Centre for
Process
Systems
Engineering

CPSE 08

The Centre for Process Systems Engineering
Annual Report 2008

Imperial College London | UCL

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CPSE CONTENTS

2008

"..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

2008

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

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

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

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

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

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

CPSE INTRODUCTION AND REVIEW OF THE YEAR
2008

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

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

Process systems engineers are concerned with systems involving physical and chemical change and aim to manage the complexity and uncertainty of such systems. The Centre's research takes a holistic, systems approach to modelling, optimization and control across many time and scale lengths. Process systems engineering then involves the development of systematic methods and computational tools for the analysis, evaluation and design of integrated processes networks, and systems. Key drivers include criteria, such as investment and opportunity costs, energy consumption, environmental impact and management of uncertainty and risk. Examples that you will find in this review include the computer aided molecular design of solvents in reactions, systematic methods to characterise the phase behaviour of surfactant mixtures, multi-scale modelling and optimization approaches for hybrid membrane/pressure swing adsorption (PSA) systems and multi-scale flash desalination (MFS) plants, systems biology and mammalion cell technology projects, and a research programme on integration of plant-wide planning, scheduling, and supervisory and regulatory control systems.

The Centre involves 19 academic staff from Imperial College and UCL, 61 PhD students and 13 research fellows and associates. In the last five years we have been managing a portfolio of grants worth more than £7 million. Of this around 40% of the awards are from Research Councils, 30% from industry, and 30% from the European Commission and other funding and charity bodies.

I am pleased to report that 2008 has been an exciting and memorable year for CPSE, with a number of highlights.

The 15th Professor R.W.H. Sargent Lecture, which was delivered by Professor Chris Floudas from Princeton University on "Discovering through Systems Engineering Thinking".

In his inspiring Lecture, Professor Floudas clearly showed how mathematical modeling, optimization theory and algorithms can be effectively employed to design novel computational approaches for the discovery of new molecules, the *de novo* design of therapeutic peptides and proteins as well as the rational selection of zeolites for catalysis and separation.

The organisation of an International Conference on Computational Management Science (CMS) at Imperial (hosted by CPSE members in the Computing Department), partially also supported by the Systems Engineering Initiative. The conference attracted around 200 participants from around the world and focused on the theory and practice of computational methods, models and empirical methods for quantitative decision modelling in economics, finance, management and engineering.

Members of CPSE co-organised and delivered plenary Lectures at the International Conference of "Foundations of Computer-Aided Process Operations", FOCAPO2008, Boston, MA, USA.

CPSE's Director was awarded a prestigious European Research Council (EPC) Advanced grant, for a five-year research programme on modelling, control and optimization of biomedical systems (MOBILE). The award, of around €2 million will allow CPSE to take a more fundamental and in-depth approach to how process systems engineering theories, algorithms and computational tools can play a significant role in biomedical problems, such as type I diabetes, anaesthesia, HIV and cancer.

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

Next year, 2009 will be the 20-year celebration of our Centre, and we will host a number of events to mark this unique milestone. I hope you will enjoy reading this report. We are always keen to collaborate with companies and organisations in the non-profit sector, and academia worldwide.

Prof Stratos Pistikopoulos
Director, Centre for Process Systems Engineering (CPSE)
http://www3.imperial.ac.uk/centreforprocesssystemsengineering

CPSE RESEARCH PROGRAMME
2008

CPSE INDUSTRIAL CONSORTIUM
2008

The CPSE Industrial Consortium currently consists of 10 members who are all major companies in their different industries. They are;

ABB Corporate Research
AkzoNobel
BASF
Bristol-Myers Squibb
BP Exploration
INEOS
Petrobras
Procter & Gamble
Shell Research & Technology
Syngenta

PRODUCT AND PROCESS DESIGN

COMPETENCE AREA 1

The Product and Process Design competence area develops systematic model-based methodologies for the rational design of processes. It encompasses a growing range of scales, from nanoscale models for materials selection, to mesoscale models for the design of processes for specific tasks, as well as overall process models for integrated plant design. The approaches we develop aim to enable engineers to meet the constraints and objectives imposed by today's business environment, in particular, in the field of sustainable development. They consider not only economic aspects, but also environmental, safety and health factors and this is exemplified both in theoretical work and in technology development projects. Part of the work is focused on early process development. Other projects are applicable to later development stages, and focus on detailed design for separation, reaction, reactive separation, or operability issues such as controllability or maintenance. Modelling spans a range of scales and includes the design of devices where material issues play an important role such as 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 researchers along four main themes (below):

Materials design for process synthesis

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

Design of novel manufacturing processes

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

Integrated process synthesis

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

Technology transfer

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

New projects and noteworthy achievements in the past year include:

Molecular Systems Engineering:

A core competence within Product and Process design is Molecular Systems Engineering. Molecular systems engineering refers to the development of methods and tools for the design of better products and processes in applications where molecular interactions play a central role, and it provides a detailed representation of the system at the microscopic level of the constituent molecules.

The activity involves the intelligent molecular design of materials for engineering applications. CPSE interfaces with experimentalists, theoreticians, and molecular and process modellers with broad expertise in thermodynamics, phase equilibria, molecular structure, and rheology.

Systematic approaches to the development of thermodynamic models for strongly associated fluids and their mixtures

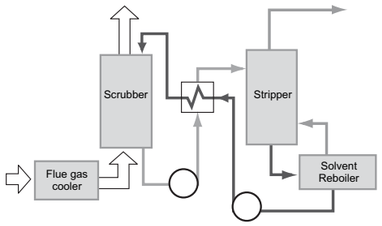
A project completed during the year focused on modelling systems containing hydrogen fluoride (HF) and replacement refrigerants, where the challenges are strong hydrogen bonding, polar interactions and the non-spherical shape of the molecules.

The Statistical Associating Fluid Theory with potentials of Variable Range (SAFT-VR) is especially well-suited for this task. In SAFT-VR, hydrogen bonding interactions are taken into account explicitly by introducing a number of short range attractive sites, which mediate this interaction, while the non-sphericity of the molecule is treated via a model of a chain of tangentially bonded segments. The non-sphericity of the molecule is obtained from quantum mechanical calculations; this is a major new contribution of this work. The work developed new molecular models for HF and a number of refrigerants and also extended to mixtures.

The systematic approach to model development established in this work is general and can be applied to other systems and advanced equations of state.

Improvements in amine-based absorption systems for the post-combustion capture of CO_2 from the flue-gases of coal-fired power stations

In this work we are focus on the optimal design and operation of flue gas scrubbing systems. The CO_2 capture medium is an amine-based solvent. As these are complex, associating fluids, they require a sophisticated thermodynamic treatment. Here we are utilising the SAFT-VR equation-of-state, which is ideally suited to this application. Furthermore, we are implementing the thermodynamic models of these systems into a rigorous rate-based simulation of the capture process. These models are implemented in gPROMS which provides the ideal platform for dynamic process simulation.



Modelling and Optimization of Polygeneration Energy Systems

Polygeneration is a potential cost-effective and environmentally friendly energy conversion technology to tackle serious energy and environmental problems faced by all human-beings in the 21st century and to release the currently huge pressure on oil oriented liquid fuel consumption. A polygeneration plant is a multi-in multi-out energy system that produces electricity, chemicals, and synthetic fuels. A generic polygeneration process, as can be seen in **Figure 1**, (**above**), starts from gasification of coal, biomass, petroleum coke, or other feedstocks, and produces electricity and synthesis fuels via integrated power generation and chemical synthesis processes.

In spite of the benefits of a polygeneration process, for instance, high energy conversion efficiency and low/zero emissions, designing such a complicated and highly-integrated system over its long-term operating horizon considering both economic and environmental performances remains a challenging problem, with the following scientific issues to be solved:

- Many technical alternatives for each functional unit
- High degree of integration among functional units
- Trade-off between profitability and environmental impacts
- Unpredictable behavior of the chemical synthesis unit due to different composition of inlet gas

These problems have been tackled from both a strategic level and a process level. At the strategic level, a polygeneration process is taken as a whole, and more focus is placed on selection of feedstocks, products, technologies, investment planning and process capacity expansion. At the process level, a polygeneration plant is divided into several functional blocks, and mass and energy balances are established for each block. First principle formulations of chemical kinetics are also introduced for chemical blocks. Modelling and optimization at this level focuses on the selection of types of equipment and technologies and their combinations, process profitability and life-cycle assessment (LCA) based environmental impacts.

Advanced Control and Optimization of a Hybrid PSA Energy System

To meet future regulations and standards, sustainable energy systems based on fossil fuels will require a significant reduction of emitted greenhouse gases and other pollutants. If CO_2 emissions are captured as a relatively pure gas, they can further be sequestered or stored appropriately, thus reducing at the source the amount emitted to the atmosphere. Unfortunately, the existing technologies for hydrogen production are not cost-effective when considered in the context of CO_2 sequestration. Usually, carbon dioxide capture is estimated to represent a large portion of the total cost of a carbon capture, storage, transport, and sequestration system. The work aims to improve, make more effective and reduce the cost, of the fossil fuel de-carbonization process, and thus reduce the cost of CO_2 capture as much as possible. An improved hybrid membrane/ Pressure Swing Adsorption (PSA) CO_2/H_2 separation process is being designed to contribute to the achievement of this target. The proposed hybrid separation process will provide a means to increase CO_2 capture rates, by capturing CO_2 from processes that currently release it in the atmosphere. A CO_2/H_2 hybrid separation process with improved separating ability will provide a way to produce a sequestration ready CO_2 stream, thus reducing the amount of CO_2 released in the atmosphere in the H_2 production.

The presence of the PSA system inside the hybrid system makes the process optimization task challenging. This is because of unique features of PSA operation, as it never reaches a true steady state and instead, a cyclic steady state (CSS) is obtained after undergoing a large number of cycles. Consequently, the computational time to achieve such a state for a given set of design variables is usually very large. New process optimization strategies, employing state of the art, mixed integer non linear programming (MINLP) techniques are being explored to overcome this challenge. Preliminary simulation based studies conducted with a CO_2 selective membrane downstream of the PSA system, handling its off-gas, show very promising results. A 10% increase in H_2 recovery has been obtained for some membrane area values, and clearly exhibits the potential of such an hybrid system.

Modelling and Optimisation of Separation Processes

The tremendous development of biotechnology in recent years has resulted in the production of more and more new active compounds such as purified sugars, enzymes, peptides, antibiotics and therapeutic macromolecules. In parallel, the constraints on product purity in drug manufacture have become increasingly stringent and this has lead to an intensified demand for efficient and economical separation technologies.

For chromatographic separations, conducting the separation continuously instead of batchwise can dramatically improve separation efficiency as well as production capacity and thereby reduce purification costs. This is particularly important for industrial applications of preparative chromatography. Continuous chromatography involves the simultaneous use of several columns. Simulating Moving Bed (SMB) chromatography simulates a counter-current contact between a solid phase and a mobile phase whereby the feed, eluent and product removal locations are switched at given intervals thus simulating the movement of the solid phase. Semi-continuous chromatography processes that are capable of separating complex mixtures of biomolecules have also recently been proposed.

The main emphasis of our work is therefore on developing techniques for the optimal design and operation of continuous and semi-continuous processes with particular emphasis on monitoring and cost efficiency. See **Figure 2**, (**overpage**).

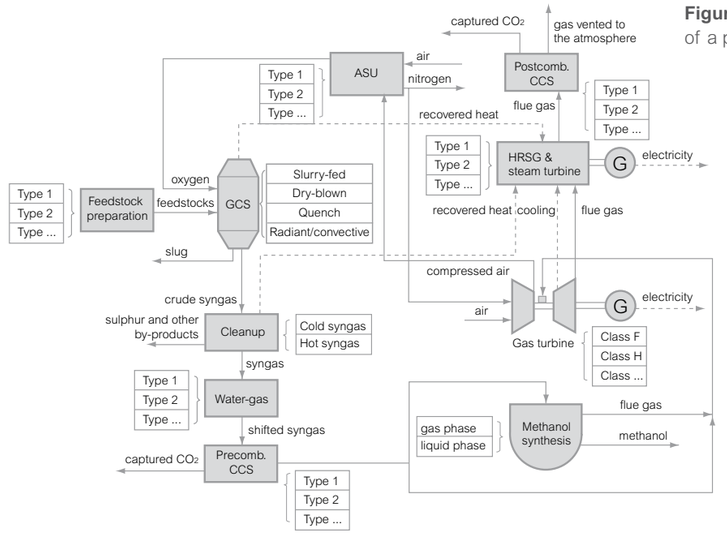


Figure 2. A superstructure representation of a polygeneration process

OPERATIONS AND CONTROL

COMPETENCE AREA 2

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, management of supply chains and of batch processing.

Process Control

Covers the theory and practice of advanced automation and control with an emphasis on application to the process industries. Applied research covers a broad spectrum including in oil & gas, reaction and absorption, granulation and polymers. Competencies feeding into applications include integration of design, operation and decision making; multiscale modelling; integrated monitoring of process, electrical and mechanical equipment; and theoretical advances in robust parametric control.

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

A highlight of 2008 was the award to Professor Pistikopoulos of a €2M Advanced Investigator award from the European Research Council. The project is called MOBILE (Modelling, control and optimization of biomedical systems) and it will support a number of researchers in modelling of insulin delivery systems, delivery of chemotherapeutic agents in cancer, anaesthesia and hemodynamic variables, and chemotherapy of HIV. Such models will lead to new fast, robust multi-parametric control algorithms. The overall goal is to develop, test and validate prototype software model-based procedures and prototype hardware controllers in the context of automation of drug delivery systems.

A selection from the broad range of other activities in the past year includes:

Unmanned Air Vehicles (UAVs)

UAVs have recently attracted attention in research due to their numerous applications where direct human intervention is undesirable. Civilian applications involve rescue missions, fire extinction, grid searching for mining, oil exploration, surveillance and reconnaissance for traffic control, marine and border inspection. The situation becomes technologically challenging if multiple UAVs (MUAVs) are involved in the task. In particular, coordinating flights of MUAVs in a predictable and verifiable way is crucial for their certification in the airspace and acceptance for safety critical missions. The project is developing and validating a rigorous, analytical framework for deriving and accessing guaranteed dynamic and kinematic performance of MUAVs. It concentrates on two different levels of control of MUAVs: (i) Trajectory planning and generation and coordinated vehicle guidance to find the optimal paths in terms of time and energy consumptions while avoiding collisions. All UAVs are considered on this level; (ii) Control of each individual UAV to avoid collision with other UAVs and environment while following the planned path. Both levels are utilizing Model Predictive Control (MPC). Initial studies have focused on the effects of

unforeseen wind conditions, since wind is particularly troublesome for small aircraft. The project is carried out in cooperation with Cranfield University. The PhD student working in the project will shortly undertake a research placement in the Cranfield laboratory to benefit from their knowledge and experience in mission control, path planning and guidance. A goal of the work is the cross over technologies from process optimization and control into aerospace research and development.

Supply chain management

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

Regulatory processes in gradient perception

Work underway at the intersection of Operations and Control with Biological Systems Engineering involves the analysis of biological pathways from a control point of view. A highlight of the year was an invited paper in as Special Issue on Systems Biology of the IEEE Transactions on Automatic Control (Krishnan and Iglesias, 2008). Of particular interest are the mechanisms of chemotaxis, when an organism exhibits direction locomotion in response to a gradient in a chemical concentration. Modelling involved firstly a minimal model reconciling gradient perception to the property of adaptation. The second model was a biochemical model of a lipid network and its regulation by enzymes. In both cases the focus was on the regulation of the modules/networks by inputs leading to some generally applicable insights. The editors of the Special Issue highlighted the central place of feedback in biological regulation and commented that control system modellers and theorists are well placed to complete explanations and make predictions of highly complex biological systems.

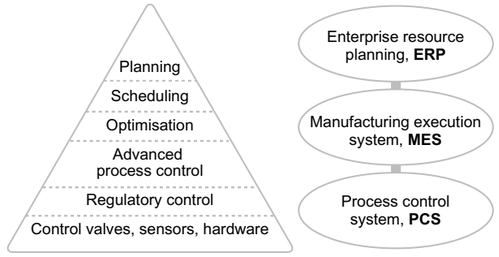


Figure 1. The old view of the CIM pyramid (left) versus the new CIM structure of ISA-95 (right). ISA-95 provides a reference model of the activities within each layer and a description of the interfaces between the MES and ERP layers.

ERP/MES/PCS integration

Control at different levels has been understood in the literature for nearly two decades leading to applications such as plant-wide planning and scheduling, model predictive control at the supervisory level and PID at the regulatory level. But in 2001 the Chairman of the ISA SP-95 Committee, said "The computer-integrated manufacturing pyramid of the 1980s has crumbled to make way for …. better models for manufacturing information technology in the 2000s." [Keith Unger, *InTech*, 03 October 2001]. The pyramid and the new manufacturing information technology structure of ISA-95 are illustrated in **Figure 1**, (**above**). While there is a well defined R&D programme for information and communication technologies to enable implementation of integrated ERP/ MES/ PCS systems, it is the research challenges for control engineers in the operation of an installed systems that are the focus of the Operations and Control programme. Work has started to draw out process control research issues in the operation of an integrated of ERP, MES and PCS. For instance, the model of manufacturing operations in ISA-95 contains structures involving tasks and information flows which resemble feedback control loops. Therefore there are requirements such as stability analysis, disturbance rejection, control loop tuning and loop performance assessment. A first step towards setting a new research agenda was to participate as co-organizer in an IChemE event which brought together end-users, vendors, consulting and contracting companies and academic researchers for two days.

Electric power transmission enhancement

A project at the intersection of the Energy Systems Engineering application area and the Operations and Control competence area is looking at the operation of electrical power transmission in collaboration with power systems experts. New wide area measurement technologies using phasor measurement units are starting to be deployed which will give real-time measurements of the high quality that have been available in chemical plants and refineries for many years. The project is investigating and adapting signal analysis methods that have been used successfully in the chemical process industries for detection of the frequency and damping of wide-area power oscillations. The student working on the project is currently on secondment with National Grid, and case studies in the Finnish sector of the Nordic transmission system are also under way. The goal is better understanding, early detection and diagnosis of instabilities in a.c. electrical power transmission systems and avoidance of situations leading to large scale power blackouts.

Urban energy systems

The Optimization and Control competence area is involved with the BP Urban Energy Systems project which is described fully elsewhere in this report. The aim is to investigate in detail how energy, people and materials flow through a city and then identify opportunities for optimising resources such as power, heating, transport and water services. For example, homes might be heated with the heat from waste water or residential and business areas might be arranged to reduce commuting traffic. The project draws upon expertise across Imperial College in modelling of complex systems, and the specific contribution from the Optimization and Control competence area is in the application of powerful global optimization techniques from supply chain and logistics, and novel supply strategies.

Krishnan, J. and Iglesias, P.A., 2008, Systems analysis of regulatory processes underlying eukaryotic gradient perception, IEEE Transactions on Automatic Control, 53, 126-138.

MODELLING AND MODEL SOLUTION TOOLS

COMPETENCE AREA 3

The activities in this area feed into all the application domains. The main objective here is to develop generic and fundamental tools to tackle the twin challenge of computational complexity and uncertainty in model parameters. To this effect many solution methodologies have been developed and tested on a wide variety of applications. A glimpse of recent and selected activities is presented as follows, several other techniques have been developed to address a broad spectrum of systems engineering problems.

Multiscale Modelling for Operation and Control of PSA Units

This research focuses on the applicability of multiscale models to solving synthesis, operations, control and/or optimization problems with emphases on spatio-temporal variable models. Multiscale Pressure Swing Adsorption (PSA) unit models, and some of their variants (e.g. Reaction and Pressure Swing Adsorption) are selected as an experimental platform for testing the proposed approaches (**see Figure 1, below**). Nevertheless, we anticipate applicability of the resulting approach to general class of problems spanning simultaneous spatio-temporal variations. A model has been developed and tested. We are now exploring four approaches to model reduction based on physical insights and approximations to be used in different applications. The main objective is to develop a model based control scheme that considers microscale effects together with unit level control where appropriate. The project will also consider operational optimization for yield maximisation and energy minimisationusing mixed integer dynamic optimization.

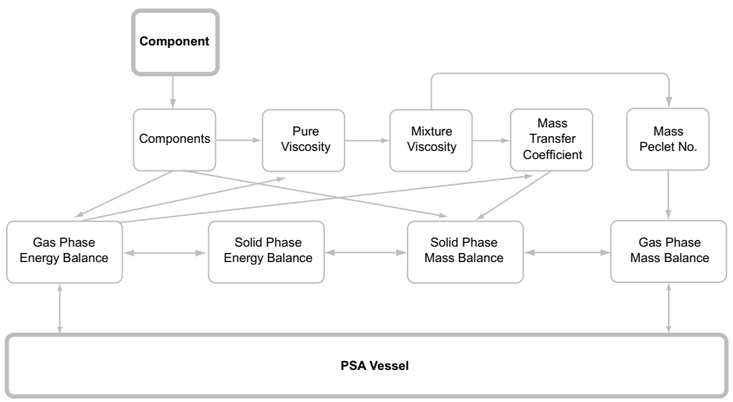


Figure 1. Length hierarchy of the developed PSA model. Each row of building blocks represents a length or detailed level in the hierarchy.

Dynamic Modelling and Control of Multi Stage Flash (MSF) Desalination Plant

The objective of this project is to develop a dynamic model of multi stage flash desalination plants for use in design and operations. The model will include links from process scale to smaller scales and will include: flashing phenomena in the stage, flow in the demister, condensation around the tube bundles, orifice flow, ejectors, and fouling and scaling in side tubes. In the last year the project has focussed on modelling of fluid dynamics and two phase flow in MSF flashing stage (including the brine pool, demister and the condenser tubes). The project is developing a full lumped model prior to a distributed model in steady state and with dynamics, using CFD to model the mixing in each stage. Through connections in Kuwait we hope to obtain commissioning data from a plant.

Multi-objective Process Design

Pressure Swing Adsorption (PSA) is a cyclic separation process whose main steps are adsorption, at high pressure, and regeneration of the adsorbent, at low pressure. For middle scale operations, PSA is a more economic and effective separation option compared with absorption, cryogenic and membrane separation. Automated tools for the design of PSA processes would be beneficial for the development of the technology due to the complex behaviour of the performance with respect to the design variables. A multi-objective design strategy can help identify and quantify the trade-offs between the different measures of performance. However, the design of PSA is a difficult task due to the complexity of the simulation and the computational effort needed to detect the performance at cyclic steady state.

A multi-criteria design framework for the design of multi-bed/multi-step PSA cycles has been developed. Computational requirements have been reduced by adopting a simplified model for the adsorption column. The column is simulated as a train of continuous stirred tank reactors (CSTRs). A faster convergence to cyclic steady state has been achieved by using a *unibed* approach. The multi-objective optimisation is addressed through a custom genetic algorithm which emphasises the generation of broad Pareto sets. A variety of case

studies has been addressed, including separation of air for N2 production and the capture of CO_2 from flue gases. The solutions obtained compare favourably with literature and demonstrate the capability of the multi-objective framework for these complex design problems. A representative solution depicting the conflicting nature of two objectives, recovery and purity, is shown in **Figure 2,** (**below**).

More recently, models for fuel cells, addressing the identification of trade-offs, such as between size and performance, in design are being developed. Another recent project addresses the design of feed pre-treatment for the production of ethanol from lignocellulosic biomass, considering a number of alternative treatments and their design options. The latter is using the Jacaranda system for process design and optimisation.

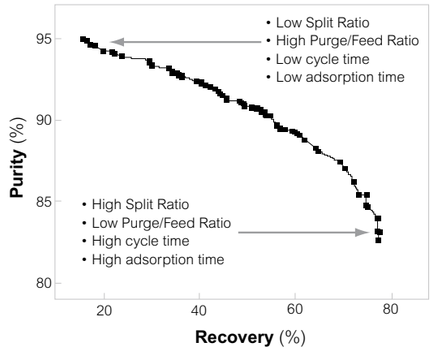


Figure 2. Multi-objective PSA process design.

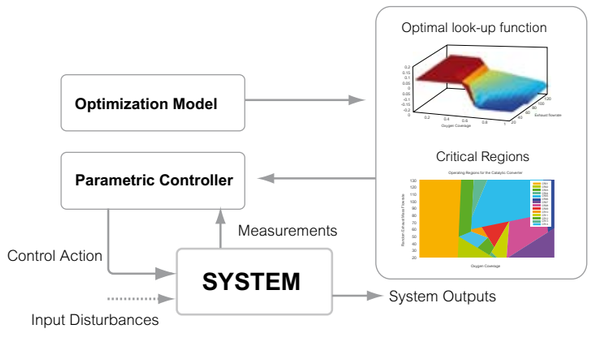


Figure 3. Parametric controller where control variables are optimization variables and state variables are parameters.

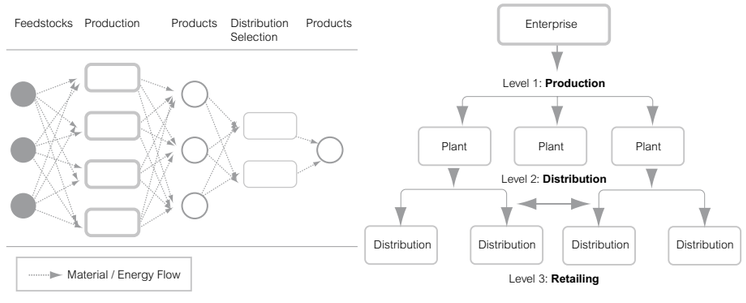


Figure 4. Design of Enterprise-wide Process Networks: Bilevel programming where decision variables from higher level are parameters for lower level.

Multiparametric Programming

A major bottleneck in the application of model-based design, control and optimization techniques is the presence of internal and external variations, where internal variations correspond to uncertainty inherent in the model parameters and external variations can come from factors such as disturbances or fluctuations into the system. A systematic incorporation of variations is important to realise the true benefits of any mathematical modelling based approach. For internal variations one is typically interested in obtaining a map of all the optimal solutions as a function of the variations and then use this map to evaluate various scenarios. For external variations the objective is to obtain the optimal solution when variations enter the system. Parametric programming is a technique that determines computationally inexpensively the exact mapping of the optimal solution profile in the space of parameters. The parameters are defined in accordance with the type of problem and variations, as shown in **Figures 3-4,** (**below left**). Recent developments in this area include robust multi-parametric model-based control, global optimization of multi-parametric mixed-integer linear programs and global optimization of mixed-integer bilevel programs.

Complexity Reduction

Model based simulation of complex processes is an efficient approach of exploring and studying systems whose experimental analysis is costly or time-consuming. Modern mathematical models of real systems often have high complexity with hundreds of variables. Straightforward modelling using such models can be computationally costly or even intractable. Good modelling practice requires sensitivity analysis (SA) to ensure the model quality by analyzing the model structure, selecting the best type of model and effectively identifying the important model parameters. Global SA is superior to other SA methods. It can be applied to any type of models for quantifying and reducing problem complexity without sacrificing accuracy and it is not dependent on a nominal point like local SA methods. A number of advanced model analysis and complexity reduction techniques based on global SA and efficient high dimensional Monte Carlo (MC) and Quasi MC methods have been developed.

The Sobol' method of global sensitivity indices is superior to other global SA methods. However, it has been applied only to low scale models because of the computational limitations of the existing technique. A number of techniques which improved the efficiency of the Sobol' method have been developed. A set of new global SA measures which are much less computationally demanding than variance based methods have also been developed.

One of the very promising developments of model analysis is the replacement of complex models and models which need to be run repeatedly on-line with equivalent operational meta models. Sampling efforts of the existing approaches grow exponentially with the number of input variables which makes them impractical in high dimensional cases. A novel approach to metamodelling using quasi random sampling - high dimensional model representation method (QRS-HDMR) which renders the original exponential difficulty to a problem of only polynomial complexity has been developed. It is proposed to solve optimization problems with high dimensional and computationally expensive objective functions by building QRS-HDMR meta models for the objective functions and set of constraints. Such meta models based optimization problems can be orders of magnitude cheaper to solve compared to the original models. **See Figure 5,** (**above right**) depicting the model reduction of a steam cracker.

The parameter estimation from experimental data remains a major bottleneck in model development. Optimal experimental design (OED) is an essential tool for improving the quality and efficiency of model identification and parameter estimation. One of the common ways to define optimal measurement sets is to use scalar functions of the Fisher Information Matrix (FIM). FIM is constructed using local sensitivities which depend on nominal values of the parameters. This approach is not sufficient for dealing with complex nonlinear problems. To overcome the limitations of the local approach to constructing FIM by the application of global SA, namely by using Sobol' sensitivity indices as elements of the FIM, was suggested. An approach based on the "global FIM" can dramatically reduce experimental cost.

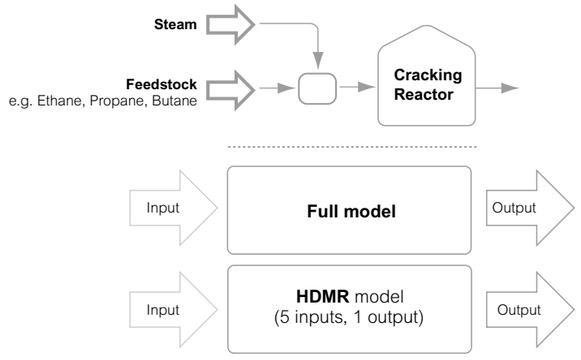


Figure 5. Model reduction of a steam cracker.

Optimal Configuration of Artificial Neural Networks

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.

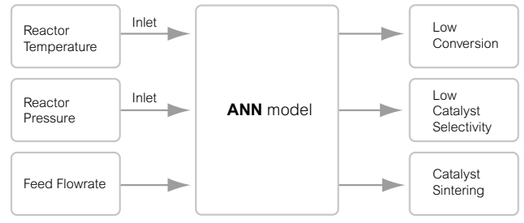


Figure 6. Demonstrates how ANN can be used to model input-output behaviour of the reactor.

Temperature, pressure and flowrate are the major input variables which determine the (output) fault characteristics of low conversion, low catalyst activity and catalyst sintering. For this example, the number of nodes has been reduced from 5 to 3. Another example demonstrates the use of ANN to predict composition of the product from the spectra. ANN is trained by giving spectra inputs for 46 different compositions. The spectra for each input composition is discretized into 30 intervals **Figure 7**, (**below**). The mixed integer approach reduces the number of nodes from 45 to 2. To summarise the key advantages of the proposed approach are: (i) a compact representation of input-output correlations and (ii) elimination of any redundant interconnections.

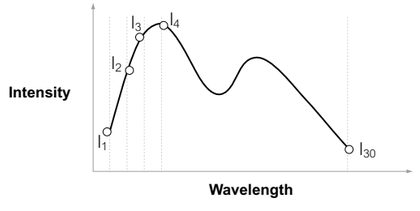


Figure 7. The spectra for each input composition discretized into 30 intervals.

CHEMICAL MANUFACTURING SYSTEMS

APPLICATION DOMAIN 1

Fundamental research across the CPSE on chemical manufacturing systems is described in each of the three competence areas of Modelling & Model Solution Tools; Operations & Control; and Product & Process Design. The process industries served can broadly be classified as bulk chemicals including petrochemicals and oil & gas; pharmaceuticals; specialty chemicals and biofuels.

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

Second generation biofuels

Lignocellulosic biomass, as a source of feedstock for the production of liquid fuels such as ethanol, is potentially an inexpensive option which is easily obtainable and renewable. Such biomass, often categorised as a *second generation* feedstock, unfortunately is difficult to process. The structure of lignocellulose requires pre-treatment before the sugars in the biomass can be converted to ethanol. There are a number of possible pre-treatment steps. One pre-treatment is based on the use of dilute acid. We have developed some initial models for such a pre-treatment, based on experimental data from the literature. These models have been incorporated into the Jacaranda process optimisation system. Results are available (see also **Figure 1**, **overleaf**), comparing the impact of the choice of acid for the pre-treatment of sugar bagasse, a widely available lignocellulosic feedstock.

Peptide tag design and downstream processing synthesis

Downstream processing for the purification of a protein product in biochemical production plants largely determines the quality of the product and is also a major component of the manufacturing and investment costs. Of all separation methods during the downstream process, chromatographic operations are of major interest in the production of high-value biomolecules. The specified purity level of the target protein product is usually achieved by applying several chromatographic steps. Such flowsheets are usually optimised on a unit per unit basis, thus creating the need for a more systematic synthesis and design procedure for purification sequences, which considers the entire process instead of each unit individually. The objective of this project is to develop novel and efficient optimisation-based apporaches for the problem of simultaneously performing an optimal synthesis of chromatographic protein purification processes and the concomitant selection of peptide purification tags that result in a maximal process improvement.

Dynamic modelling and control of multistage flash desalination plant

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

Modelling of reaction/adsorption systems

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

Hydrate prediction in oil-and-gas flows

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

Computer-aided tools for process heat integration

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

Other activities

Other projects within the Chemical Manufacturing Systems application area include air separations and emulsion

polymerisation. There are more details of these projects in the reports on the Product and Process Design and Process Operation and Control competence areas.

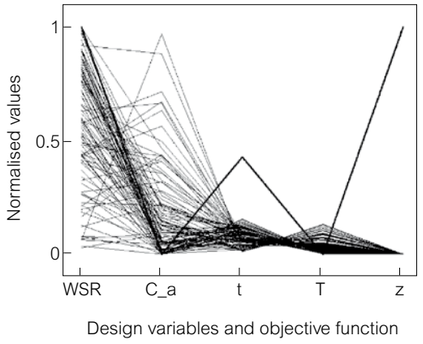
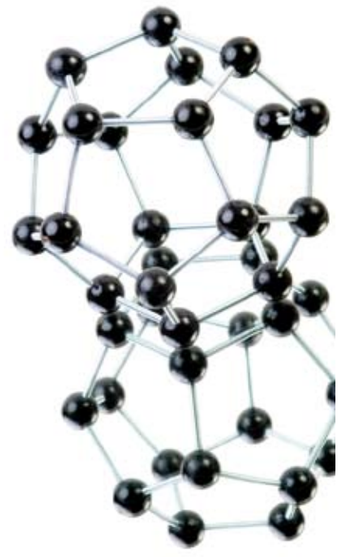


Figure 1. This graph presents a parallel co-ordinate system representation of the 4 dimensional design space with the objective function for the feed pre-treatment in the production of ethanol from lignocellulosic biomass. Each line represents a single point in the design space. The thick line is the initial solution presented to the optimiser in the Jacaranda system. All other lines are the solutions obtained, using a stochastic optimisation method, for a number of runs. All solutions obtained have the same objective function value yet cover a wide region of the domain. The figure shows that the first design variable, WSR, for instance, has little impact on the objective function value whereas the residence time, t, has to be small to achieve the best performance.



MOLECULAR SYSTEMS ENGINEERING

APPLICATION DOMAIN 2

WP1.1: Design of solvents for maximum selectivity and yield

Computer aided molecular design of solvents – Spyridon Konstantinidis

Computer Aided Molecular Design (CAMD) is a powerful method to get to the "Holy Grail" by finding the optimal conditions that will lead you there. The methodology has been used for process wide operations and the results are promising. My work is currently focused on designing solvents for optimal reaction rate constants. Before the CAMD problem is formulated one needs a model of the reaction giving quantitative and qualitative information on how solvents affect the rate constants of reactions. The model employed is empirical and accessible without the need for expensive and complicated calculations. However it is not perfect. To optimize the performance of the model a careful selection of solvents is necessary. Such a selection is based on Design of Experiments (DoE). Alternative models can also be constructed by multivariate projection methods (PCA, PCR, PLS) addressing the deficiencies of the model maintaining at the same time its simple basic structure. Combining DoE with multivariate methods can yield an optimal model. The model can then be used in CAMD to generate the solvents that will maximise the reaction rate constant.

Solvent design for organic reactions – Heiko Strubing

Solvents are widely used in industry (e.g. pharmaceutical industry) and fulfil a variety of roles, such as increasing the reaction rate or facilitating separations. Solvent choice is therefore crucially important to process performance. The current methodology for solvent selection is mainly based on using experimental data in combination with experience. The aim of the project is to develop a computer-aided methodology that accelerates the solvent design process, with a particular focus on the effect of solvent on reactions. By optimising solvents for multistep reactions, "stage-telescoping" can reduce the number of steps in a process, possibly leading to capital cost savings and a reduction in operational complexity. In the past, solvent selection has been approached using computer-aided molecular design, however, significant amounts of solvent and reaction data are required experimentally.
To quantify the solvent effects on reaction performance (indicators could be reaction rate, selectivity and yield), a range of different theoretical chemistry approaches is used for the Menschutkin reaction. The method considered combines empirical models (e.g. the solvatochromic equation) and first-principle calculations (DFT calculations of activation energy and reaction rate, using continuum solvation models). We investigate how such modelling tools can be embedded within a solvent design algorithm, which uses mixed-integer optimisation to identify the molecular structure of the optimal solvent.

WP1.2: Design of functional polymers, block co-polymer and blends

Development of DFT theories to the study of interfacial behaviour – Felix Llovell

This work is focused on the modelling of phase equilibrium and interfacial properties of crude oil mixtures and other complex fluids of industrial interest, through the application of density functional theories (DFT) coupled with molecular SAFT-type equation of state (SAFT-VR). The functional is constructed by partitioning the free energy density into a reference term, described by the use of the Local Density Approximation (LDA), and an attractive perturbation (which incorporates the long-range dispersion interactions). The development to multicomponent mixtures and the improvement of the capability predictions of density profiles, interfacial tension and capillary waves are the current main goals of this research.

Recent Achievements:

Extension of the SAFT-DFT theory to binary mixtures, using some reasonable approximations for short- and long-range molecular interaction terms.

Testing of the new equation to a wide variety of pure fluids, including alkanes (from methane to decane), carbon dioxide, ammonia and water. Calculation of density profiles and surface tension data.

Testing the new equation to several binary mixtures alkane-alkane, CO_2-alkane, alkane-alkanol and alkane-perfluoroalkane. Calculation of density profiles and interfacial tension data.

Extension of Onsager type density functional theories for hard body fluid mixtures – Alexandr Malijevsky

Onsager's second virial theory of hard rods is extended for mixtures of nonspherical hard bodies with finite length-to-breadth ratios using the decoupling approximations of Parsons and Lee. In addition to the second-order approach of Onsager, three different theories are developed from the virial expansion and the virial theorem of the free energy. A scaling approach onto a one component hard-sphere fluid results in the well-known Parsons-Lee theory, while the multi-component hard-sphere decoupling approximation gives two different theories. We refer to the first as the Lee theory of the mixture, and the second one as the Parsons theory. A binary mixture of hard Gaussian overlap (HGO) particles is chosen to test the accuracy of four different theories, namely the Onsager, Parsons-Lee, Lee and Parsons theories. A comparison with the simulation data of Zhou et. al. (Journal of Chemical Physics, 120, 1832 (2004)) suggests that the Parsons theory describes most accurately the properties of the ordering transition and density (pressure) dependence of the order parameters.

A density functional study of interfacial properties of spherical fluid interfaces – Alexandr Malijevsky

The determination of the interfacial tension of planar interfaces between fluid phases is relatively straightforward within classical statistical mechanics. In the case of molecular simulation the mechanical route of Irving and Kirkwood, which requires a knowledge of the tangential and normal components of the pressure, is commonly employed. Within density functional theories (DFTs) one makes use of the thermodynamic identity for the excess grand potential per unit area. The situation is less obvious in the case of curved interfaces: according to the Laplace relation there is a pressure difference on either side of a curved interface which causes complication for the evaluation of the tension via a mechanical route; in the case of small drops of liquid the density (and local pressure) one cannot strictly talk of a uniform value as the density profile can be oscillatory; an evaluation of the tension from the thermodynamic relation of Tolman (to first order in the curvature) is only formally valid for large drops. These complications lead to problems in the determination of the interfacial tension of spherical drops in computer simulation. From the perspective of a DFT approach one can unambiguously define the interfacial tension as the excess grand potential per unit area using a suitably chosen hypothetical bulk reference system. We provide an in depth analysis of the interfacial properties of liquid drops and bubbles of particles interacting via a Lennard-Jones potential (truncated at 2.5) within a fundamental measure theory (FMT). The attractive interactions are treated at the mean-field level using a WCA split of the potential to define a reference hard-sphere fluid. The drop or bubble is stabilised by confining a finite number of particles within a fixed sample volume so that the DFT is formulated in the canonical ensemble. Systems with an external field (hard central spherical repulsive or attractive substrate) are also examined with in grand canonical ensemble. We examine the effect of system size and temperature on the density profiles making a connection with the planar interface which is recovered in the limit of very large drops. At low temperatures an oscillatory profile is obtained which is particularly marked for the small drops making it difficult to define a liquid density. The density of the gas in coexistence with a liquid drop is always found higher than for the planar interface as would be expected from the Kelvin relation (indicating a higher vapour pressure). The interfacial tension is also examined in some detail as a function of the drop size and comparisons are made with the corresponding values obtained for bubbles and systems with external fields. Some preliminary results are also presented for mixtures where liquid drops rich in a given component are dispersed in a liquid which is rich in another component.

Accurate perturbation theories for soft core chains – Thomas Lafitte

This research focuses on the study of the thermodynamic behavior and physical properties of complex mixtures by using equation of state based on Statistical Associating Fluid Theory (SAFT). We have recently developed a new version which models molecules as chains of spherical segments interacting through Mie potentials. This new SAFT-VR equation of state has been applied to real substances (associating and non-associating) for which we show the importance of using a variable repulsive range to simultaneously describe vapour-liquid equilibrium and second derivative properties. In the special case of the Lennard-Jones chains, the theory is seen to provide accurate estimates of the complete vapour-liquid diagram for chains up to 100 segments. The highly accurate representation obtained here for homonuclear chains, will be extended for heteronuclear molecules formed from Mie segments of different type by coupling the current development with the SAFT- gamma group contribution approach (previously developed for square-well potentials).

Recent Achievements:

Development of an accuration perturbation theory for soft core chains which gives comparable results with the Johnson EOS in the special case of the 12-6 fluid.

Extension for heteronuclear molecules formed from Mie segments of different types.

Phase behaviour of surfactant mixtures
– Jens Schreckenberg

The phase behaviour of surfactant mixtures is of great interest, both from the scientific and industrial perspective. Surfactants are used, for example, in pharmaceutical and in oil recovery applications in which they act as emulsifier or adhesive. The liquid phase behaviour, especially, is relevant in many processes. Under certain conditions surfactant mixtures exhibit liquid-liquid separation which, dependent on the process, is beneficial or detrimental. A general problem to be solved in applications dealing with microemulsions (mixtures consisting of water, oil and surfactant) is, for instance, to prepare a stable homogeneous solution of water and oil with as little surfactant as possible. We model the liquid-liquid phase behaviour of water and non-ionic n-alkyl polyoxyethylene ether surfactants, which are often denoted by CiEj. The number of carbons in the hydrophobic alkyl and number of hydrophilic ethoxy groups in the surfactant chain can take any value which allows a wide field of applications in different areas. The phase behaviour of aqueous solutions of these kinds of surfactants is complex. This includes micellization, liquid-liquid immiscibility and formation of liquid crystal structures. In terms of the liquid-liquid immiscibility, this is bounded at higher temperature by an upper critical solution temperature (UCST) and at lower temperature by a lower critical solution temperature (LCST) giving rise to closed-loops of immiscibility. We provide a model for CiEj within the statistical association fluid theory of variable range (SAFT-VR). A SAFT-VR model for (water + oil + CiEj surfactant) microemulsions is also proposed. The phase behaviour of multicomponent mixtures is heavily determined by the features of the respective binary mixtures. SAFT-VR allows to transfer pure component parameters onto component mixtures for which additional cross interaction parameters may need to be specified. The aim is to transfer the surfactant model achieved from aqueous surfactant solutions onto ternary water + n-alkane + CiEj systems.

Recent Achievements:

SAFT-VR calculations dealing with the solubility of CO_2 in polystyrene. Co solubility effects of other gases have also been examined.

WP1.3: Design of organic crystals for enhanced bioavailability

Design of organic crystal structures, chiral separation agents and solvents for organic reactions – Panagiotis (Panos) Karamertzanis

The project focuses on the application of molecular systems engineering approaches to:

(a) Improve the crystalline properties of drug molecules by co-crystal formation. We will design pharmaceutically acceptable excipients for co-crystal formation so that co-crystallisation is thermodynamically feasible and, secondly, the co-crystals have desired properties (including, but not limited to, solubility, morphology and mechanical stability).

(b) Improve the performance of chiral separation processes by diastereomeric salt formation. We will design chiral resolving agents to maximise the thermodynamic stability difference, and hence solubility ratio, of the crystal structures of the resulting diastereomeric salt pair.

(c) Enhance yield and selectivity of organic reactions by solvent design. We will advance the prediction of solvent properties from the molecular structure and subsequently use these predicted properties as input in implicit-solvent quantum mechanical calculations to predict reaction mechanisms and kinetics. We will then aim to invert the mapping between molecular structure and reaction rate to design optimal solvents for given reactions.

The project's scope encompasses both the development of rigorous models for the modelling of interactions at the atomic/molecular level and numerical methods. In particular, research strands (a) and (b) involve the development of a state-of-the-art lattice modelling package to minimise the Gibbs free energy and compute the properties of crystals using accurate, theoretically well-justified models for the intermolecular forces and molecular distortions. Research strand (c) involves the development of robust and efficient numerical strategies to identify transition states on complex, ab-initio derived potential energy surfaces.

Design of organic crystals for enhanced bioavailability – Andrey Kazantsev

Many organic molecules form multiple crystalline forms ("polymorphs"). The precise crystal structure has a significant effect on the properties of the crystalline material. In the case of active pharmaceutical ingredients (APIs), different polymorphs often have widely different solubilities, which results in significant differences in the bioavailability of the corresponding drug. A given API will form only a relatively small number of polymorphs which may not, in themselves, have the desired combination of bioavailability and stability. However, it is often possible to combine the API with other species to form different crystal structures without affecting the intrinsic biological efficacy of the API. To date, the task of finding appropriate combinations for a given API has been carried out in a semi-empirical fashion, relying heavily on both experience and experimentation. The aim of this project is to develop effective computational techniques which can complement and accelerate existing approaches, and enhance their reliability. As salts and co-crystals can exhibit a high degree of polymorphism, the computational techniques will aim to reduce the time required for screening any molecule proposed as a candidate for combining with the API within a crystal, identifying all possible polymorphs and assessing their relative stability.

Recent Achievements:

Proposed a methodology to minimise stable packing arrangements of cocrystals containing flexible molecules. The results from the study provide a significant step towards the rationalisation of cocrystal formation.

Developed a computationally efficient lattice energy minimisation algorithm for flexible molecules. The method allows optimisation of large set of flexible molecular degrees of freedom and/or the use of more accurate quantum mechanical basis sets.

WP1.4: Design of microemulsions and liquid crystal mixtures

Self assembly of liquid crystals
– Andrew J. Crane

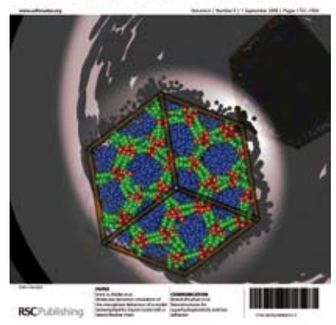
We have performed coarse-grained simulations of a model of a bolaamphiphile liquid crystal molecule with a grafted flexible side chain. The coarse-graining approach employed is based on minimising the attractions present in the system, on the premise that the most important features of the liquid structure stem from the balance between the close range repulsions and the strong directional forces typical of hydrogen bonding and association. The model consists of six fused rigid spheres, where the two end spheres have a significant attraction amongst themselves while the rest are repulsive in nature. A weakly self-attracting lateral chain consisting of fully flexible tangently bonded spheres is attached to one of the central spheres. A parametric study is made of the configurations of collectives of these molecules at temperatures that span from the isotropic fluid range down to the onset of crystallization. The underlying rigid core molecules (with no side chain) are set up to exhibit a smectic liquid crystal behaviour. Upon increasing the number of spheres in the lateral chains from 1 to 12, the liquid regions exhibit a rich variety of self-assembled structures; for small number of lateral spheres columnar arrays of different cross sections (triangular, square, rectangular, hexagonal) are obtained and for the longer chains lamellar structures of different interlayer spacing are observed. We showcase and give a rational physical explanation for the global phase behaviour of the model, based on pertinent order parameters and apparent diffusivities of the several regimes encountered. The model is inspired in the reported synthesis of a family of T-shaped polyphilic molecules (C. Tschierske, Chem. Soc. Rev., 2007, 36, 1930-1970) where some of the above mentioned phases have been inferred from experimental measurements.

Recent Achievements:

The coarse-grained Bolaamphiphile work has been extended to mixtures with coarse-grained solvent particles. Here the effect of solvent on phase geometry has been investigated, with the results showing that solvents may aid the tuning of the system to the required structured phase.

Work into the systematic coarse-graining of small molecules has begun. Programs to calculate both angular averaged potentials and potentials that reproduce all-atom structural data have been developed. An investigation of the validity of these approximation schemes has begun, through molecular dynamics gas-liquid coexistence simulation studies.

A study into how attractive end groups effect the liquid crystalline phase behavior of rod molecules has begun. A thermodynamic integration scheme has been produced to accurately determine phase coexistence points between the liquid crystalline phases. A Gibbs-Duhem type program to trace the coexistance lines is being developed. These are the tools required to study this system.



Soft Matter v4 p1820 (2008)

Computer simulation of ionic and dipolar systems – Carlos Avendaño

Dispersions of anisotropic colloids and several ionic and dipolar liquids can show liquid crystalline phases. Examples of these kinds of systems are rodlike colloidal particles and rodlike viruses that can exhibit orientational and positional order. An accurate description of these complex materials is very important due to their broad applications in many advanced technologies and in connection with relevant theoretical issues. Over the years, theoretical work on charged and dipolar elongated molecules has been published; however, the analysis of these systems by molecular simulation is more demanding due to the high computational time needed to handle the long-range interaction and all the degrees of freedom presented in the systems. By these reason we are interested in the computer simulation of charge and dipolar systems with spherical and non-spherical geometries using coarse-grained models in order to reduce the complexity of the systems to make the simulation a tractable approach.

Recent Achievements:

Development of different methodologies to represent the properties of water using Molecular simulation and SAFT-related models.

Coarse grain models of discotic liquid crystal molecules to study the self-assembly process using moleclar dynamics.

Phase diagram of mixtures of hard body particles to represent the properties of lyotropic liquid crystals.

Extension of Onsager type density functional theories for hard body fluid mixtures – Alexandr Malijevsky

Onsager's second virial theory of hard rods is extended for mixtures of nonspherical hard bodies with finite length-to-breadth ratios using the decoupling approximations of Parsons and Lee. In addition to the second-order approach of Onsager, three different theories are developed from the virial expansion and the virial theorem of the free energy. A scaling approach onto a one component hard-sphere fluid results in the well-known Parsons-Lee theory, while the multi-component hard-sphere decoupling approximation gives two different theories. We refer to the first as the Lee theory of the mixture, and the second one as the Parsons theory. A binary mixture of hard Gaussian overlap (HGO) particles is chosen to test the accuracy of four different theories, namely the Onsager, Parsons-Lee, Lee and Parsons theories. A comparison with the simulation data of Zhou et. al. (Journal of Chemical Physics, 120, 1832 (2004)) suggests that the Parsons theory describes most accurately the properties of the ordering transition and density (pressure) dependence of the order parameters.

BIOLOGICAL SYSTEMS ENGINEERING

APPLICATION DOMAIN 3

CPSE's research in the area of Biological Systems Engineering currently involves activities in the fields of systems biology, mammalian cell biotechnology and biomedical engineering.

Systems Biology

Research in Dr. Krishnan's group has focussed on different aspects of biological modelling and systems biology. One aspect has been the modelling of signalling networks involved in chemotaxis in eukaryotes, both chemoattraction and chemorepulsion. This involves the development of models of signal transduction which involves biochemical complexity, combined feedforward and feedback regulation and a spatial aspect to signalling. A second aspect has been the investigation of translation in yeast, in particular the role of feedback effects in translation termination and how this regulates the translation process. This project involves modelling and non-linear dynamical analysis of this naturally occurring feedback control system in collaboration with biologists at the School of Medical Sciences at the University of Aberdeen. A third aspect is the theoretical analysis of signal processing features and capabilities of minimal signalling modules in different contexts.

In Prof. Bogle's group, work is underway on modelling endothelial cell response to fluid flow. ***In vitro*** endothelial cells respond to fluid flow by elongating in the direction of flow. The most studied and crucial aspects to this response are; actin filament alignment, mechano-transduction, signal transduction, RhoGTPase localised activation and lamellipodia formation. The goal of this project is to understand how these separate facets interact and lead to a coordinated response. The flow is modelled over a 3D virtual cell, which naturally gives the force the flow exerts on the cell surface via a boundary integral representation. This force is coupled to a Kelvin-body model of mechano-transduction which links, via a focal adhesion associated protein- Src, to a PDE model of the Rho GTPases Rac and Rho. The PDEs are integrated over a 2D projection of the 3D cell a giving a time course for protein concentration at any point in the cell. It is demonstrated that a mechano-transducer that can respond to the normal component of the force is likely to be necessary (though perhaps not sufficient) component of the signalling network.

Moreover, the group is working on the task of model evaluation and validation in Systems Biology of physiological systems, and in particular the liver. The focus has been on the assessment of the uncertainty in the output of the glucose homeostasis models, as a result of uncertainty in model inputs, and how to apportion the source of this uncertainty to the different inputs. In most applications of sensitivity analysis the model output of interest is a scalar value, however here we are interested in the entire time-course of the model output. To look at the entire time-course, we have expanded the model output using some form of basis set representation (in the first instance the principal components of the output) and to look at how the coefficients of this expansion (themselves scalar values) vary with the model inputs by applying standard sensitivity analysis techniques.

Mammalian Cell Biotechnology

Research in biotechnology focuses on the systematic integration of mathematical modelling with cell culture experimentation and analytical techniques. Dr. Kontoravdi's group is working on product quality and metabolic flux analysis. Specifically, we are working on assessing and modelling the interactions between bioprocess conditions and protein glycosylation in antibody-producing mammalian cell cultures by employing a combination of bioprocessing and glycoproteomics techniques. A number of experimental studies have identified a relationship between extracellular conditions in cell cultures, oligosaccharide production and the sugar profile of the proteins produced. This becomes particularly important when the protein product of interest is a therapeutic, such as a monoclonal antibody, the *in vivo* efficacy of which highly depends on its sugar structure.

We are also working on elucidating the metabolic pathways in GS-CHO cells. The glutamine synthetase (GS) expression system is one of the most efficient mammalian ones and is used by over eighty biotechnology and pharmaceutical companies for the production of therapeutic products. However, our knowledge about how this system alters the cellular metabolic pathways, in particular those responsible for the synthesis of glutamine – one of the major nutrients – is limited. Our work aims to identify and model the metabolic pathways responsible for glutamine synthesis in CHO cells transfected with the GS system. It functionally combines model-based engineering tools with NMR analysis of isotope-labelled metabolite distribution to tackle the research problem.

At the same time, we are continuing our research in the application of advanced analysis methods to models of biological systems. Our efforts are focusing on advanced, variance- and derivative-based global sensitivity methods for parameter analysis at a reduced computational load, as well as optimal experiment design applications for model validation and parameter estimation. A future goal is the development and validation of metamodels, derived using high dimensional model representation techniques, for online applications such as process optimisation and control.

Biomedical Engineering

Dr Mantalaris and his group are continuing their work on stem cell bioprocessing. Our efforts are focusing on improving bioreactor design for a variety of biomedical applications, such as the differentiation of stem cells to pneumocytes and the stimulation of bone or cartilage tissue engineering. Moreover, work is ongoing on the systematisation and standardisation of stem cell differentiation techniques and systems through the use of high-throughput screening methods.

Professor Pistikopoulos and his team are aiming to create new computer-based systems that can calculate the most effective, safe dose of a drug or anaesthetic for an individual patient by using novel mathematical programming methods that can take account of and control for a multitude of different parameters. These systems would use information about the patient's makeup and medical history, together with data on how different drugs perform and interact with each other. They would provide fast and reliable methods to help doctors devise the best tailor-made drug regimes for conditions such as cancer and HIV. The new systems would also help anaesthetists to decide on the best dosage of anaesthetic for each patient, prior to an operation. The researchers also want to explore whether a similar system could be used to create a device to help people with diabetes who inject themselves with insulin to manage their condition. This device would read the patient's blood sugar level and then calculate and deliver the most effective dose of insulin, depending on this readout. This research into the Modelling, optimisation and control of biomedical devices – MOBILE – is funded by the highly prestigious Advanced Grant awarded by the European Research Council.

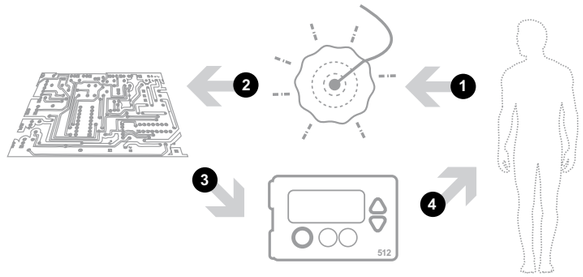


Figure 1. Overall vision of integrated insulin delivery systems based on MOBILE's developments.

Step 1: The sensor measures the glucose concentration from the patient. **Step 2**: The sensor then inputs the data to the controller which analyses it and implements the algorithm. **Step 3**: After analyzing the data the controller then signals the pump to carry out the required action. **Step 4**: The insulin pump delivers the required dose to the patient intravenously.

SUPPLY CHAINS OF THE FUTURE

APPLICATION DOMAIN 4

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

Sustainability

- Exploiting new energy and material sources;
- Cleaner exploitation of existing sources (e.g. high-carbon fossil fuels);
- Resource efficiency to deal with increasing scarcity of non-fuel resources (e.g. water and minerals);
- Decarbonised supply chains;
- Reduction of waste and landfill.

Supporting Healthcare

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

Exploiting the advances in biosciences to develop customised healthcare products.

Commercialising Innovation

Exploiting rapid advances in the physical and biological sciences (e.g. nanotechnology) along with new manufacturing techniques to translate these into mass customised innovative products. These challenges will require a holistic approach to the underlying science, the process engineering and the structuring of the supply chain, and therefore fall squarely into the remit of multi-scale process engineering. Some examples of our work in this area include:

Energy and materials from biomass

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

focussing on a whole-systems approach to bioenergy via multi-scale modelling to address questions such as these.

Carbon dioxide infrastructures

Long-term infrastructure planning must also account for improvements in technology and processes. A good example of this is carbon dioxide. The growing international pressures for low-carbon economies are likely to lead to the emergence of CO_2 infrastructures, based around carbon capture and storage (CCS). The objective of our research in this area is to develop a holistic optimisation-based methodology for CCS network infrastructure in countries such as the Netherlands and the UAE that takes into account: optimum performance under different targets, policies and time; life cycle CO_2 emissions; safety, operability and controllability. This complex goal can be achieved by integrating multi-scale optimization models namely: CO_2 source plant, CO_2 capture plant and CO_2 network design coupled with the data, models, and experiments linked mainly with the storage site.

Key decisions outlined from the detailed optimisation-based model are to answer the following questions:

What are the existing CO_2 sources included in the model?

And what is the CO_2 capture level necessary to meet the objective function (e.g. cost or life cycle CO_2 emissions)?

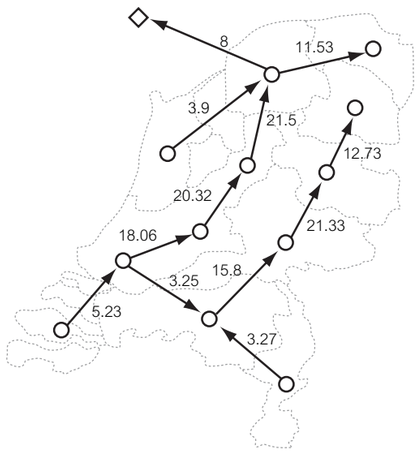
Where might new CO_2 sources emerge in the future?

What is the optimum CO_2 network design of the model (e.g. transportation modes, layout)?

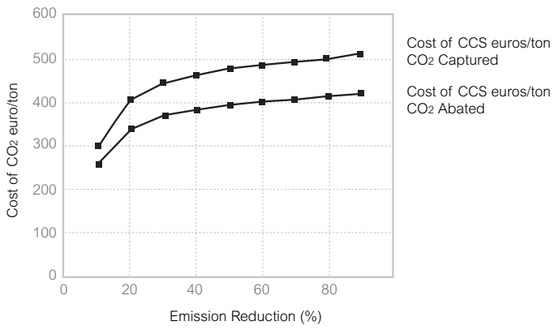
Is there any opportunity to integrate between capture plant and process plant ?

How to deal with the uncertainty in the future CO_2 reduction targets, which are usually governed by legalisation, potential for EOR, capacity and dynamics of reservoirs ?

An example of our results is below and above right. It shows a CO_2 infrastructure for the Netherlands and illustrates how the total cost per ton varies with degree of emissions reduction.



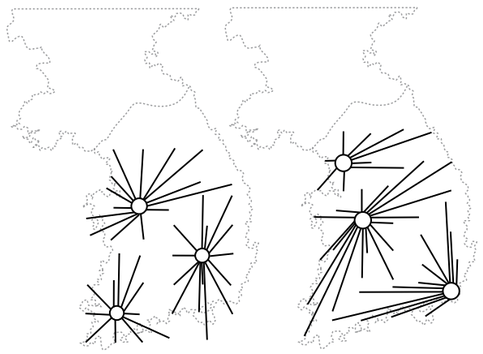
Scenario 4 - emission reduction 90% Gasfields only.



Closed loop supply chains

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

The diagrams below show our redesign of a fluorescent lamp recycling network; the optimised network has a 60% reduction in transport energy and emissions.



South Korea – Existing network Optimised network

ENERGY SYSTEMS ENGINEERING

APPLICATION DOMAIN 5

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

Energy-related activities at Imperial College span several departments and centres including the Energy Futures Laboratory which coordinates college-wide initiatives in this area, the Centre for Transport Studies, the Innovation Studies Centre, the Centre for Environmental Policy, the Control and Power group in E&E Engineering, the Departments of Earth Sciences and Engineering, Civil Engineering and Chemical Engineering.

CPSE personnel contribute to a new interdepartmental MSc in Sustainable Energy Futures, run by the Faculty of Engineering on behalf of Imperial College. Energy systems research within the CPSE relates to oil and gas production, clean routes to fossil fuel production, electric grids, fuel cells, and energy-integrated cities.

Overall, our methodology involves combining and integrating models and goes by the title “Energy Systems Engineering”. Two examples of this include the design of polygeneration systems and urban energy systems.

Design of clean coal polygeneration systems

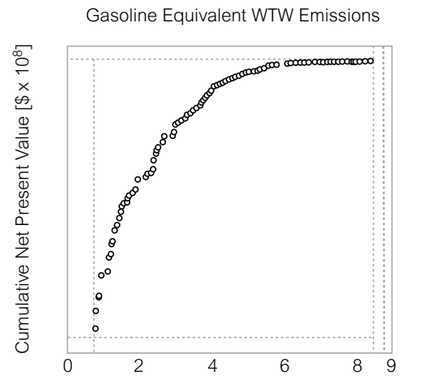
Coal-based alternative fuels and chemicals are expected to play a crucial role in countries such as China’s near-term (up to 2020) transition of conventional energy and chemical industry to a more sustainable and environmentally benign mode. Many important issues need to be tackled during this fast developing stage for a successful and efficient transition, in terms of resource availability, allocation of production sites, adoption of technologies, arrangement of transportation methods and routes, and future market and other uncertainties.

Coal (and biomass) polygeneration systems involve gasification, separation and chemical conversion. This results in large scope for alternative configurations and pathways, many of which result in CO_2 streams which are relatively easy to sequester. The complex option space and opportunities for optimisation mean that this is an ideal system for the application of energy systems engineering. Here, we use a superstructure to embed the different alternatives and explore how different optimisation criteria (e.g. economic, environmental) give rise to different structures. **Figure 1**, (**right**) shows the superstructure for a combined power generation/ methanol production system and a greenhouse gas/economics tradeoff curve.

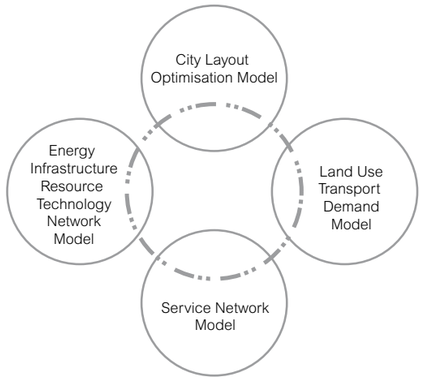
Urban energy systems

The BP Urban Energy Systems project at Imperial will identify the benefits of a systematic, integrated approach to the design and operation of urban energy systems, with a view to at least halving the energy intensity of cities.

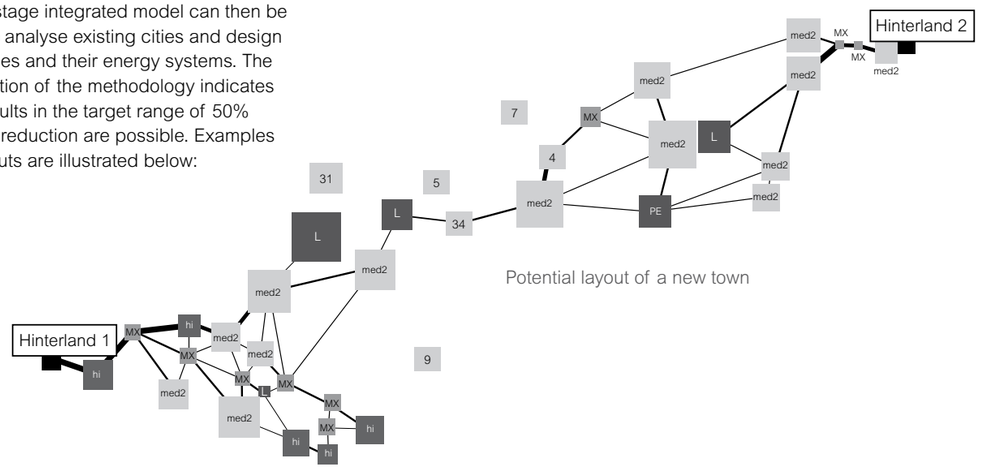
This challenging, multidisciplinary project is organised into three overlapping phases. The first phase (2006-2010) is concerned with identifying in broad terms the potential of the proposed modelling and optimisation approach, will deliver an estimate of the potential benefits to different classes of cities, and will identify the means and business models required to achieve these objectives. Later phases will address detailed design issues and implementation.



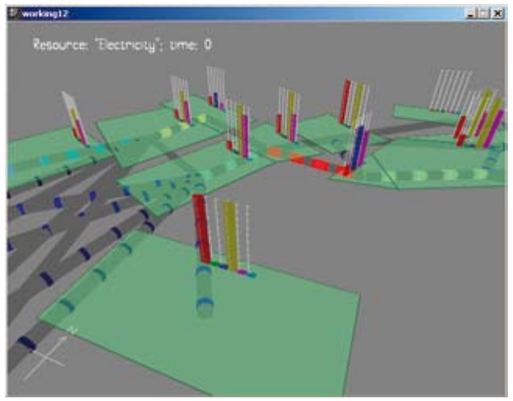
The Synthetic City toolkit has arisen out of our conceptual framework for the modelling of urban energy systems. It combines an integrated data management and simulation executive with four interacting modelling tools in a hierarchical framework, as in the figure (**overpage**).



This 4-stage integrated model can then be used to analyse existing cities and design new cities and their energy systems. The application of the methodology indicates that results in the target range of 50% energy reduction are possible. Examples of outputs are illustrated below:



Potential layout of a new town



3-D visualisation of optimisation results


Dr Claire Adjiman p.29


Professor Roger Benson p.30


Professor David Bogle p.31


Professor Nigel Brandon p.31


Dr Vivek Dua p.32


Professor Eric Fraga p.32


Dr Amparo Galindo p.33


Dr Michael C. Georgiadis p.33


Dr Charles D. Immanuel p.35


Professor George Jackson p.36


Dr Cleo Kontoravdi p.39


Dr J.Krishnan p.39


Dr Daniel Kuhn p.40


Professor Geoffrey Maitland p.40


Dr Athanasios Mantalaris p.41


Professor Costas C. Pantelides p.42


Dr Lazaros Papageorgiou p.42


Professor Efstratios N Pistikopoulos p.43


Professor Berc Rustem p.45


Professor Paul Rutter p.46


Professor Roger W. H. Sargent p.46


Professor Nilay Shah p.47


Dr Eva Sørensen p.47


Professor Nina Thornhill p.47

STAFF PROFILES

2008

CLAIRE S. ADJIMAN

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

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). Model-based assessment of design of energy conversion systems. Development of property prediction techniques integrating different scales of modelling (from quantum mechanics to advanced equations of state). Global analysis techniques, such as global optimisation or global sensitivity analysis.

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

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

Other Activities

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

Reviewer for

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

Academic Collaborations

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

Industrial Collaborations

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

ROGER BENSON

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

Industrial Positions prior to semi retirement

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

Industrial positions

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

Qualifications

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

Awards and Distinctions

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

Other activities

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

Academic Collaborations

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

Publications
Book

Benchmarking in the Process Industries; Prof. M. Ahmed, Prof. R.S. Benson. Published by I Chem E in May 1999. ISBN 0 85295 411 5

Journal Articles

Passing the agility test, Professor Roger Benson, FREng and Dr Peter Norman, The Chemical Engineer, Issue 804, June 2008, Page 22-23

Off Shoring Lifecycle Production is not the only answer, Professor Roger Benson, FREng, ISPE Journal, Volume 27, Number 4, July/August 2007, Page 22- 32

Batch cycle time – a forgotten opportunity; Professor Roger Benson, FREng, Speciality Chemicals Magazine, December 2006

Off Shoring production is not the only answer; Professor Roger Benson, FREng, Speciality Chemicals Magazine, April 2006

From World Class Research to World Class Manufacturing: The Challenges; Professor Roger S Benson FREng; Pharmaceutical Engineering, September/ October 2005, Page 100

Benchmarking – An Art or a Science?; Professor Roger Benson, FREng, ABB Eutech, UK; Lynne McGregor, Maintenance and Asset Management, Volume 20 No 1, Spring 05

Patient heal Thyself; Editorial, Drug Discovery Today, Volume 10, Number 3, pp.159 – 161, February 1 2005

From Good Manufacturing Practice to Good Manufacturing Performance, Professor R S Benson, Jim D J McCabe; Pharmaceutical Engineering; July/August 2004

Conference Contributions
Invited Lectures and Seminars

Why Operastional Excellence is Essential for Survival, Professor Roger Benson FREng, Operational Excellence in Pharmaceuticals & Medical Devices, London, 16 October 2008

Future Challenges – Process Control, Professor Roger Benson FREng, Institute of Chemical Engineers PMCSG , London, 25th September 2008

Maintaining Your Momentum; Professor Roger Benson FREng, PHARMATEX 2008, Cork, Ireland, 16 September 2008

Offshoring Life Science Production is Not the Only Answer; Professor R S Benson FREng, Pharmaceuticals Manufacture Survival in the 21st Century, Institute of Mechanical Engineers, 5 June 2008

A Business Perspective on the Benefits of Real-Time Data Integration, Professor R S Benson FREng; The Institute of Engineering and Technology Seminar on Enterprise Integration and Control Systems; The University of Warwick, 23 November 2006

Meeting the Far Eastern Challenge Through Innovative Manufacturing; Professor R S Benson FREng; European Fine Chemicals Conference, 1 - 2 December 2005, Manchester

How Management and Workforce Can Combine to Create World Class Manufacturing and Service Business; Professor R S Benson; Print 2005 Congress; 3 - 4 October , London

Ensuring Process Manufacturing Remains Competitive in the Future; Professor R S Benson FREng & M Grady; World Chemical Engineering Congress, Glasgow, 10 – 14 July 2005

Meeting the Far Eastern Challenge; Professor R S Benson FREng, PICME Conferences; Edinburgh, Humberside, Slough, Huddersfiled; Profiting from Manufacturing Excellence – Developing Lean and Agile Manufacturing. 2005

I DAVID L. BOGLE

Professor of Chemical Engineering.

Qualifications

BSc (Eng) Hons MSc PhD DIC CEng

Awards and Distinctions

FREng FIChemE.

Research Interests

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

Other Activities

Head of the UCL Graduate School. Member of College of Engineering for the Engineering & Physical Sciences Research Council (EPSRC). Member of BBSRC Integrative and Systems Biology Strategy Panel. Member of BBSRC Bioscience Skills and Careers Panel, Chair BBSRC Working Group on Systems Biology Training, University of Sheffield Chemical Engineering at the Life Science Interface International Advisory Board.

Committee member of Computer Aided Process Engineering Subject Group of Institution of Chemical Engineers. Member of European Federation of Chemical Engineers Working Party on Computer Aided Process Engineering (UK representative). Member of Board of Engineering Council UK. Member of International Federation of Automatic Control (IFAC) Technical Committees on Chemical Process Control and on Control of Environmental Systems. Member of Natural Sciences Committee of the U.K.'s National Commission for UNESCO. Member of Board of the Engineering Council UK.

Reviewer for

BBSRC, EPSRC, Leverhulme Trust, AIChEJ, Chemical Engineering Science, Industrial and Engineering Chemistry

Academic Collaborations

Centre for Mathematics and Physics in the Life Sciences and Experimental Biology (UCL), University of Palermo, University of Kuwait

Publications
Book Chapters

Zilinskas J. and Bogle I.D.L. (2007) A **Survey of Methods for the Estimation of Ranges of Functions Using Interval Arithmetic**. In Models and Algorithms for Global Optimization, Springer.

Journal Articles

Repke, J.-U., Klein, A., Bogle I.D.L and Wozny G. (2007) **Pressure Swing Batch Distillation for Homogeneous Azeotropic Separation**, TransIChemE, PartA 85/ (A4) 492-501

Saffrey P., Margoninski O., Hetherington J , Varela Rey M., Yamaji S., Bogle I.D.L, Finkelstein A., and Warner A. (2007) **End to end information management in Systems Biology**. Trans on Comput. Syst. Biol.VIII, LNBI 4780, 77-91.

Zilinskas J. and Bogle I.D.L. (2007) **Global Optimization: Interval Analysis and Balanced Interval Arithmetic**. In Encyclopedia of Optimization ed Pardalos and Floudas, Kluwer.

Conference Contributions

Laftah Z., Abdul Aziz T.Z.T., Bogle I.D.L. (2007) **Identifying Added Value in Integrated Oil Supply Chain Companies – A Case Study**. In Proc. ESCAPE17 Bucharest 769-774 ed. V. Plesu and P.S. Agachi, Elsevier.

Gomes, M.V.C., Bogle I.D.L., Biscaia JR E.C., and Odloak D. (2008) **Using kriging models for real-time process optimization**. In Proc ESCAPE 18, Lyon 361-366, Elsevier. Invited Lectures and Seminars

Bogle I.D.L. and Warner A.W., **A Systems Approach to Glucose Homestasis** presented at BBSRC Workshop on Adopting a Systems Approach to Animal Physiology

Bogle I.D.L., **Nonlinearity and Multiplicity in Intensified Processes**, Keynote lecture at IWPI 2008, International Workshop on Process Intensification, Tokyo, Sept 2008

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 2007 Silver Medal Royal Academy of Engineering

Research Interests

Fuel cell science, engineering and technology. Energy systems analysis

Nigel Brandon's research involves the quantitative analysis of energy systems, with a particular focus on the design, characterisation, modelling, control and optimisation of fuel cells. His present research work encompasses high temperature Solid Oxide Fuel Cells (SOFCs), metal supported Intermediate Temperature-SOFCs, and lower temperature Polmyer Fuel Cells. He collaborates extensively with industry in this field, as well with other research centres and universities around the world. He leads the EPSRC 'Supergen' Fuel Cell consortia, and the fuel cell topic within the UK Energy Research Centre

Other Activities

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

VIVEK DUA

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

Qualifications

PhD in Chemical Engineering, Imperial College London, MTech in Chemical Engineering, Indian Institute of Technology, Kanpur. BE (Honours) in Chemical Engineering, Panjab University, Chandigarh Research Interests Optimal Configuration of Artificial Neural Networks, Variable Horizon Model Based Control

Other Activities

Member Synthetic Biology Network

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

Academic Collaborations Eastman Dental Institute

Publications
Book Chapters

V. Dua, K. Kouramas, S. Pistikopoulos (2009) **Global Optimization Issues in Parametric Programming and Control**, Fields Communications Series, Volume #55 - Workshop on Global Optimization, P.M. Pardalos and C.A. Floudas (eds.).

Dua, P., Dua, V., Pistikopoulos, E. N. (2009) **Model based control for drug delivery systems**, Encyclopaedia of Optimization, Editors: C. A. Floudas and P. M. Pardalos.

Dua, V., Pistikopoulos, E. N. (2009) **Self dual parametric method for linear programs: criss cross method**, Encyclopaedia of Optimization, Editors: C. A. Floudas and P. M. Pardalos.

Dua, V., Pistikopoulos, E. N. (2009) **Parametric mixed integer nonlinear optimization**, Encyclopaedia of Optimization, Editors: C. A. Floudas and P. M. Pardalos.

Dua, V., Pistikopoulos, E. N. (2009) **Parametric linear programming: cost simplex algorithm**, Encyclopaedia of Optimization, Editors: C. A. Floudas and P. M. Pardalos.

Dua, V., Pistikopoulos, E. N. (2009) **Multiparametric mixed integer linear programming**, Encyclopaedia of Optimization, Editors: C. A. Floudas and P. M. Pardalos.

Dua, V., Pistikopoulos, E. N. (2009) **Multiparametric linear programming**, Encyclopaedia of Optimization, Editors: C. A. Floudas and P. M. Pardalos.

Dua, V., Pistikopoulos, E. N. (2009) **Bounds and solution vector estimates for parametric NLPs**, Encyclopaedia of Optimization, Editors: C. A. Floudas and P. M. Pardalos.

Conference Contributions

Dua, V. (2008) **Automatic Selection of Optimal Configuration of Artificial Neural Networks**, Population Approach Group in Europe, Marseille.

Dua, V. (2008) **Modelling and control of intracellular gene delivery**, 2nd International Symposium on Cellular Delivery of Therapeutic Macromolecules.

Invited Lectures and Seminars

Hybrid Modelling Strategies for Biological Systems (2008), IChemE Systems Biology Workshop, Imperial College London.

ERIC S. FRAGA

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

Qualifications

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

Research interests

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

Other Activities

EPSRC: Member of Peer Review College. Member of the International Editorial Board for the Information Technology and Control journal. External examiner for the undergraduate programme in Information Technology, University of Kingston

Reviewer for

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

Academic Collaborations

University of Edinburgh, UK; University of Teesside, UK.

Publications
Journal Articles

T A M Barakat, E S Fraga & E Sørensen (2008), **Multi-objective optimisation of batch separation processes**, Chemical Engineering & Processing 47:2303-2314, doi:10.1016/j.cep.2008.01.005.

A Yang, B Braunschweig, E S Fraga, Z Guessoum, W Marquardt, O Nadjemi, D Paen, D Piñol, P Roux, S Sama, M Serra & I Stalker (2008), **A Multi-Agent System for Facilitating Component-based Process Modelling**, Computers & Chemical Engineering 32:2290-2305, doi:10.1016/j.compchemeng.2007.11.005.

Conference Contributions

A Abiola, E S Fraga & P Lettieri (2008), **Sustainability Assessment of Ethanol Production**, in A Sayigh (editor), World Renewable Energy Congress – WREC X, paper BM50, ISBN: 978 008 056 8973.

I D Stalker, E S Fraga, A Yang & N D Mehandjiev (2008), **Service-oriented CAPE: A new direction for software applications, in B Braunschweig & X Joulia (editors)**, 18/th/ European Symposium on Computer Aided Process Engineering (ESCAPE-18), Computer-aided Chemical Engineering 25:611-616 (Elsevier), paper FP-00282, ISBN: 978-0-444-53227-5.

I D Stalker & E S Fraga (2008), **Towards an interface standard for automated synthesis tools: a proposal**, in B Braunschweig & X Joulia (editors), 18/th/ European Symposium on Computer Aided Process Engineering (ESCAPE-18), paper FP-00283, ISBN: 978-0-444-53228-2.

E S Fraga (2008), **A Lindenmayer system for heat exchanger network design with stream splitting, in I C Parmee (editor)**, Adaptive Computing in Design and Manufacture 2008: Proceedings of the Eighth International Conference. Paper 2.2 (10 pages). ISBN: 978-0-9552885-1-7.

G Fiandaca, E S Fraga & S Brandani (2008), **A multi-objective genetic algorithm for the design of Pressure Swing Adsorption**, in I C Parmee (editor), ``Adaptive Computing in Design and Manufacture 2008: Proceedings of the Eighth International Conference.'' Paper 2.3 (10 pages). ISBN: 978-0-9552885-1-7.

Invited Lectures and Seminars

Invited workshop participation in data analytics with BP; Keynote presentation at Stinkfest 2008; Invited presentation at special session of ESCAPE-18, Lyon; seminars in the departments of Chemical Engineer at the University of Newcastle and the University of Alberta.

AMPARO GALINDO

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

Qualifications

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

Awards and Distinctions

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

Research Interests

My research interests are two-fold: the development of statistical mechanical approaches for complex systems, and their application to processes relevant to industry.

The tools of statistical mechanics and computer simulations offer a privileged molecular perspective of increasingly complex systems. My interest in this field is to develop fundamental approaches to contribute to the understanding of experimental systems, with a special focus on chemical processes. The goal is to be able to truly predict complex phase behaviour.

The types of problems I am interested in at the moment include charged systems, near-critical and supercritical separations, mixtures of polymers and liquid crystals, and solid phases of chain molecules. The impact and exposure of this work is maximised through collaborative efforts in which the aim is to promote the transfer of the theoretical developments into tools for the design and synthesis of chemical processes and products.

Other Activities

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

Reviewer for

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

MICHAEL C. GEORGIADIS

Associate Professor of Process Optimization, Department of Engineering Informatics and Telecommunications, University of Western Macedonia, Kozani 50100, Greece.

Qualifications

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

Awards and Distinctions

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

Research Interests

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

Other Activities

Independent Expert of the European Commission (evaluator of RTD projects under the NMP/FP7 and ENERGY/FP7 programmes). Member of the Scientific Committer of the European Congress of Chemical Engineering 7. Copenhagen September 2007. Member of the Scientific Committee of PRES'2008, 24 - 28 August 2008, Prague - Czech Republic

Reviewer for

Chemical Engineering Research and Design; AIChE Journal; Computational Management Science, Chemical Engineering Science, European Journal of Operational Research; Chemical Engineering Research and Design; Computers and Operations Research

Academic Collaborations

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

Industrial Collaboration

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

Publications
Books

Co-editor (with Dr. Panos Seferlis) of the special Computer-Aided Chemical Engineering Book **The Integration of Process Design and Control** ELSEVIER B.V., May 2004, ISNB: 0-444-51557-7

M.C. Georgiadis and E.N. Pistikopoulos (2006). **Energy and process integration** Textbook. Begell House Inc, Connecticut, USA. ISBN: 1-56700-228-5

E.N. Pistikopoulos, M.C. Georgiadis, V. Dua (2007). Process Systems Engineering. Volume I. **Multi-parametric Programming: Theory, Algorithms and Applications**. WILEY-VCH, ISBN: 978-3-527-31691-5

E.N. Pistikopoulos, M.C. Georgiadis, V. Dua (2007). **Process Systems Engineering. Volume II. Multi-parametric Model-Based control: Theory and applications**. WILEY-VCH ISBN: 978-3-527-31692-2

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M.C. Georgiadis, E.S. Kikkinides, E.N. Pistikopoulos (2008). **Process Systems Engineering. Volume V. Energy Systems Engineering**, WILEY-VCH, ISBN: 978-3-527-31694-6

Chapters in Books

P. Seferlis and M.C. Georgiadis, **The Integration of Process Design and Control – Summary and Future Directions**, In: The Integration of Process Design and Control, pp. 1-9, Elsevier, 2004. ELSEVIER, ISBN: 0-444-51557-7.

Georgiadis, M.C. and E.N. Pistikopoulos. **Process Synthesis** In Computer-Aided Process and Product Design (L. Puigjaner and G. Heyen, editors), Wiley-VCH Publisher, ISBN 3-527-30804-0.

Georgiadis M.C. and P. Tsiakis. **Resources Planning**. In Computer-Aided Process and Product Design (L. Puigjaner and G. Heyen, editors), Wiley-VCH Publisher ISBN 3-527-30804-0.

Georgiadis M.C., M. Kostoglou and E. Kikkinides. **Modelling Frameworks** In "Computer-Aided Process and Product Design" (L. Puigjaner and G. Heyen, editors), Wiley-VCH Publisher, ISBN 3-527-30804-0

P. Dua and M.C. Georgiadis. **Multi-parametric Mixed-Integer Linear Programming**. In: Multi-parametric programming: Theory, Algorithms and Applications (E.N. Pistikopoulos, M.C. Georgiadis and V. Dua, editors), Wiley-VCH Publisher. ISBN: 978-3-527-31691-5 p 53-71.

M.C. Georgiadis and E.N. Pistikopoulos. **Multi-Objective Energy and Environmental Analysis**. In: Multi-parametric programming: Theory, Algorithms and Applications (E.N. Pistikopoulos, M.C. Georgiadis and V. Dua, editors), Wiley-VCH Publisher. ISBN: 978-3-527-31691-5, p. 255-305.

D. Narciso, N. Faisca, K. Kouramas and M.C. Georgiadis. **Continuous-time Parametric Model Based Control**. In: Multi-parametric model-based control: Theory and Applications (E.N. Pistikopoulos, M.C. Georgiadis and V. Dua, editors), Wiley-VCH Publisher. ISBN: 978-3-527-31692-2, p. 105-132.

V. Sakizlis and M. C. Georgiadis. **Integration of Design and Control**. In: Multi-parametric model-based control: Theory and Applications (E.N. Pistikopoulos, M.C. Georgiadis and V. Dua, editors), Wiley-VCH Publisher. ISBN: 978-3-527-31692-2, p. 135-171.

P. Dua and M.C. Georgiadis. **Model based Control of a Pilot Plant Reactor**. In: Multi-parametric model-based control: Theory and Applications (E.N. Pistikopoulos, M.C. Georgiadis and V. Dua, editors), Wiley-VCH Publisher. ISBN: 978-3-527-31692-2, p. 217-229.

N. Faisca and M.C. Georgiadis. **Planning and Material Design Under Uncertainty**. In: Multi-parametric programming: Theory, Algorithms and Applications (E.N. Pistikopoulos, M.C. Georgiadis and V. Dua, editors), Wiley-VCH Publisher. ISBN: 978-3-527-31691-5, p. 229-254.

P. Dua, M.C. Georgiadis and E.N. Pistikopoulos. **Flexibility Analysis via Parametric Programming**. In: Multi-parametric programming: Theory, Algorithms and Applications (E.N. Pistikopoulos, M.C. Georgiadis and V. Dua, editors), Wiley-VCH Publisher. ISBN: 978-3-527-31691-5. p. 175-228.

P. Tsiakis, L.G. Papageorgiou **Optimal Design of Supply Chain Networks using Mathematical Programming** In: Supply Chain Optimization. (L.G. Papageorgiou and M.C. Georgiadis, editors) WILEY-VCH ISBN,: 978-3-527-31693-9.

M.C. Georgiadis and E.N. Pistikopoulos. **Integrated Optimization of Oil and Gas Processes**. In: Energy Systems Engineering. (M.C. Georgiadis, E.S. Kikkinides and E.N. Pistikopoulos editors) WILEY-VCH, ISBN: 978-3-527-31694-6.

Journal Articles

D. Nikolic, A. Giovanoglou, M.C. Georgiadis and E.S. Kikkinides (2008). **A generic modelling framework for multi-bed pressure swing adsorption systems**. Ind. Eng. Chem. Res. 47, 3156-3169.

M. C. Georgiadis, E. S. Kikkinides , S. S. Makridis, K. Kouramas and E. N. Pistikopoulos (2008). **Design and Optimization of Advanced Materials and Processes for Efficient Hydrogen Storage**. Computers & Chemical Engineering, To appear.

F. Aller, D. Kukanj, V. Jovan, M. Georgiadis (2008). **Modelling the semi-batch vinyl acetate emulsion polymerization in a real-life industrial reactor**. To appear in Mathematical and Computer Modelling of Dynamical Systems

D. Nikolic, E.S. Kikkinides, M.C. Georgiadis. **Optimisation of Multi-Bed PSA Processes**. To appear in Industrial Engineering Chemistry Research, November 2008.

Refereed Conference Contributions

E.N. Pistikopoulos, M.C. Georgiadis and V. Dua. **Parametric Programming and Control: From Theory to Practice** (Invited talk). Proceeding of the 17th European Symposium on Computer-Aided Process Engineering, Bucharest, Romania, 29 May – 1 June 2007, pp 569-574.

Nikolic D., A. Giovanoglou, M.C. Georgiadis, E.S. Kikkinides. **Modelling and simulation of multi-bed pressure swing adsorption processes**. Proceeding of the 17th European Symposium on Computer-Aided Process Engineering, Bucharest, Romania, 29 May – 1 June 2007, pp 159-164.

M. Kostoglou, M.C. Georgiadis. **On a new family of sectional methods for the soluation of the coagulation populations balance**. Proceeding of the 17th European Symposium on Computer-Aided Process Engineering, Bucharest, Romania, 29 May – 1 June 2007, pp 117-122.

D. Nikolic, A. Giovanoglou, M.C. Georgiadis, E.S. Kikkinides. **Modeling and optimization of single and multi-layer pressure swing adsorption systems**. Presented in the European Congress of Chemical Engineering – 6. Copenhagen, 16-21 September 2007.

C.O. Akinlabi, D.I. Gerogiorgis, M.C. Georgiadis and E.N. Pistikopoulos. Modelling, **Design and Optimisation of Hybrid PSA-membrane Gas Separation Processes**. Proceeding of the 17th European Symposium on Computer-Aided Process Engineering, Bucharest, Romania, 29 May – 1 June 2007, pp 363-370.

D. Nikolic, M.C. Georgiadis, E.S. Kikkinides. **An Optimisation Framework of Multi-Bed PSA processes**. Proceeding of the 18th European Symposium on Computer-Aided Process Engineering, Lyon, France, 1-4 June 2008, pp 265-270.

CHARLES D. IMMANUEL

Lecturer, Department of Chemical Engineering, Imperial College London.

Qualifications

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

Research Interests

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

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

Other Activities

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

Reviewer for

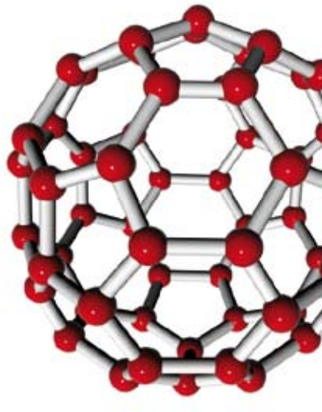
Chemical Engineering Science. AIChE Journal. Industrial & Engineering Chemistry Research. Computers & Chemical Engineering. Journal Applied Polymer Science. Journal Chemical Technology & Biotechnology. International Journal of Systems Sciences. Chemical Engineering Research & Development. Transactions of Institute of Measurement & Control. Polymer International

Academic Collaborations

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

Industrial Collaboration

ICI, BASF



GEORGE JACKSON

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

Qualifications

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

Awards and Distinctions

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

Research Interests

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

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

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

Other activities

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

Reviewer for

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

Industrial Collaborations

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

Publications
Book chapters

Pereira, F. E., Keskes, E., Galindo, A., Jackson, G., and Adjiman, C. S., **Integrated design of CO_2 capture processes from natural gas**, Energy Systems Engineering, Georgiadis, M. C., Kikkinides, E. S., and Pistikopoulos, E. N., Editors (ISBN 3-527-31694-6, Wiley-VCH) 2008.

Journal publications

Deschamps, J., Trusler, J. P. M., and Jackson, G., **Vapor pressure and density of thermotropic liquid crystals: MBBA, 5CB, and novel fluorinated mesogens**, J. Phys. Chem. B, 112, (2008), 3918-3926.

Haslam, A. J., Galindo, A., and Jackson, G., **Prediction of binary intermolecular potential parameters for use in modelling fluid mixtures**, Fluid Phase Equilibria, 226, (2008), 105-128.

Franco-Melgar, M., Haslam, A. J., and Jackson, G., **A generalisation of the Onsager trial-function approach: describing nematic liquid crystals with an algebraic equation of state**, Molec. Phys., 106, (2008), 649-678

de Wijn, A. S., Vesovic, V., Jackson, G., and Trusler, J. P. M., **A kinetic theory description of the viscosity of dense fluids consisting of chain molecules**, J. Chem. Phys., 128, (2008), 204901 (1-8)

Clark, G. N. I., Galindo, A., Jackson, G., Rogers, S., and Burgess, A. N., **Modelling and understanding closed-loop liquid-liquid immiscibility in aqueous solutions of poly(ethylene glycol) using the SAFT-VR approach with transferable parameters**, Macromolecules, 41, (2008), 6582-6595

Lymperiadis, A., Adjiman, C. S., Jackson, G., and Galindo, A., **A generalisation of the SAFT-gamma group contribution method for groups comprising multiple spherical segments**, Fluid Phase Equilibria, 274, (2008), 85-104

Malijevsky, A., Jackson, G., and Varga, S., **Many-fluid Onsager density functional theories for orientational ordering in mixtures of anisotropic hard-body fluids**, J. Chem. Phys., 129, (2008), 144504 (1-15)

Blas, F. J., González MacDowell, L., de Miguel, E., and Jackson, G., **Vapor-liquid interfacial properties of fully-flexible Lennard-Jones chains**, J. Chem. Phys., 129, (2008), 144703 (1-9).

Cuetos, A., Galindo, A., and Jackson, G., **Thermotropic biaxial liquid crystalline phases in a mixture of attractive uniaxial rod and disc particles**, Phys. Rev. Lett., in press (2008).

Giovanoglou, A., Galindo, A., Jackson, G., and Adjiman, C. S., **Fluid phase stability and equilibrium calculations in binary mixtures - Part I: Theoretical development for non-azeotropic mixtures**, Fluid Phase Equilibria, in press (2009). doi:10.1016/j.fluid.2008.08.017

Giovanoglou, A., Adjiman, C. S., Jackson, G., and Galindo, A., **Fluid phase stability and equilibrium calculations in binary mixtures - Part II: Application to single-point calculations and the construction of phase diagrams**, Fluid Phase Equilibria, in press (2009). doi:10.1016/j.fluid.2008.08.018

Pollock, M., Adjiman, C. S., Galindo, A., Jackson, G., and Filipe, E. J. M., **Integrating modelling of mixture fluid phase equilibrium experiments using SAFT-VR applied to xenon + diborane, xenon + cyclopropane, xenon + boron trifluoride**, Ind. Eng. Chem. Res., in press (2009).

Conference Abstracts

Lymperiadis, A., Adjiman, C. S., Galindo, A., and Jackson, G., **A heteronuclear group contribution method for associating chain molecules (SAFT-gamma)**, Proceedings of the 18th European Symposium on Computer-Aided Process Engineering ESCAPE 18, B. Braunschweig and X. Joulia, Editors, Elsevier Science, Computer-Aided Chemical Engineering (2008).

J. Jover, A. Galindo, A. J. Haslam, G. Jackson, and E. A. Müller, **Simulation of athermal demixing in systems containing large chains and colloidal-like particles**, Europhys. Conf. Abst., PI:26, (2008).

P. Brumby, G. Jackson, and S. Varga, **An examination on the effect of molecular chirality and confinement on the orientational and positional order of liquid crystalline phases**, Europhys. Conf. Abst., C:8, (2008).

G. N. I. Clark, A. Galindo, G. Jackson, and C. Vega, **The use of spectroscopic data for the degree of association to determine optimal models for water in theoretical and computer simulation methods**, Europhys. Conf. Abst., PB:33, (2008).

A. Cuetos, A. Galindo, and G. Jackson, **Thermotropic biaxial liquid crystalline phases in a mixture of attracting uniaxial rod and disc particles**, Europhys. Conf. Abst., PC:19, (2008).

M. Franco-Melgar, A. J. Haslam, and G. Jackson, **Algebraic description of nematic order in attracting rod-like particles and the Maier-Saupe model of liquid crystals using the Onsager trial-function approach**, Europhys. Conf. Abst., PC:20, (2008).

F. Llovell, G. Jackson, and F. J. Blas, **SAFT-VR density functional theory and step-function profile approximation for the prediction of the vapour-liquid interfacial tension of real fluids**, Europhys. Conf. Abst., PG:59, (2008).

A. Malijevsky, G. Jackson, and S. Varga, **Extension of Onsager type density functional theories for hard body fluid mixtures**, Europhys. Conf. Abst., PC.21, (2008).

A. Malijevsky and G. Jackson, **A density functional study of interfacial properties of spherical fluid interfaces**, Europhys. Conf. Abst., PG:60, (2008).

F. J. Blas, L. González MacDowell, E. de Miguel, and G. Jackson, **Determination of the vapour-liquid interfacial properties of freely jointed tangent Lennard-Jones chains**, Europhys. Conf. Abst., PG:61, (2008).

J. Schreckenberg, G. N. I. Clark, C. S. Adjiman, A. Galindo, and G. Jackson,, **Understanding the thermodynamic drivers for fluid phase separation in aqueous solutions of polymers and non-ionic surfactants**, Europhys. Conf. Abst., PD:38, (2008).

J. G. Sampayo, E. A. Müller, G. Jackson, F. J. Blas, and E. de Miguel, **Direct simulation of the interfacial tension using the test area method. Diatomic fluids and spherical interfaces**, Europhys. Conf. Abst., PG:64, (2008).

T. Lafitte, M. M. Piñeiro, D. Bessières, C.S. Adjiman, A.Galindo, and G.Jackson, **Analysis of anomalies in thermodynamic properties of liquid water for associating models with hard and soft cores**, Europhys. Conf. Abst., PB:41, (2008).

Conference contributions

A. Lymperiadis, C. S. Adjiman, A. Galindo, and G. Jackson, **Building molecules from fused heteronuclear groups – A SAFT based group contribution model (SAFT-gamma) (talk)**, 18th European Symposium of Computer Aided Process Engineering (ESCAPE-18), Lyon, France, 2 June 2008.

J. Jover, A. Galindo, A. J. Haslam, G. Jackson, and E. A. Müller, **Simulation of athermal demixing in systems containing large chains and colloidal-like particles** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

P. Brumby, G. Jackson, and S. Varga, **An examination on the effect of molecular chirality and confinement on the orientational and positional order of liquid crystalline phases** (talk), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 28 June 2008.

G. N. I. Clark, A. Galindo, G. Jackson, and C. Vega, **The use of spectroscopic data for the degree of association to determine optimal models for water in theoretical and computer simulation methods** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

A. Cuetos, A. Galindo, and G. Jackson, **Thermotropic biaxial liquid crystalline phases in a mixture of attracting uniaxial rod and disc particles** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

M. Franco-Melgar, A. J. Haslam, and G. Jackson, **Algebraic description of nematic order in attracting rod-like particles and the Maier-Saupe model of liquid crystals using the Onsager trial-function approach** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

F. Llovell, G. Jackson, and F. J. Blas, **SAFT-VR density functional theory and step-function profile approximation for the prediction of the vapour-liquid interfacial tension of real fluids** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

A. Malijevsky, G. Jackson, and S. Varga, **Extension of Onsager type density functional theories for hard body fluid mixtures** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

A. Malijevsky and G. Jackson, **A density functional study of interfacial properties of spherical fluid interfaces** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

F. J. Blas, L. Gonzalez MacDowell, E. de Miguel, and G. Jackson, **Determination of the vapour-liquid interfacial properties of freely jointed tangent Lennard-Jones chains** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

J. Schreckenberg, G. N. I. Clark, C. S. Adjiman, A. Galindo, and G. Jackson,, **Understanding the thermodynamic drivers for fluid phase separation in aqueous solutions of polymers and non-ionic surfactants** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

J. G. Sampayo, E. A. Müller, G. Jackson, F. J. Blas, and E. de Miguel, **Direct simulation of the interfacial tension using the test area method. Diatomic fluids and spherical interfaces** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

T. Lafitte, M. M. Piñeiro, D. Bessières, C.S. Adjiman, A.Galindo, and G.Jackson, **Analysis of anomalies in thermodynamic properties of liquid water for associating models with hard and soft cores** (poster), European Physical Society (EPS), 7th Liquid Matter Conference, Lund, Sweden, 26 June - 1 July 2008.

F. Llovell, F. J. Blas, A. Galindo, and G. Jackson, **SAFT-VR EOS coupled with DFT for the prediction of interfacial phenomena in real fluids** (talk), 20th International Conference on Chemical Thermodynamics (ICCT), Warsaw, Poland, 5 August 2008. F. Llovell winner of IACT Junior Award.

G. N. I. Clark, A. Galindo, and G. Jackson, **Study of the closed-loop immiscibility of polyethylene glycol aqueous solutions with the statisitcal associating fluid theory** (talk), American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 17 November 2008.

F. Llovell, A. Galindo, G. Jackson, and F. J. Blas, **Modelling interfacial properties of real fluids involved in enhanced oil recovery through the use of a density functional theory based on the SAVT-VR EOS** (talk), American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 17 November 2008.

J. M. A. Schreckenberg, C. S. Adjiman, A. Galindo, and G. Jackson, **Modelling the fluid phase behaviour in aqueous surfactant and water + oil + surfactant solutions and the effects of added salts** (poster), American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 17 November 2008.

T. Lafitte, C. S. Adjiman, A. Galindo, and G. Jackson, **Accurate perturbation theory for chains of soft-core attractive segments of arbitrary softness** (poster), American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 17 November 2008.

A. J. Haslam, A. Galindo, and G. Jackson, **Predicting binary interaction parameters for use in modelling fluid mixtures** (talk), American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 18 November 2008.

F. E. Pereira, E. Keskes, C. S. Adjiman, A. Galindo, and G. Jackson, **A physical absorption process for the capture of CO_2 from CO_2-rich natural gas streams using hydrocarbon solvents with post-capture CO_2 recompression** (talk), American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 18 November 2008.

A. Lymperiadis, C. S. Adjiman, A. Galindo, and G. Jackson, **Molecular based group contribution approaches for the prediction of the thermophysical properties of fluids** (talk), John O'Connell 70th Birthday Celebration, American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 19 November 2008.

N. Mac Dowell, C. S. Adjiman, A. Galindo, and G. Jackson, **Modeling CO_2 Capture In Amine Solvents with An Advanced Association Model: Process Optimisation and a Platform for Solvent Design** (talk), American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 20 November 2008.

B. Giner, T. Sheldon, M. Pollock, C. S. Adjiman, A. Galindo, G. Jackson, D. Jacquemin, V. Wathelet, and E. A. Perpète, **An approach for developing intermolecular models for use within SAFT-VR from quantum mechanical calculations and experimental data** (talk), American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 20 November 2008.

P. Ahlström (Borås, Sweden), K. Aim, (Prague, Czech Republic), R. Dohrn, (Bayer, Leverkusen, Germany), R. Elliott (Akron, USA), G. Jackson (Imperial College London, UK), J.-N. Jaubert (Nancy, France), M. E. Rebello de A. Macedo (Porto, Portugal), J.-P. Pokki (Helsinki, Finland), K. Reczey (Budapest, Hungary), A. Victorov (St Petersburg, Russia), L. F. Žilnik (Ljubljana, Slovenia), and I. G. Economou (Demokritos, Greece), **A survey of thermodynamics and transport properties in chemical engineering education in Europe and the USA** (talk), A Century of Chemical Engineering Thermodynamics Education, American Institute of Chemical Engineers (AIChE), 2008 Annual Meeting & Centennial Celebration, Philadelphia, USA, 21 November 2008.

G. Jackson, **Theories of the liquid state**, UK Theoretical Chemistry Summer School, Engineering and Physical Sciences Research Council (EPSRC) Postgraduate School, University of Oxford, Oxford, 15-16 September 2008.

Invited seminars

Molecular based group contribution approaches for the prediction of the thermophysical properties of fluids, Department of Chemical and Biochemical Engineering, Danish Technical University, Lyngby, Denmark, 22 February 2008.

Modelling of CO_2 separation and capture, Presentation to Fujitsu, Grantham Institute for Climate Change & Energy Futures Laboratory, Imperial College London, 5 March 2008.

The SAFT equation of state – new power and accuracy for thermophysical properties, gPROMS Annual Meeting, PSe Ltd., Blackfriars, London, 16 April 2008.

Modelling complex fluids: asphaltenes and flow assurance, BP, Sunbury Research Centre, 5 June 2008.

CLEO KONTORAVDI

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

Qualifications

MEng, PhD

Research Interests

Biotechnology

Reviewer for

Biotechnology and Applied Biochemistry
Academic Collaborations: Institute of Biomedical Engineering and Division of Medicine (SORA), Imperial College
Industrial Collaborations: Lonza Biologics

Publications
Journal Articles

Kontoravdi C., **Asprey S.P. et al. Systematic development of predictive mathematical models for animal cell cultures**. Computers and Chemical Engineering, in peer review.

Kontoravdi C., Lee Y.Y. et al. (2007). **Modelling amino acid metabolism in mammalian cells – towards the development of a model library**. Biotechnology Progress 23: 1261-1269.

Kontoravdi C., Asprey S.P. et al. (2007). **Development of a dynamic model of monoclonal antibody production and glycosylation for product quality control**. Computers and Chemical Engineering 31(5-6): 392-400.

Kontoravdi C., Asprey S.P. et al. (2005). A**pplication of global sensitivity analysis to determine goals for design of experiments: An example study on antibody-producing cell cultures**. Biotechnology Progress 21: 1128-1135.

Conference Contributions

CM Lam, K Sriyudthsak, C Kontoravdi et al. (2008). **Cell Cycle Modelling for Off-Line Dynamic Optimisation of Mammalian Cultures**. In: Proceedings of the 18th European Symposium on Computer Aided Process Engineering.
Kontoravdi C., Asprey S.P. et al. (2005). **Dynamic model of MAb production and glycosylation for the purpose of product quality control**. In: Proceedings of the 15th European Symposium on Computer Aided Process Engineering.

Kontoravdi C., Asprey S.P. et al. (2005). **Application of the Sobol´ global sensitivity analysis method to a dynamic model of MAb-producing mammalian cell cultures**. In: Proceedings of the 24th IASTED International Conference on Modelling, Identification and Control..

Kontoravdi C., Asprey S.P. et al. (2004). **Towards the optimisation of the production of monoclonal antibodies**. In: Proceedings of the 9th International Symposium on Computer Applications in Biotechnology.

Invited seminars

A Systems Engineering approach to the production of Biologics. IChemE workshop on 'Systems Biology with an Industrial Focus', London 26 June 2008.

J. KRISHNAN

Lecturer, Department of Chemical Engineering, Imperial College London.

Qualifications

PhD

Research Interests

Mathematical modelling of cell signalling in the context of different processes such as directed cell migration, polarity generation and genetic processes; development of systems approaches to understand signal transduction; systems biology; non-linear dynamics and pattern formation in biological and physico-chemical systems

Reviewer for

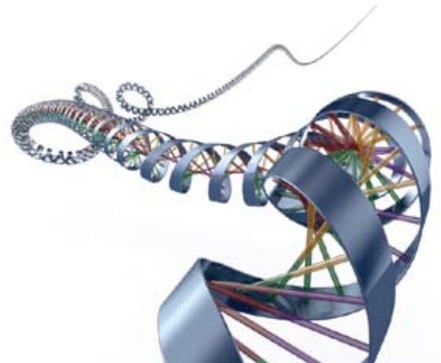
Interface Journal of the Royal Society, PLOS Computational Biology
Academic Collaborations School of Medical Sciences Univ. of Aberdeen, Cell Biology, King's College London.

Publications
Journal Articles

Signal processing via a generalized module of adaptation and spatial sensing", Journal of Theoretical Biology (submitted)

Invited Lectures and Seminars

Dept. of Chemical Eng Cambridge University, Actin and Cell Polarity Workshop, University of Warwick (other lectures at AIChE, Cold Spring Harbour International Conference)



DANIEL KUHN

Lecturer, Department of Computing, Imperial College London.

Qualifications

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

Awards and Distinctions

Fellowships from Swiss National Science Foundation (2004-2006).
Polya Award of ETH Zurich for Best MSc Examination Result in Theoretical Physics (1999)

Research Interests

Stochastic optimization (development of approximation schemes and solution algorithms)

Computational finance (derivatives pricing, portfolio optimization)

Energy market modeling (power system operation and scheduling, risk management)

Other Activities

Member of Mathematical Programming Society

Reviewer for

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

Academic Collaborations

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

GEOFFREY C. MAITLAND

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

Qualifications

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

Awards and Distinctions

Fellow of the Royal Academy of Engineering
Fellow of the IChemE
Fellow of the Royal Society of Chemistry
Salters' Scholar 1969-72
ICI Fellowship 1972-74
Hutchison Medal of the IChemE, 1999

Research Interests

Clean production and use of fossil fuels
Recovery of non-conventional hydrocarbons. Real-time control and management of oil and gas reservoirs
Thermophysical properties of fluids
Rheology of complex fluids and soft materials. Rock-fluid interactions
Chemical characterisation of multi-component fluids. The development of new hydrocarbon recovery processes
The application of biological processes to oil recovery.

My research is built around three main themes:

- more efficient recovery of existing hydrocarbons
- exploitation of non-conventional sources of hydrocarbons
- mitigating the environmental impact of fossil fuels and managing the transition to alternative energies

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

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

Other Activities

Institut Francais du Petrole: Member of Scientific Council. EPSRC: Member of Peer Review College. Soft Matter Journal: Founder Member of Editorial Board. Member US National Petroleum Council Technology Task Group on Carbon Capture and Storage. Sheffield Hallam University: Chairman, Materials and Engineering Research Institute Scientific Advisory and Policy Boards. Associate member University of Wales Institute of Non-Newtonian Fluid Mechanics Chair, EPSRC Steering Group, Portfolio Grant on Complex Fluids and Complex Flows, Swansea University. Chair, International Advisory Board, SoftComp EU Network.

Reviewer for

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

Industrial Collaboration

Schlumberger and Shell

ATHANASIOS MANTALARIS

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

Qualifications

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

Awards and Distinctions

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

Secondments

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

Research Interests

My research interests cover the advancement of an integrated systems engineering platform for the generation of solutions/strategies through the development of adaptive algorithms for the model-based design of experiments, prediction, control, and optimisation of complex biological/biomedical problems. They integrate experimentation with modelling from molecules into cell populations and to link the in silico with the *in vitro* through:

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

Mammalian cell bioprocessing:

Commercial synthesis of monoclonal antibodies (MAB) represents one of the most important products in the biopharmaceutical industry because of their diagnostic and clinical applications. However, the production of industrial scale quantities of MAB is an expensive and challenging task.

Complications arising in these systems include the requirement to grow cultures in complex media, the lack of on-line measurements for many of the key substrates, metabolites, and products, the limited and noisy nature of much of the available experimental data and the extremely complex underlying reaction system.

Our research programme sets out to integrate modelling, experiment design and validation, and control and optimisation into a single framework that would lead to increased productivity, regulated product quality, and reduced costs for mammalian cell culture systems.

Stem cell bioprocessing:

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

Other Activities

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

Reviewer for

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

Academic Collaborations

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

Industrial Collaborations

NovaThera

COSTAS C. PANTELIDES

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

Qualifications

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

Awards and Distinctions

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

Research Interests

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

Other Activities

Reviewer for

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

Technology Director, Process Systems Enterprise Ltd.

Member of the committee for the establishment of the new University of Applied Sciences and Arts, Cyprus

LAZAROS PAPAGEORGIOU

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

Qualifications

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

Research Interests

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

Other Activities

Member of IChemE CAPE Subject Group Committee. Co-editor, Vol 3 and 4 "Supply Chain Optimization" of book series in Process Systems Engineering, Wiley-VCH
Invited lecture in FOCAPO 2008 conference “Supply Chain Optimisation for the Process Industries: Advances and Opportunities”

Reviewer for

Industrial & Engineering Chemistry Research,Computers and Chemical Engineering, AIChE Journal, Chemical Engineering Research and Design, Chemical Engineering Science, Biotechnology Progress.

Academic Collaborations

Imperial College, Department of Chemical Engineering. King's College, Centre for Bioinfromatics. Polytechnic University, Othmer-Jacobs Department of Chemical and Biological Engineering. University College London, Department of Biochemical Engineering

Industrial Collaborations

Syngenta (supply chain network design for agrochemicals)

Publications
Book Chapters

E.S. Fraga and L.G. Papageorgiou, **A Two Step Hybrid Optimization Procedure for the Design of Optimal Water Distribution Networks**, in “Models and Algorithms for Global Optimization” (A. Torn and J. Zilinskas, editors), Springer's book series on Optimization and Its Applications, 4, 311-332 (2007).

L.G. Papageorgiou and M.C. Georgiadis (editors), **Supply Chain Optimization**, Vol. 3 and 4, Wiley-VCH, 2008.

P. Tsiakis, L.G. Papageorgiou and M.C. Georgiadis, **Optimal Design of Supply Chain Networks using Mathematical Programming**, in “Supply Chain Optimization: Part I” (L.G. Papageorgiou and M.C. Georgiadis, editors), 157-184, Wiley-VCH (2008).

R.T. Sousa, N. Shah and L.G. Papageorgiou, **Supply Chain of High Value Low Volume Products**, in “Supply Chain Optimization: Part II” (L.G. Papageorgiou and M.C. Georgiadis, editors), 1-27, Wiley-VCH (2008).

Journal Articles

G. Xu and L.G. Papageorgiou, **A Construction-based Approach to Process Plant Layout using Mixed-integer Optimization**, Ind. Eng. Chem. Res., 46, 351-358 (2007).

L.G. Papageorgiou and E.S. Fraga, **A Mixed Integer Quadratic Programming Formulation for the Economic Dispatch of Generators with Prohibited Operating Zones**, Electric Power Systems Research, 77, 1292-1296 (2007).

A.A. Levis and L.G. Papageorgiou, **Active Demand Management for Substitute Products through Price Optimisation**, OR Spectrum, 29, 551-577 (2007).

J. Westerlund, L.G. Papageorgiou and T. Westerlund, **A MILP Model for N-dimensional Allocation**, Comput. Chem. Eng., 31, 1702-1714 (2007).

K. Lakhdar, J. Savery, L.G. Papageorgiou and S. Farid, **Multiobjective Long Term Planning of Biopharmaceutical Manufacturing Facilities**, Biotechnology Progress, 23, 1383-1393 (2007).

G. Xu, S. Tsoka and L.G. Papageorgiou, **Finding Community Structures in Complex Networks using Mixed Integer Optimisation**, Eur. Phys. J. B., 60, 231-239 (2007).

P. Tsiakis and L.G. Papageorgiou, **Optimal Production Allocation and Distribution Supply Chain Networks**, International Journal of Production Economics, 111, 468-483 (2008).

K. Lakhdar and L.G. Papageorgiou, **An Iterative Mixed Integer Optimisation Approach for Medium Term Planning of Biopharmaceutical Manufacture under Uncertainty**, Chem. Eng. Res. Des., 86, 259-267 (2008).

P. Chen and L.G. Papageorgiou and J.M. Pinto,, **Medium-term planning of single-stage multiproduct plants using a hybrid discrete/continuous-time MILP model**, Ind. Eng. Chem. Res., 47, 1925-1934 (2008).

T. Al-Ameri, N. Shah and L.G. Papageorgiou, **Optimization of Vendor-Managed Inventory Systems in a Rolling Horizon Framework**, Comput. Ind. Eng., 54, 1019-1047 (2008).

R.T. Sousa, N.Shah and L.G. Papageorgiou, **Supply Chain Design and Multilevel Planning – an Industrial Case**, Comput. Chem. Eng., 32, 2643-2663 (2008).

S. Liu, J.M. Pinto and L.G. Papageorgiou, **A TSP-based MILP Model for Medium-Term Planning of Single-Stage Continuous Multiproduct Plants**, Ind. Eng. Chem. Res., 47, 7733-7743 (2008).

Conference Contributions

G. Xu and L.G. Papageorgiou, **An Iterative Solution Approach to Process Plant Layout using Mixed Integer Optimisation**, Escape-17 Conference, V. Plesu and P.S. Agachi (editors), 291-296 (2007).

G. Xu, N. Shao and L.G. Papageorgiou, **A Mixed Integer Optimisation Approach for DataClassification with Multiple Groups**", Escape-17 Conference, V. Plesu and P.S. Agachi (editors), 419-424 (2007).

J.M. Pinto, P. Chen and L.G. Papageorgiou, "**A Discrete/Continuous-time MILP Model for Medium-term Planning of Single Stage Multiproduct Plants**, Escape-17 Conference, V. Plesu and P.S. Agachi (editors), 685-690 (2007).

K-M. Bjork and L.G. Papageorgiou, **Global optimization of water distribution systems**, Hawaii International Conference on System Sciences (HICSS)-41, 88 (2008).

M.C. Georgiadis and L.G. Papageorgiou, **Algorithmic methods for the optimal lumping of analytical data for compositional studies**, Escape-18 Conference, FP-00103 (2008).

L.G. Papageorgiou, **Supply Chain Optimisation for the Process Industries: Advances and Opportunities**, FOCAPO-2008 Conference, M. Ierapetritou, M. Bassett and E.N. Pistikopoulos (editors), 33-42 (2008).

S. Liu, J.M. Pinto and L.G. Papageorgiou, **A New MILP Model for Medium-Term Planning of Single-Stage Continuous Multiproduct Plants**, 5th International Conference on Computational Management Science, London, U.K. (2008).

G. Xu and L.G. Papageorgiou, **Evaluating Credit Risks of Business Entities using Mixed Integer Optimisation**, 5th International Conference on Computational Management Science, London, U.K. (2008).

C-G. Lee, N. Shah and L.G. Papageorgiou, **Strategic Design and Planning of Reverse Supply Chain with Model-based Decision Support Tools**, 5th International Conference on Computational Management Science, London, U.K. (2008).

EFSTRATIOS N. PISTIKOPOULOS

Professor of Chemical Engineering CPSE Director.

Qualifications

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

Awards and Distinctions

Royal Academy of Engineering, Mac Robert Award, 2007 (part of PSE Ltd’s 5-member team). Fellow, Institution of Chemical Engineers, 2005. Imperial College, Rector’s Award for Research Excellence, 2005. ICI/Royal Academy of Engineering Fellowship, 1991-1996

Research Interests

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

Other activities

Co-Editor, Book Series in Process Systems Engineering, Wiley-VCH. Editorial Board, Computers and Chemical Engineering, Elsevier. Editorial Board, Journal of Global Optimization, Kluwer. Editorial Board, Computational Management Science, Springer. Co-Founder and Senior Consultant, PSE Ltd. Founder and Director, PAROS Ltd Co-organiser, Global Optimization Workshop, December 2007, Imperial College London. Plenary Lectures – ESCAPE-17 (Bucharest, Romania), ECCE-6 (Copenhagen, Denmark). International Programme Committee member – ESCAPE-17, PRES’07, ECCE-6. Invited Presentations – University of Manchester, National University of Singapore, University of Pannonia, University of Coimbra, Tsinghua University. External Examiner - DTU, UPC Reviewer – AIChE J, IECR, CCE, JOGO, CMS, IEEE Transactions, Process Control J, OR. Invited Member, Computer Aided Process Engineering (CAPE) Working Party, European Federation

of Chemical Engineers. Member of the Advisory Scientific Committee, European Enterprise Institute (EPPED Association). Involved in 14 ongoing projects – 4 EPSRC funded (two as PI), 1 BBSRC-funded, 2 BP-funded, 1 BASFfunded, 5 EU-funded (1 as Coordinator), Systems Engineering Initiative (Imperial, Faculty of Engineering).

Academic Collaborations

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

Industrial Collaborations

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

Conference publications

Samaraweera, M., Shah, N. and Pistikopoulos, E. N. (2008), '**Modelling and optimisation of urban energy systems**' In Foundations of Computer-Aided Process Operations (Eds, Ierapetritou, M., Bassett, M. and Pistikopoulous, E. N.) Cambridge, USA, pp. 213-216.

ChemPor 2008, Braga, Portugal: **Molecular Weight Distribution in Free-Radical Polymerisation – Model Development, Experimental Validation and Process Optimisation** Bruno Amaro (Imperial College London), Charles Immanuel (Imperial College London), Efstratios Pistikopoulos (Imperial College London), Andreas Daiß (BASF, Germany), Florian Becker (BASF, Germany), Klaus Hungenberg (BASF, Germany), Pedro Saraiva (Depart. Eng.Quimica, FCTUC)

2008 AIChE Conference Philadelphia, PA, USA **Global Optimization of Mixed-integer Bi-level Problems via Multiparametric Programming** Session: Computers in Operations and Information Processing #198 - Advances in Optimization I

Global Optimization Workshop 2008, Imperial College London

A combined Balanced Truncation and Multi-Parametric Programming approach for Linear Model Predictive Control, ESCAPE 18

A framework for Multi-Parametric programming and control – an overview, IEMC - Europe 2008

A combined Balanced Truncation and Multi-Parametric Programming approach for Linear Model Predictive Control, ESCAPE 18, June 2008, Lyon, France

Nonlinear Multiparametric Model-based Control, Nonlinear Model Predictive Control Conference, September 2008, Pavia, Italy

Nonlinear MPC via Novel Multiparametric Programming Techniques, PROMATCH End Symposium, November 2008, Frankfurt, Germany

ESCAPE 18, June 2008, Lyon, France
IEMC - Europe 2008, June 2008, Estoril, Portugal
Nonlinear Model Predictive Control Conference, September 2008, Pavia, Italy
PROMATCH End Symposium, November 2008, Frankfurt, Germany

Journal publications

P. Liu, E. N. Pistikopoulos, and Z. Li (2008). **A mixed-integer optimization approach for polygeneration energy systems design**. Computers & Chemical Engineering. In press.

Z. Li, D. Gao, L. Chang, P. Liu and E. N. Pistikopoulos (2008). **Hydrogen infrastructure design and optimization: a case study of China**. International Journal of Hydrogen Energy, 33(20): 5275-5286

Z. Li, D. Gao, L. Chang, P. Liu and E. N. Pistikopoulos (2008). **Coal-derived methanol for hydrogen vehicles in China: energy, environment, and economic analysis for distributed reforming**. Chemical Engineering Research and Design. Submitted.

P. Liu and E. N. Pistikopoulos (2008). **A multi-period mixed integer optimization formulation for polygeneration energy systems**. Proceeding of FOCAPO 2008 (Foundations of Computer-Aided Process Operation), Cambridge, Massachusetts, USA.

P. Liu, E. N. Pistikopoulos, and Z. Li (2009). **Environmentally benign process design of polygeneration energy systems**. FOCAPD 2009 (Foundations of Computer-Aided Process Design), Breckenridge, Colorado, USA. Abstract accepted.

P. Liu, E. N. Pistikopoulos, and Z. Li (2009). **An energy systems engineering approach to polygeneration and hydrogen infrastructure systems analysis & design**. PRES 09 (12th International Conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction), Rome, Italy. Abstract accepted.

Chapters in books

P. Liu, E. N. Pistikopoulos and Z. Li (2008). **Polygeneration systems engineering**, in E. N. Pistikopoulos (ed.) Energy Systems Engineering. WILEY-VCH, Weinheim.

Z. Li, L. Chang, D. Gao, P. Liu and E. N. Pistikopoulos (2008). **Hydrogen energy systems**, in E. N. Pistikopoulos (ed.) Energy Systems Engineering. WILEY-VCH, Weinheim.

P. Liu and E. N. Pistikopoulos (2008). **Mixed-integer optimization for polygeneration energy systems design**, in J. Kallrath etc. (ed.) Optimization in the Energy Industry, Springer. In press.

BERC RUSTEM

Professor, Department of Computing, Imperial College London.

Qualifications

B.S. MSc, PhD, FIMA, CMath

Awards and Distinctions

President of Society of Computational Economics, 2002-04

Research Interests

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

Other Activities

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

Academic Collaborations

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

Industrial Collaborations

Ericsson; Lehman Brothers; JP Morgan

Research Projects

1. Algorithms for Worst Case Design: (with Professor Pistikopoulos)
2. Algorithms for Safe Food Processes: (with Professor Pistikopoulos)

3 a. DTC: Software for Uncertain Systems & UV's

3 b. DTC: Renewed Aug 08 - Aug 11

4. "COMISEF" http://www.comisef.eu/
5. Systems Engineering Initiative
6. DTI Feasibility Study for Houshold Energy Optimisation
7. EPSRC Global Optimisation Workshop
8. iHealth (EPSRC) Guo-Rustem

Competence Areas

Optimisation algorithms
Minimax algorithms
Global optimisation
Stochastic optimisation
Robust decisions under uncertainty
Risk management

Editorships

Editor
Automatica

Editor
Computational Management Science

Editorial Advisory Board
Journal of Economic Dynamics & Control

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

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

Organiser & Programme Committee Co-Chair

EPSRC Global Optimisation Workshop, Imperial College, Dec 07.
http://gow2007.ps.ic.ac.uk/

Computational Management Science, Imperial College London, Mar 08
http://cms2008.ps.ic.ac.uk/

Programme Committee Member

International Conference on Nonconvex Programming 2007 - Rouen

International Conference on Applied Mathematical Programming and Modelling 2008, Bratislava

Stochastic Programming XI 2007, Vienna
Keynote Talk

Computational Finance - Toronto, Jul 2007.

Publications - Edited Book

Computational Methods in Financial Engineering, (E. Kontoghiorghes, B. Rustem, P. Winker Eds), Springer-Verlag, 2008.

Chapters in Books

Kuhn, D. P. Parpas, B. Rustem (2008). **Threshold Accepting Approach to Improve Bound Based Approximations for Portfolio Optimization**, in Computational Methods in Financial Engineering, (E. Kontoghiorghes, B. Rustem, P. Winker Eds), Springer-Verlag, 2008, 3-26.

Gulpinar, N, B. Rustem, S. Zakovic (2007) **Stochastic Optimization and Worst-case Decisions**, in "Cooperative Systems: Control and Optimization", (D. Grundel, R. Murphey, P. Pardalos, O. Prokopyev Eds), Springer-Verlag, Berlin & New York.

Daniel Kuhn, Panos Parpas, Berç Rustem (2008), **Stochastic Optimization of Investment Planning Problems in the Electric Power Industry**, Daniel Kuhn, Panos Parpas, Berç Rustem, in (Pistikopoulos, E., Georgiadis, M., Kikkinides, E. S. Eds.) Process Systems Engineering, Volume 5: Energy Systems Engineering, J Wiley.

Conferences Talks/Papers
(selected subset)

Partitioning Procedure for Polynomial Optimisation: Application to Portfolio Decisions with Higher Order Moments P. M. Kleniati, P. Parpas and B. Rustem, Presented at NCP07 (International conference on Nonconvex Programming), 17-21 December 2007, National Institute for Applied Sciences, Rouen, France Submitted to Journal of Global Optimisation, special issue dedicated to NCP07

Decomposition-based method for sparse SDP relaxations of polynomial problems P. M. Kleniati, P. Parpas and B. Rustem Working Paper Presented at CMS08 (International conference on Computational Management Science), 26-28 March 2008, Imperial College London, UK

Maximizing the Net Present Value of a Project under Uncertainty at CMS 2008 (London); submitted to European J Operations Research. (W. Wieseman, D. Kuhn, B. Rustem)

Multi-Resource Allocation in Stochastic Project Scheduling, International Conference on Applied Mathematical Programming and Modelling. 2008 (Bratislava); (W. Wieseman, D. Kuhn, B. Rustem) to be submitted to Annals of OR.

Robust Scenario Trees, Computational Finance, Toronto, (D. Kuhn, P. Parpas, B. Rustem) submitted to Computational Finance.

Journal Papers

Faısca, N. P., P. M. Saraiva, B. Rustem and E. N. Pistikopoulos. **A multi-parametric programming approach for multilevel and decentralised optimisation problems**, Computational Management Science, (2008) (forthcoming)

Parpas, P., B. Rustem, E.N Pistikopoulos, **Global optimization of robust chance constrained problems**, J of Global Optimization (2008) (forthcoming)

M. Osorio, N. Gülpinar, B. Rustem, **A General Framework for Multi-Stage, Mean-Variance, Post-Tax Optimization**, Annals of Operations Research, 157(1) (2008).

Faísca, Nuno P., K.I. Kouramas, P.M. Saraiva, B. Rustem and E.N. Pistikopoulos (2008). **A multi-parametric programming approach for constrained dynamic programing problems** Optimization Letters 2 (2), pp. 267-280."

Parpas, P. and B. Rustem. **A pricing mechanism for resource management in grid computing**, forthcoming in: Computational Economics. (2008) forthcoming

B. Rustem, S. Zakovic, P. Parpas, **An interior point algorithm for continuous minimax: Implementation and Computation**, forthcoming in: Optimization Methods and Software, 2009

Kuhn, D. P. Parpas, B. Rustem (2008) **Bound Based Decision Rules in Multi-stage Stochastic Programming**, Kibernetika, 44, 134-150.

Tsoukalas, A., B. Rustem, **A smoothing algorithm for finite min-max-min problems**, forthcoming in: Optimization Letters, (2009).

Activities

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

Systems Engineering Initiative, Research Director, Faculty of Engineering, Imperial College

PAUL RUTTER

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

Qualifications

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

Research Interests

The impact of Climate Change on industrial infrastructure. The development of urban energy systems. Energy economics: My principal interest is the reason why countries move from one system of energy supply to another e.g. the change from gas to electricity for lighting in the UK and whether parallels can be drawn for new energy systems like wind and hydrogen Climate Change: Interest in the impact of climate change to industrial operations and infrastructures. Environmental engineering: General interest in applying environmental principles to engineering without losing economic competitiveness.

Other Activities

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

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

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

ROGER W. H. SARGENT

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

Qualifications

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

Awards and Distinctions

Royal Academy of Engineering-Founder Fellow,1976. Honorary Fellowship of the City and Guilds of London Institute,1977 Docteur honoris causa, Institut National Polytechnique de Lorraine,1987 Fellow of the Royal Society of Arts,1989 AIChE CAST Division “Computing in Chemical Engineering Award”, 1990 Foreign Associate of the United States National Academy of Engineering, 1993 Honorary DSc(Edinburgh), 1993. Fellowship of Imperial College London, 1994. Docteur honoris causa, Universite de Liege, 1995

Research Interests

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

Other Activities

Associate Editor of Journal of Optimization Theory and Applications

Reviewer for

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

NILAY SHAH

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

Qualifications

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

Awards and Distinctions

Fellow of the IChemE. RSC/SCI/IOM Beilby Medal 2005. ICI/RAE Fellowship (1997-2002)

Research Interests

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

Other Activities

Co-founder of Process Systems Enterprise Ltd. Director of Ashe Morris Ltd. Director of Britest Ltd. Defra panel member EPSRC college member. IChemE Transactions editorial board member

Reviewer for

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

Academic Collaborations

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

Industrial Collaborations

Ashe Morris (Novel reactor modeling and experimentation). BP (Urban Energy Systems Project). ICI (Supply chain management under uncertainty). Ineos (Supply chain study). Shell (H_2-CO_2 project) Syngenta (Supply chain network design)

EVA SØRENSEN

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

Qualifications

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

Awards and Distinctions

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

Research Interests

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

Other Activities

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

Academic Collaboration

University College London, Department of Biochemical Engineering

Industrial Collaboration

BP, Novasep

NINA F. THORNHILL

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

Qualifications

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

Awards and Distinctions

Fellow of the IChemE. Fellow of the IET Winner of the Journal of Process Control Best Paper Award in the category methodology/theory for the period 2002 to 2005. UCL Faculty of Engineering Teaching Award, 2002

Secondments

Royal Academy of Engineering Global Research Award with ABB Corporate Research, Norway, April-Sept 2005. Royal Society Industry Fellowship with BP International, 1992-5

Research interests

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

Other activities

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

Reviewer for

AIChE Journal. Biotechnology and Bioengineering. Chemical Engineering Research and Design. Computers & Chemical Engineering. Control Engineering Practice. IEE Proceedings D. Industrial and Engineering Chemistry Research. Institution of Mechanical Engineers Journal of Systems and Control Engineering. International Journal of Adaptive Control

and Signal Processing. ISA Transactions. Journal of Process Control

Academic Collaborations

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

Industrial collaboration

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

Publications
Book and book chapter

Choudhury, M.A.A.S., Shah, S.L., and Thornhill, N.F., 2008, **Diagnosis of Process Nonlinearities and Valve Stiction: Data Driven Approaches**, Springer, ISBN: 978-3-540-79223-9.

Thornhill, N.F., 2007, **Locating the source of a disturbance, In Process Control Performance Assessment; From Theory to Implementation**, Chapter 6, Eds: D.O. Uduehi, A. Ordys and M.A. Johnson, Springer-Verlag (London) Ltd, ISBN 1846286239.

Refereed journal papers

Bauer, M., and Thornhill, N.F., 2008, **A practical method for identifying the propagation path of plant-wide disturbances**, Journal of Process Control, 18, 707-719.

Thornhill, N.F., Patwardhan, S.C. and Shah, S.L., 2008, **A continuous stirred tank heater simulation model with applications**, Journal Of Process Control, 18, 347–360.

Edwards-Parton, S., Thornhill, N.F., Bracewell, D.G., Liddell, J.M., and Titchener-Hooker, N.J., 2008, **Principal component score modeling for the rapid description of chromatographic separations**, Biotechnology Progress, 24, 202-208.

Bauer , M., Cox, J.W., Caveness, M.H., Downs, J.J., and Thornhill, N.F., 2007, **Nearest neighbors methods for root cause analysis of processes with plant-wide disturbances**, Industrial Engineering and Chemistry Research, 46, 5977-5984.

Conference presentations

Beez, S., Fay, A., and Thornhill, N.F., 2008, **Automatic generation of bond graph models of process plants**, 13th IEEE International Conference on Emerging Technologies and Factory Automation (IEEE ETFA), 12-15 September, Hamburg.

Thornhill N.F. and Huang, B., 2008, **Management and monitoring of process assets**, Advanced Control of Industrial Processes AdConIP, Jasper, Canada, May 4-7, keynote paper.

CPSE ACADEMICS
2008

Imperial College London

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

Department of Computing

Daniel Kuhn
Berc Rustem

Department of Earth Science & Engineering

Nigel Brandon

Visiting Professors

Roger Benson
John Perkins
Paul Rutter

University College London

Department of Chemical Engineering

David Bogle
Vivek Dua
Eric Fraga
Lazaros Papageorgiou
Eva Sørensen

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CPSE RESEARCH PROJECT LIST

2008

Name: **Mr Allen, Richard**
Supervisor: Prof D Bogle and Anne Ridley
Title: **Modelling Endothelial Cells Response to Fluid Flow**
Starting Date: Sep-05
Finishing Date: Oct-08

Name: **Ms Al Fulaij, Hala**
Supervisor: Prof David Bogle
Title: **Dynamic Modelling and Control of Multi Stage Flash (MSF) Desalination Plant**
Starting Date: Apr-07
Finishing Date: Apr-12

Name: **Mr Al Soudani, Tareg**
Supervisor: Prof David Bogle
Title: **Multiscale Modelling for Operation and Control of PSA Units**
Starting Date: Apr-05
Finishing Date: Apr-10

Name: **Ms Sheila Mae Ang**
Supervisor: Prof Eric Fraga & Dr Dan Brett (UCL Chemical Engineering)
Title: **Modelling and multi-criteria optimisation of PEM fuel cells with experimental validation.**
Starting Date: Sep-08.
Finishing Date: Sep-12

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

Name: **Mr Bianco, Nicola**
Supervisor: Dr C Immanuel
Title: **Control of Particle Size Distribution in Emulsion Polymerisation**
Starting Date: Oct-04
Finishing Date: Dec-08

Name: **Mr Brumby, Paul**
Supervisor: Prof G Jackson
Title: **Characterisation of the Link Between Molecular Chirality and Bulk Phase Chirality in Systems of Liquid Crystals**
Starting Date: Oct-05
Finishing Date: Oct-09

Name: **Mr Chen, Ning**
Supervisor: Dr Cleo Kontoravdi and Dr Andy Racher (Lonza Biologics)
Title: **Modelling of protein-producing Chinese hamster ovaries cells**
Starting Date: Oct-08
Finishing Date: Oct-11

Name: **Mr Cheung, Kwok Yuen**
Supervisors: Prof N Shah & Prof CC Pantelides
Title: **Site-wide and Supply Chain Optimisation for Continuous Chemical Processes**
Starting Date: Oct-04
Finishing Date: Sep-07

Name: **Mr Crane, Andrew**
Supervisors: Dr E Muller & Prof G Jackson
Title: **Molecular Systems Engineering**
Starting Date: Jul-07
Finishing Date: Jul-11

Name: **Mr Dominguez, Luis**
Supervisor: Prof EN Pistikopoulos
Title: **Multiparametric Mixed Integer Dynamic Optimization of Process Systems**
Starting Date: Jul-07
Finishing Date: Jul-10

Name: **Mr Dunnett, Alexander**
Supervisors: Prof N Shah & Dr C Adjiman
Title: **Biofuel Supply Chain**
Starting Date: Oct-05
Finishing Date: May-08

Name: **Mr Faisca, Nuno**
Supervisors: Prof EN Pistikopoulos & Dr V Dua
Title: **Parametric Programming and Control**
Starting Date: Oct-04
Finishing Date: Apr-08

Name: **Ms Fiandaca, Giovanna**
Supervisors: Prof E Fraga & Prof S Brandani (University of Edinburgh)
Title: **Optimal Design of Pressure Swing Adsorption for CO_2 Capture**
Starting Date: Apr-06
Finishing Date: Mar-09

Name: **Ms Fonseca, Raquel**
Supervisor: Berc Rustem
Title: **Robust Optimization applied to a Currency Portfolio.**
Starting Date: Sep-07
Finishing Date: Sep-11

Name: **Mr Gueddar, Taoufiq**
Supervisor: Dr Vivek Dua
Title: **Optimization under Uncertainty**
Starting Date: Mar-08
Finishing Date: Feb-13

Name: **Mr Jimenez del Val, Ioscani**
Supervisor: Dr Cleo Kontoravdi and Dr Judit M. Nagy (Institute of Biomedical Engineering)
Title: **Assessment of the interactions between bioprocess conditions and protein glycosylation in antibody-producing mammalian cell cultures**
Starting Date: Oct-08
Finishing Date: Oct-11

Name: **Mr Khajuria, Harish**
Supervisor: Prof EN Pistikopoulos
Title: **Advanced Control and Optimization of PSA Hybrid System**
Starting Date: Oct-07
Finishing Date: Jan-11

Name: **Ms Kleniati, Polyxeni**
Supervisor: Berc Rustem
Title: **Global Optimisation of Polynomials and Decompositions Schemes**
Starting Date: Sep-05
Finishing Date: Sep-09

Name: **Mr Hosseini, Seyed Ali**
Supervisor: Prof N Shah
Title: **Multiscale modelling of bio?**
Starting Date: Sep-07
Finishing Date: Sep-10

Name: **Mr Ikram, Waqas**
Supervisor: Prof NF Thornhill
Thesis: **Plant-wide and wireless process control and automation**
Starting Date: Oct-08
Finishing Date: Sept-11

Name: **Mr Iyun, Oluwatope Ebenezer**
Supervisor: Prof NF Thornhill
Title: **Plant-wide Fault Diagnosis: Cause-and-effect analysis using process connectivity**
Starting Date: Dec-07
Finishing Date: Nov-10

Name: **Mr Kazantsev, Andrei**
Supervisors: Dr C Adjiman & Prof C Pantelides
Title: **Design of Organic Crystals for enhanced Bioavailability**
Starting Date: Oct-07
Finishing Date: Oct-10

Name: **Mr Kiparissides, Alexandros**
Supervisor: Prof EN Pistikopolus & Dr S Mantalaris
Title: **Development of a Combined Mathematical and Experimental Framework for the Control and Optimisation of Mammolian Cell Cultures**
Starting Date: Jan-07
Finishing Date: Jan-10

Name: **Mr Konda, Naga**
Supervisor: Prof N Shah
Title: **H_2-CO_2 Infrustructure Design**
Starting Date: Aug-06
Finishing Date: Jul-09

Name: **Mr Laakso, Gunilla**
Supervisor: Dr LG Papageorgiou
Title: **Supply chain management for the paper industry**
Starting Date: Feb-04
Finishing Date: Feb-07

Name: **Ms Lam, Ming-Chi (Carolyn)**
Supervisors: Dr A Mantalaris & Prof EN Pistikopoulos
Title: **Creating a Predictive in Silico Model of Mammation Cell Cultures**
Starting Date: Oct-04
Finishing Date: Apr-08

Name: **Mr Lee, Chang-Gun Colin**
Supervisor: Prof N Shah
Title: **Optimisation of Closed-loop supply chain**
Starting Date: Jun-07
Finishing Date: Jun-10

Name: **Mr Liu, Cong**
Supervisors: Dr Krishnan
Title: **Mathematical Modelling of Drug Delivery in Cancer Tumors**
Starting Date: Jan-08
Finishing Date: Jun-11

Name: **Mr MacDowell, Niall**
Supervisors: Prof G Jackson, Dr C Adjiman & Dr A Galindo
Title: **Improvements in Amine Based Absorption Systems for Post Combustion CO_2 Capture**
Starting Date: Oct-06
Finishing Date: Oct-09

Name: **Mr Palma Rosillo, Javier**
Supervisors: Prof N Shah & Prof EN Pistikopoulos
Title: **Model Predictive Control of Supply Chain Systems**
Starting Date: Oct-06
Finishing Date: Oct-09

Name: **Mr Paopo, Idtisak**
Supervisors: Dr S Mantalaris & Dr Xu
Title: **Design and Modelling of 3D Perfusion Bioreactor for Stem Cell Bioprocessing**
Starting Date: Oct-07
Finishing Date: Feb-11

Name: **Mr Patel, Mayank**
Supervisor: Prof N Shah
Title: **Design, Operation & Control of the Next Generation Flexible Process Plant**
Starting Date: Jun-07
Finishing Date: Jun-10

Name: **Ms Pereira, Frances**
Supervisors: Prof G Jackson, Dr C Adjiman and Dr A Galindo
Title: **From CO_2 Capture to Advanced Oil Recovery**
Starting Date: Oct-06
Finishing Date: Oct-09

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

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

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

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

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

Name: **Melanie Ramirez Jaramillo**
Supervisor: Prof Eric Fraga
Title: **Waste processing options for biofuel production**
Starting Date: Mar-08
Finishing Date: Mar-12

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

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

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

Name: **Mr Sampayo-Hernandez, Jose Guillermo**
Supervisor: Prof G Jackson
Title: **Theory and Simulation of Interfacial Systems**
Starting Date: Oct-05
Finishing Date: Sep-08

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

Name: **Mr Seaton, Daniel**
Supervisor: Dr Krishnan
Title: **Mathematical modelling and systems-based understanding of cell polarity**
Starting Date: Oct-08
Finishing Date: Oct-12

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

Name: **Mr Soh, Boon Seng**
Supervisors: Dr A. Mantalaris, Dr A. E. Bishop & Dr L. Bing (Genome Institute of Singapore)
Title: **Directed differentiation of human embryonic stem cells to lung bronchioalveolar stem cell**
Starting Date: Apr-06
Finishing Date: Apr-09

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

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

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

Name: **Mr Sweetman, Stephen**
Supervisor: Dr C Immanuel
Title: **Population Balance Modelling of Emulsion Polymerisation Systems'**
Starting Date: Nov-04
Finishing Date: Nov-08

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

Name: **Mr Thambirajah, Jegatheeswaran**
Supervisor: Prof NF Thornhill
Title: **A Wide-Area System for Power Transmission Security Enhancement using a Process Systems Approach**
Starting Date: Jul-07
Finishing Date: Jul-10

Name: **Mr Tsoukalas, Angelos**
Supervisor: Berc Rustem
Title: **Global Optimization Algorithms for Multi-level and Generalized Semi-Infinite problems**
Starting Date: Sep-05
Finishing Date: Sep-09

Name: **Mr Sumner, Tom**
Supervisor: Prof D Bogle
Title: **Evaluating Uncertainty in Computational Models of Biological Systems**
Starting Date: Oct-06
Finishing Date: Oct-09

Name: **Ms Voelker, Anna**
Supervisor: Prof EN Pistikopoulos
Title: **Control of MUAVs**
Starting Date: Oct-07
Finishing Date: Oct-10

Name: **Mr Wiesemann, Wolfram**
Supervisor: Berc Rustem
Title: **Optimisation of Temporal Networks under Uncertainty?**
Starting Date: Sep-06
Finishing Date: Sep-10

Name: **Mr Ye, Kai**
Supervisor: Berc Rustem
Title: **Applications of Semidefinite Programming in Finance**
Starting Date: Sep-05
Finishing Date: Sep-09

NOTES

NOTES

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