, Journal of Process Control, 2005, Vol: 15, Pages: 729-740, ISSN: 0959-1524.

Westerlund J, Papageorgiou LG and Westerlund T, **"A Problem Formulation for Optimal N-dimensional Allocation"**, ICheaP-7 Conference, S. Pierucci (editor), Chemical Engineering Transactions, 6, 185-190 (2005).

Westerlund J, Papageorgiou LG and Westerlund T, **"A Problem Formulation for Optimal Mixed-sized Box Packing"**, ESCAPE-15 Conference, L. Puigjaner and A. Espuna (editors), 913-918 (2005).

Xia C, Howell J and Thornhill NF, **Detecting and isolating multiple plant-wide oscillations via spectral independent component analysis**, Automatica, 2005, Vol: 41, Pages: 2067-2075, ISSN: 0005-1098.

Yan L, and. Bogle IDL, (2006) **A visualisation method for operating optimisation**. Comput chem. Engng in press.

Zilinskas J, Bogle IDL, (2006) **Balanced random interval arithmetic in market model estimation**, European Journal of Operational Research, Volume 175, Issue 3 , 16 December 2006, Pages 1367-1378

Zilinskas J, Bogle IDL, (2005) **Stochastic global optimisation in chemical engineering**. In Proc 7th World Congress of Chemical Engineering Paper O170-002

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| Research Project List |

Competence Areas

Product and Process Design (Chem MFG SYS)

Name Mr Taj Barakat **Supervisor** Dr E Sorensen **Competence Area** Product and Process Design **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Optimal Design and Operation of Hybrid Separation Processes **Starting Date** Oct-03 **Finishing Date** Oct-06

Name Mr Rodrigo Blanco-Gutierrez **Supervisors** Dr CS Adjiman & Prof CC Pantelides **Competence Area** Product and Process Design **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Managing Technological Risk In Process Design **Starting Date** Nov-02 **Finishing Date** May-06

Name Mr Bruno Amaro **Supervisors** Dr C. Immanuel and Prof ENP Pistikopoulos **Competence Area** Product and Process Design **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Modelling and Optimisation of Molecular Weight Distribution for Free-Radical Solution Polymerisation in batch reactors **Finishing Date** Dec-08

Name Ms Milica Folic **Supervisors** Dr CS Adjiman & Prof EN Pistikopoulos **Competence Area** Product and Process Design **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Solvent selection for reaction **Starting Date** Nov-02 **Finishing Date** Nov-06

Name Mr Emmanuel Keskes **Supervisors** Dr CS Adjiman, Dr A Galindo & Prof G Jackson **Competence Area** Product and Process Design **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Integrated Process and Solvent Design for CO_2 removal from natural gas **Starting Date** Nov-03 **Finishing Date** Nov-06

Name Mr Hsien-His (Kenny) Kao **Supervisors** GJ/JSH **Competence Area** Product and Process Design **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Theory and experiment of polymer solutions and blends **Starting Date** Oct-03 **Finishing Date** Sep-06

Name Mr Westerlund Joakim **Supervisors** Dr LG Papageorgiou **Competence Area** Product and Process Design **Applications Domain** Chemical Manufacturing **Title of Thesis** Systems Facility and Process Plant Layout **Starting Date** Mar-03 **Finishing Date** Mar-06

Name Mr Zahoor Kashif **Supervisors** Dr E Sorensen **Competence Area** Product and Process Design **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Optimal design and operation of batch distillation **Starting Date** Jan-05 **Finishing Date** Jan-08

Product and Process Design (Biological SE)

Name Mr Xu Gang **Supervisors** Dr LG Papageorgiou & /KF **Competence Area** Product and Process Design **Applications Domain** Biological Systems Engineering **Title of Thesis** Optimisation-based Analysis of Biochemical Systems **Starting Date** Oct-04 **Finishing Date** Oct-07

Name Miss Cleo Kontoravdi **Supervisors** Prof EN Pistikopoulos & Dr A Mantalaris **Competence Area** Product and Process Design **Applications Domain** Biological Systems Engineering **Title of Thesis** Towards the Optimisation of the Production of Monoclonal Antibodies – Advanced Modelling, Experimental Validation and Control Optimisation Studies **Starting Date** Oct-02 **Finishing Date** Mar-06

Name Miss Teresa Mortera-Blanco **Supervisor** Dr A Mantalaris **Competence Area** Product and Process Design **Applications Domain** Biological Systems Engineering **Title of Thesis** Development of an Ex-vivo Leukaemic 3-D culture system **Starting Date** Oct-04 **Finishing Date** Sep-07

Name Miss Laleh Safinia **Supervisor** Dr A Mantalaris **Competence Area** Product and Process Design **Applications Domain** Biological Systems Engineering **Title of Thesis** Preparation and surface characterization of polymer constructs for tissue engineering applications' **Starting Date** Oct-04 **Finishing Date** Sep-07

Operation and Control (Chem MFG SYS)

Name Mr Nicola Bianco **Supervisor** Dr C Immanuel **Competence Area** Operations and Control **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Control of particle size distribution in emulsion polymerisation **Starting Date** Oct-04 **Finishing Date** Mar-08

Name Mr Tareg Al-Soudani **Supervisor** Prof Bogle **Competence Area** Operations and Control **Applications Domain** Chemical Manufacturing Systems Operations, **Title of Thesis** Multi-scale Modelling for Control of Reaction-Adsorption Systems, **Starting Date** Feb-05 **Finishing Date** Feb-10

Name Mr Dario Luis **Supervisors** LSK/AA **Competence Area** Operations and Control **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Design & Implementation of Nonlinear Robust Controller for an extohermic reaction system **Starting Date** Apr-02 **Finishing Date** Jun-06

| Research Project List |

Competence Areas

Operation and Control (Chem MFG SYS) (cont'd)

Name Rohit Ramachandran **Supervisors** Dr C Immanuel & Dr Stepanek **Competence Area** Operations and Control **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Control of Distributed Parameter Systems **Starting Date** Oct-05 **Finishing Date** Sep-08

Name Mr Hlyur Stefansson **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Multiscale planning and scheduling in the pharmaceutical industry **Starting Date** Oct-03 **Finishing Date** Oct-06

Operation and Control (Molecular SE)

Name Ms Margaret Bauer **Supervisor** Mrs NF Thornhill **Competence Area** Operations and Control **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Data-driven methods for process analysis **Starting Date** Nov-02 **Finishing Date** Jan-06

Operation and Control (Biological SE)

Name Mrs Pinky Dua **Supervisor** Prof EN Pistikopoulos **Competence Area** Operations and Control **Applications Domain** Biological Systems Engineering **Title of Thesis** Model Based and Parametric Control for Drug Delivery Systems **Starting Date** Oct-01 **Finishing Date** May-06

Name Mr Michalis Koutinas **Supervisors** Andrew Livingstone & Dr A Mantalaris **Competence Area** Operations and Control **Applications Domain** Biological Systems Engineering **Title of Thesis** Microbial Strain Dynamics and Bioreactor Stability in an Intensive Absorber-Bioscrubber Process **Starting Date** Apr-02 **Finishing Date** Oct-06

Name Mr Robin Kumar **Supervisor** Dr A Mantalaris **Competence Area** Operations and Control **Applications Domain** Biological Systems Engineering **Title of Thesis** Oxygen Transport Simulation in the Human Bone Marrow Microcirculation **Starting Date** Oct-01 **Finishing Date** Oct-06

Name Mr Mark Pinto **Supervisor** Dr C Immanuel **Competence Area** Operations and Control **Applications Domain** Biological Systems Engineering **Title of Thesis** Modelling and controll of biological systems **Starting Date** Oct-04 **Finishing Date** Mar-08

Operation and Control (Supply Chains)

Name Mr Kwok Yuen Cheung **Supervisors** Prof N Shah & Prof CC Pantelides **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Site-wide and supply chain optimisation for continuous chemical processes **Starting Date** Oct-04 **Finishing Date** Sep-07

Name Ms Gunilla Laakso **Supervisor** Dr LG Papageorgiou **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Supply chain management for the paper industry **Starting Date** Feb-04 **Finishing Date** Feb-07

Name Mr Edric Margono **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Supply Chain Optimisation **Starting Date** Oct-03 **Finishing Date** Sep-06

Name Mr Yongyut Meepetchdee **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Supply chain optimisation **Starting Date** Oct-04 **Finishing Date** Sep-07

Name Mr Javier Palma Rosillo **Supervisors** Prof N Shah & Prof EN Pistikopoulos **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Model predictive control of supply chain systems

Name Ms Gabriela Pereira **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Supply Chain Modelling **Starting Date** Oct-05 **Finishing Date** Sep-08

Name Mr Yoong See Toh **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Paints supply chain optimisation **Starting Date** Oct-03 **Finishing Date** Sep-06

Name Mr Rui Sousa **Supervisors** Prof N. Shah & Dr LG Papageorgiou **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Global network planning for pharmaceuticals **Starting Date** Oct-03 **Finishing Date** Oct-07

Name Mr Pasant Suwanapal **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Chemical Complex Supply Chain **Starting Date** Oct-05 **Finishing Date** Sep-08

| Research Project List |

Competence Areas

Operation and Control (Supply Chains) (cont'd)

Name Mr Tsang King Hei **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Supply Chains of the Future **Title of Thesis** Vaccine supply chain optimisation **Starting Date** Oct-02 **Finishing Date** Jan-06

Operation and Control (Energy Systems)

Name Mr Javier Aguilar **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Energy Systems **Title of Thesis** Engineering Strategic Development in the Petrochemical Industry **Starting Date** Nov-01 **Finishing Date** Dec-06

Name Mr Sufian Ali **Supervisor** Prof EN Pistikopoulos **Competence Area** Operations and Control **Applications Domain** Energy Systems **Title of Thesis** Engineering Oil & gas Production Optimization **Starting Date** Feb-03 **Finishing Date** Feb-06

Name Mr Ali Al-Mansoori **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Energy Systems Engineering **Title of Thesis** Design and operation of a future hydrogen supply chain **Starting Date** Nov-02 **Finishing Date** Aug-06

Name Mr Lee Chang **Supervisors** Prof N Shah & Stratos Pistikoupolous **Competence Area** Operations and Control **Applications Domain** Energy Systems Engineering **Title of Thesis** Modelling and optimization of China hydrogen infrastructure **Starting Date** Oct-06 **Finishing Date** Jan-07

Name Mr Alexander Dunnett **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Energy Systems Engineering **Title of Thesis** Biofuel Supply Chain **Starting Date** Oct-05

Name Mr Naga V. N. M Konda **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Energy Systems Engineering **Title of Thesis** H_2-CO_2 Infrustructure Design **Starting Date** Aug-06 **Finishing Date** Jul-09

Name Mr Javier Rodriguez Perez **Supervisors** Dr C Immanuel & Dr CS Adjiman **Competence Area** Operations and Control **Applications Domain** Energy Systems **Title of Thesis** Engineering Optimal Sensor Location **Starting Date** Jan-09

Name Mr Milinda Sanjeewa Samaraweera **Supervisors** Prof N. Shah & Prof E.N Pistikopoulos **Competence Area** Operations and Control **Applications Domain** Energy Systems Engineering **Title of Thesis** Modelling and optimisation of urban energy systems **Starting Date** Oct-06 **Finishing Date** Oct-09

Name Mr Panthot Suwanapal **Supervisor** Prof N. Shah **Competence Area** Operations and Control **Applications Domain** Energy Systems Engineering **Title of Thesis** Energy Systems with Application to Thailand **Starting Date** Oct-05 **Finishing Date** Sep-08

Modelling and Model Solution Tools (Chem MFG SYS)

Name Mr Sujan Balendra **Supervisor** Prof IDL Bogle **Competence Area** Modelling and Model Solution Tools **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Global Optimisation of Modular Systems **Starting Date** Oct-01 **Finishing Date** Sep-06

Name Mr Bernardino Pereira Lo **Supervisor** Dr CS Adjiman **Competence Area** Modelling and Model Solution Tools **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Parameter estimation for a model of polymer rheology **Starting Date** Oct-02 **Finishing Date** Dec-06

Name Mr Jonathon Poon **Supervisor** Dr C Immanuel **Competence Area** Modelling and Model Solution Tools **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Modelling and control of granulation processes employing population balances **Starting Date** Oct-04 **Finishing Date** Mar-08

Name Mr Stephen Sweetman **Supervisor** Dr C Immanuel **Competence Area** Modelling and Model Solution Tools **Applications Domain** Chemical Manufacturing Systems **Title of Thesis** Population Balance Modelling of Emulsion Polymerisation Systems' **Starting Date** Nov-04 **Finishing Date** Nov-07

Modelling and Model Solution Tools (Molecular SE)

Name Mr Paul Brumby **Supervisor** Prof G. Jackson **Competence Area** Modelling and Model Solution Tools **Applications Domain** Molecular Systems Engineering **Title of Thesis** 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 Gary Clark **Supervisors** Dr A Galindo & Prof G Jackson **Competence Area** Modelling and Model Solution Tools **Applications Domain** Molecular Systems Engineering **Title of Thesis** Phase Behaviour of Water-soluble polymers using the SAFT Equation of State **Starting Date** Oct-04 **Finishing Date** Sep-07

| Research Project List |

Competence Areas

Modelling and Model Solution Tools (Molecular SE) (cont'd)

Name Mr Hugh Docherty **Supervisor** Dr A Galindo **Competence Area** Modelling and Model Solution Tools **Applications Domain** Molecular Systems Engineering **Title of Thesis** Computer simulation of aqueous electrolyte solutions **Starting Date** Oct-03 **Finishing Date** Oct-06

Name Mr Nikolaos P Kakalis **Supervisor** Prof CC Pantelides **Competence Area** Modelling and Model Solution Tools **Applications Domain** Molecular Systems Engineering **Title of Thesis** Reliable and Efficient Use of the SAFT Equation of State in Process Modelling **Starting Date** Oct-01 **Finishing Date** Apr-06

Name Mr Alexandros Lymperiadis **Supervisors** Dr A Galindo, Prof G Jackson & Dr CS Adjiman **Competence Area** Modelling and Model Solution Tools **Applications Domain** Molecular Systems Engineering **Title of Thesis** A new group contribution method for solvent design **Starting Date** Apr-04 **Finishing Date** Apr-07

Name Mr Niall MacDowell **Supervisors** Proj. Jackson, Dr.s Adjiman & Galindo **Competence Area** Modelling and Model Solution Tools **Applications Domain** Molecular Systems Engineering **Title of Thesis** Improvements in amine based absorption systems for post combustion CO_2 capture **Starting Date** Oct-06 **Finishing Date** Oct-09

Name Miss Michaela Pollock **Supervisors** Dr A Galindo, Prof G Jackson & Dr CS Adjiman **Competence Area** Modelling and Model Solution Tools **Applications Domain** Molecular Systems Engineering **Title of Thesis** Predictive thermodynamic models for replacement refrigerants and blends **Starting Date** Oct-04 **Finishing Date** Oct-07

Name Mr Jose Guillermo Sampayo-Hernandez **Supervisor** Prof G. Jackson **Competence Area** Modelling and Model Solution Tools **Applications Domain** Molecular Systems Engineering **Title of Thesis** Theory and simulation of Interfacial Systems **Starting Date** Oct-05 **Finishing Date** Sep-08

Modelling and Model Solution Tools (Biological SE)

Name Mr Richard Allen **Competence Area** Modelling and Model Solution Tools **Applications Domain** Biological Systems **Title of Thesis** Engineering Modelling Endothelial Cells

Name Mr Sandeep Chandarana **Supervisor** Dr A Mantalaris **Competence Area** Modelling and Model Solution Tools **Applications Domain** Biological Systems **Title of Thesis** Engineering Fluid Dynamics in Microgravity Bioreactors **Starting Date** Oct-03 **Finishing Date** Oct-06

Name Miss Ming-Chi (Carolyn) Lam **Supervisors** Dr A Mantalaris & Prof EN Pistikopoulos **Competence Area** Modelling and Model Solution Tools **Applications Domain** Biological Systems Engineering **Title of Thesis** Creating a predictive in silico model of mammation cell cultures **Starting Date** Oct-04 **Finishing Date** Apr-08

Name Mr Fabio Sidoli **Supervisors** Prof N Shah & Dr A Mantalaris **Competence Area** Modelling and Model Solution Tools **Applications Domain** Biological Systems Engineering **Title of Thesis** Systematic Development of a Coupled Population-Balance-Single-Cell Model for Mammalian Cell Cultures **Starting Date** Oct-01 **Finishing Date** May-06

Name Mr Boon Seng Soh **Supervisors** Dr A. Mantalaris, Dr A. E. Bishop & Dr L. Bing (Genome Institute of Singapore) **Competence Area** Modelling and Model Solution Tools **Applications Domain** Biological Systems Engineering **Title of Thesis** Directed differentiation of human embryonic stem cells to lung bronchioalveolar stem cell **Starting Date** Apr-06 **Finishing Date** Apr-09

Modelling and Model Solution Tools (other)

Name Mr Amit Manthanwar **Supervisor** Prof EN Pistikopoulos **Competence Area** Modelling and Model Solution Tools **Title of Thesis** Model-based Control and Parametric Programming **Starting Date** Oct-03 **Finishing Date** Oct-06

Name Mr Mohamed Al-Hosani **Supervisor** Prof EN Pistikopoulos **Competence Area** Modelling and Model Solution Tools **Title of Thesis** Novel Parametric Programming Algorithms and Applications **Starting Date** Nov-02 **Finishing Date** Nov-06

Name Mr Nuno Faisca **Supervisors** Prof EN Pistikopoulos & Dr V Dua **Competence Area** Modelling and Model Solution **Title of Thesis** Tools Parametric Programming and Control **Starting Date** Oct-04 **Finishing Date** Oct-07 cpse

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