Imperial College London

UCL

Centre for Process Systems Engineering

PSE@ResearchDayUK

Friday 7 September 2018, 08:30 - 16:00

Opening Lecture

"Process Systems Engineering from an Industrial and Academic Perspective"

Professor Anton Kiss
University of Manchester

Lecture Theatre 266, Level 4, Roderic Hill Building,
South Kensington Campus, Imperial College London SW7 2AZ.

Lunch and refreshments will be served in Room 265, Level 4, Roderic Hill Building.

WELCOME TO THE 2018

PSE@ResearchDayUK

Why PSE@ResearchDayUK was started?

The Centre of Process Systems Engineering (CPSE), from Imperial College London and University College London started the PSE@ResearchDayUK to try to bring together researchers and leading United Kingdom's academics. Our aim was to enable them to explore the latest technological advances in core and emerging application areas in PSE and to build their personal networks for future collaborations. Postgraduate students are given opportunity to showcase their research results and share visions with leading researchers and academics in the UK.

Centre of Process Systems Engineering (CPSE)

CPSE is a Multi-institutional research centre of world-class departments at Imperial College London and University College London. CPSE was inaugurated in 1989 by Professor Roger W.H. Sargent, the founding Director of the Centre from 1989 to his retirement in 1992. Since then, CPSE has continued the legacy of Professor Sargent and remains a Centre of Excellence.

Message from CPSE Director, Professor Claire S. Adjiman

"Welcome to the third PSE@ResearchDayUK! This year, we have a new programme lined up, where we will have oral presentations without the posters. We hope you will enjoy the new programme and I look forward to welcoming United Kingdom's leading academics and researchers to the Centre.

For more information, please email Professor Claire S. Adjiman: c.adjiman@imperial.ac.uk or Dr Benoît Chachuat: b.chachuat@imperial.ac.uk

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2018 Programme

08.30 *Registration – Refreshments* served

09.00 **Welcome** by Professor Claire S. Adjiman, Director of CPSE (LT266 Auditorium)

09.10 **Opening Lecture** by Professor Anton Kiss, University of Manchester, *"Process Systems Engineering from an Industrial and Academic Perspective"*

Oral Session 1 (LT266 Auditorium)

10.00 Fabian Neumann, "*Modelling the European Energy System to Fulfil the Paris Agreement Targets: The Role of Informatics*", Karlsruhe Institute of Technology

10.20 Patrick Brandl, *"Techno-Economic Screening of CO_2 Capture Solvents and their Marginal Cost"*, Imperial College London

10.40 Andrés González Garay, *"Optimal Design of Sustainable Chemical Processes"*, Imperial College London

11.00 *Coffee Break – Refreshments served*

Oral Session 2 (LT266 Auditorium)

11.20 Mark Jones, *"Superstructure Optimisation with General Disjunctive Programming and Surrogate Models"*, Technical University of Denmark

11.40 Johannes Wiebe, "*Data-Driven Optimization of Processes with Degrading Equipment*", Imperial College London

12.00 Gyula Dörgő, "Hierarchical Frequent Sequence Mining Algorithm for the Improvement of Advanced Alarm Management Solutions", University of Pannonia

12.20 Panagiotis Petsagkourakis, *"Equation-Free Model Reduced Multiparametric Model Predictive Control"*, University of Manchester

12:40 Panagiotis Demis, *"Global Sensitivity Analysis for Problems with Inequality Constraints"*, University of Surrey

13.00 *Lunch Break*

Oral Session 3 (LT266 Auditorium)

14.00 Govind Menon, *"Unraveling Modularity and Compartmentalization of Biochemical Pathways: Systems Engineering Approaches at the Intersection of Systems and Synthetic Biology"*, Imperial College London

14.20 Federico Lozano Santamaria, "Refinery Case Study of Optimal Cleaning Scheduling for Fouling Mitigation in the Preheat Train," Imperial College London

14.40 Michael Ehrenstein, *"Strategic Planning of Supply Chains Considering Extreme Events: Novel Heuristic and Application to the Petrochemical Industry"*, Imperial College London

15.00 Yukun Wang, "*Optimization-Based Analysis of a Thermofluidic Engine for Low-grade Heat Recovery"*, Imperial College London

15.20 Pedro I. O. Filho, *"Design and Scale-up of an Industrial AACVD under Uncertainty: MINLP Formulation and Solution"*, University College London

15.40 *Announcement of Prize Winners – Refreshments* served

16.00 *Close*

Opening Lecture

Process Systems Engineering from an Industrial and Academic Perspective

Professor Anton Kiss
University of Manchester

Tony Kiss is a professor and chair in chemical engineering at The University of Manchester, and a *Royal Society Wolfson Research Merit Award* holder. His early passion for chemistry led him to win several awards at Olympiads and to become member of the National Chemistry Olympic Team. He holds an MSc degree in Chemical Engineering from the Babes-Bolyai University of Cluj-Napoca, where he graduated as the best student and also worked for several years as teaching assistant. Afterwards, he successfully earned a PhD at the University of Amsterdam (UvA). He worked as PostDoc fellow at DeltChemTech (TU Delft) on PSE projects, and then again as PostDoc at UvA focusing on catalysis. Tony has over a decade of industrial experience, working as Senior Project Manager/ Leader + RD&I Specialist in Separation Technology at AkzoNobel – Research, Development & Innovation (RD&I). Next to his industrial role, he was also appointed as part-time professor of Separation Technology at University of Twente, in the Sustainable Process Technology group. During the past decade, he carried out many research & industrial projects, supervised graduation projects, published several textbooks, book chapters, and over 100 scientific articles. For the pioneering work and remarkable achievements in his area of scientific research, he was rewarded in 2013 with the *Hoogewerff Jongerenprijs* – a very prestigious award recognizing the most promising young scientist in The Netherlands. He also led his team to receive in 2013 the *AkzoNobel Innovation Excellence Award* for the most successful industrial innovation. More information is available at: www.tonykiss.com

Abstract: Process Systems Engineering (PSE) deals with methods and tools to support decision-making for the creation and operation of chemical supply chains, including the discovery, design, manufacturing, processing, and distribution of chemical products. In other words, PSE is about educated decision-making, at all levels and (size/time) scales, by understanding complex systems using a holistic view. This lecture aims to provide an informative industrial and academic perspective on PSE, from a personal viewpoint of the author - a seasoned professional with more than 20 years of combined industrial and academic experience. The main topics covered include: brief history, PSE in academic education vs industrial needs, PSE research vs industrial projects, personal perspectives, lessons learned in industry, global challenges and trends, professional skills, role and opportunities for PSE.

Modelling the European Energy System to Fulfil the Paris Agreement Targets: The Role of Informatics

Fabian Neumann
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Abstract

1 Problem Statement

To investigate the best ways to reduce greenhouse gases in the energy sector, researchers build models that represent many aspects of the energy system. These models typically use optimisation to minimise the total system costs (made up of investment and operation costs) under the condition that all technical and environmental constraints are met. But also political and social constraints are increasingly receiving attention.

For systems based on renewable energy, whose greatest expansion potentials are found for wind and solar generation, the chief challenge is dealing with the variability and volatility of these energy sources. Different approaches can be found in the literature to tackle this challenge: smoothing renewable feed-in in space with large transmission networks; smoothing the variability in time with storage; and demand-side management, which is particularly effective when electricity models are coupled to other energy sectors like heating, transport and industrial demand. Since wind and solar dominate the expandable potentials for low-carbon energy provision electrification of these sectors also is essential. Fortunately, these sectors can also offer crucial flexibility back to the electricity system.

However, all aspects of the energy system at all levels of detail cannot currently be contained in a single optimisation model because of computational constraints. Researchers, thus, have to simplify crucial aspects of modelling.

An advanced energy system model would need high spatial resolution to represent variations in the availability of renewable energy and transmission constraints, as well as continental scope to capture energy markets and large-scale smoothing. Similarly, it would need to combine high temporal resolution and multi-year time series to represent load and variable renewable energy resource variability, correlations and extreme events. This gives rise to the research question of what simplifications largely retain accuracy and reduce complexity.

Optimising parts of the model independently may not capture the large number of interacting interdependencies between places, times and sectors. For instance, with added use of cross-sector flexibility, the benefit of cross-border power transmission may become weaker. The strong interacting relationship between generation, storage and transmission extension leads to the question which decisions should be cooptimised and which can be treated separately.

2 Informatics in Energy System Modelling

The contribution of informatics is twofold: (1) it can contribute to data quality e.g. by processing big weather datasats, performing geographical potential analyses as well as merging open data sources fostering model openness and (2) it can contribute on the algorithmic side with e.g. data reduction techniques such as clustering and principal component analysis, new optimisation routines for speed and accuracy, and information theory to trace interdependencies in the optimisation model.

PyPSA-Eur is an exemplary open and increasingly crosssectoral energy model for the joint optimisation of the European transmission system [H¨orsch et al., 2018]. Its grid data is based on an extraction of the ENTSO-E interactive map, it combines open databases on power plants using a matching algorithm, and derives geographic potentials for renewables from land use. It constitutes a tool for investigating methods to increase the model detail while remaining computationally performant, so that large systems can be studied which have both a continental scope and fine-scaled temporal and spatial resolution. Moreover, in the future it will include non-linearities of transmission network expansion problems allowing the consideration of reactive power flows and demand as well as line losses, that can scale up to large networks with coupling between multiple energy sectors.

3 Conclusion and Outlook

It is apparent that the energy transition is an urgent challenge for science, society and industry. Initial studies show that the energy transition is feasible, but due to computational complexity, researchers have to simplify crucial aspects of modelling. Energy system optimisation may leverage new algorithms and interdisciplinary methodologies to tackle this complexity as taking account of European interactions, spatial as well as temporal detail, and sector coupling are all crucial for assessing the number of feasible and near-optimum pathways to reducing CO_2 emissions. Since the energy system is complex and contains major uncertainties (e.g. cost developments, scaleability of storage, social acceptance and consumer behaviour), openness about assumptions and model implementation is critical.

References

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Techno-Economic Screening of CO_2 Capture Solvents and their Marginal Cost

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Abstract

Carbon Capture and Sequestration (CCS) is widely regarded as being a vital technology for the cost-effective mitigation of anthropogenic climate change [1]. Chemical solvent-based post-combustion capture is the most mature technology, which could be deployed near-term and at large scale. A vast research effort focused on increasing a solvent's equilibrium capacity to absorb CO_2 or on reducing the inherent energy requirement of regenerating the solvent, has resulted in thousands of new materials being proposed in the last decades.

This heuristic methodology might miss the point of accelerating CCS technologies from the lab/ pilot plants to widespread large-scale deployment, which are dominated by costs [2]. Transport properties, such as *e.g.,* viscosity or heat capacity, contribute to the total costs, which include the capital expenditure (CAPEX) and operating expenditure (OPEX). Previous results indicate that viscosity dominates the installed costs and even limits the usability of ionic liquids as post-combustion capture solvents [3]. However, multi-dimensional trade-offs between thermodynamic- and transport-properties (*e.g.,* increased equilibrium constant and increased viscosity) are highly non-linear and require a systematic screening approach.

Amine scrubbing is the predominant technology and usually utilises aqueous blends of primary, secondary, tertiary, sterically hindered or cyclic amines. Common examples are monoethanolamine (MEA), diethanolamine (DEA), methyl diethanolamine (MDEA), 2-amino-2-methyl-1-propanol (AMP) and piperazine. State-of-the-art proprietary amine solvents have shown workable capacities up to 5000 tonnes CO_2 per day at commercial-scale plants at Boundary Dam and Petra Nova. The insights that we seek are to compare new solvents of interest with state-of-the-art proprietary amine solvents, which have shown workable capacities up to 5000 tonnes CO_2 per day at commercial-scale plants at Boundary Dam and Petra Nova.

In this study, we present a techno-economic assessment of solvents of interest with the literature's benchmark, a 30 wt-% aqueous monoethanolamin (MEA) solvent, for gas-fired power plant flue gas conditions, *e.g.,* $y\mathrm{co}_2$ =4% and determine the impact of exhaust gas recycling on the capture costs. Our reduced order model includes rate-based phenomena and uses monetised and non-monetised performance indicators, such as *e.g.,* column height, heat of regeneration and costs. While screening and computer aided molecular design (CAMD) approaches have been followed previously [4], this work introduces parameter for a fair comparison of solvents based on costs. The economic calculation (CAPEX, OPEX) is physically based on properties such as *e.g,* column height, material or flowrates and is condensed into the total annualised costs (TAC, total cost of ownership) $\$\mathrm{ton}CO_2$ /. We perform a multi-dimensional cost optimisation covering operating parameter such as *e.g.,* lean loading or capture rate. We report the OPEX and CAPEX cost-breakdowns for each solvent and quantify the marginal cost of capturing more than 90% of the to be treated flue gas stream.

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Optimal Design of Sustainable Chemical Processes

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Abstract
Developing effective tools for process design is of paramount importance in the transition towards a more sustainable chemical industry. In this work, we present a framework to incorporate sustainability principles in process design that combines a palette of tools, including life cycle assessment, surrogate modeling, objective reduction, multi-objective optimization, and data envelopment analysis (DEA). The latter methodology facilitates the post-optimal analysis of the Pareto front by narrowing down the number of designs and ranking them without the need to define weights in an explicit manner. Additionally, DEA also provides improvement targets for the suboptimal alternatives that if attained would make them optimal, thereby guiding retrofit efforts towards the most effective actions based on benchmarking them against the best technologies available. The capabilities of the framework are demonstrated in a case study based on the production of methanol from CO_2 and hydrogen. The results showed how the substitution of the original model by surrogates (Neural Networks) and the objective-reduction stage (reduction from11 to five indicators) enhanced the multi-objective optimisation. A multi-objective genetic algorithm was used during the optimization retrieving a total of 126 optimal solutions. By applying DEA in the analysis of the Pareto frontier, a total of 9 optimal designs were identified as the most promising configurations. The further use of DEA allowed the final ranking of the solutions, which are presented and discussed.

Superstructure Optimisation with General Disjunctive Programming and Surrogate Models

Mark Jones[a,b], Hector Forero-Hernandez[a,b], Bent Sarup[a] and Gürkan Sin[b]*
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[b]Process and Systems Engineering Center (PROSYS); Technical University of Denmark

Abstract

In this work we present a framework to generate surrogates from rigorous process models embedded in a modelling environment or a process simulator. These unit operations (i.e. process flowsheet subsystems) are treated as black-box models to generate data for fitting and deriving surrogate functions. Further, the methodology includes the formulation of a superstructure optimisation problem in form of a general disjunctive program (GDP) and the identification of the optimal process flowsheet structure and point of operation from the possible alternatives. The superstructure optimisation incorporates selection and interconnection of each unit operation in form of disjunctions and with the objective to maximize profit or to minimize total cost. In this paper we highlight the surrogate building step of the methodology with a rigorous counter-current spray column model and a continuous stirred tank reactor (CSTR). We assess the performance of different surrogate modelling methods such as multivariate regression splines, polynomial chaos expansion and Gaussian process regression in respect to the coefficient of determination (R2), the mean squared error (MSE) and the learning curve performance. The GDP is either solved by transforming it to a MINLP via convex-hull and then solving the problem with a nonlinear solver or by applying directly the GDPopt solver which makes use of the logic based outer-approximation (OA) algorithm. We show that superstructure generation with surrogate models elevates rigorous process design to the upper layer of optimisation where the best sequence of unit operations is determined and raw material input streams, unit operation conditions and product purity are optimized simultaneously. Our proposed methodology and software tool helps engineers to concentrate on the formulation and data retrieval tasks while trial and error simulations of different process configurations is prevented. A spreadsheet interface allows for easy data input and hides the underlying Fortran, Python and Pyomo scripts which can be accessed if the more sophisticated user wants to add new features to the framework.

Data-Driven Optimization of Processes with Degrading Equipment

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Abstract
Process planning and scheduling frequently assumes perfect equipment availability and performance. In reality, equipment degradation can cause deteriorating process performance or equipment failure if maintenance is not carried out frequently enough. Process performance and equipment availability are therefore dependent on the selected maintenance strategy. Furthermore, the rate at which equipment health degrades may be partially random and affected by the selected operating strategy. Process scheduling and planning are both known to be hard problems. Integrating them and including effects of maintenance and uncertain equipment degradation is therefore challenging.

Multiple authors have addressed planning and scheduling with equipment degradation by proposing integrated process and maintenance models which explicitly incorporate unit degradation, e.g. [1–4]. Most of these works assume deterministic relationships between degradation, process performance, operating variables, and/or time. In contrast, the field of Condition-based maintenance (CBM) has attracted significant attention in recent years by using data-informed, stochastic degradation models to infer equipment health, albeit mainly at unit level [5]. We argue that properly accounting for equipment degradation requires new integrated process and maintenance planning and scheduling models which exploit the more sophisticated data-driven stochastic degradation models developed in CBM.

To this end, we show how Lévy type models [6], a class of stochastic processes commonly used for degradation modelling in CBM, can be incorporated into a MILP scheduling and/or planning model using the Lappas and Gounaris [7] adjustable robust optimization approach. Robust optimization has been applied to scheduling and planning by multiple authors, e.g. [7, 8], but it has not been applied, to the best of our knowledge, to uncertainty in equipment degradation. We account for effects of the operating strategy on degradation by allowing the Lévy models parameters to depend on a set of discrete operating modes. As demonstrated by Li and Li [10], selecting an appropriate uncertainty set size in robust optimization is challenging and may be treated as its own optimization problem. We describe the uncertainty set size through a single parameter which we optimize by solving the robust MILP model repeatedly. Since this model can be computationally expensive, we propose using Bayesian optimization, which is known to work well for low dimensional problems with expensive to evaluate objective functions [11]. Bayesian optimisation can also manage the noise introduced when some of the MILP sub-solves cannot be solved to optimality in a reasonable amount of time.

We furthermore propose a cheap way of estimating probabilities of equipment failure. We generate data regarding the relative frequency of occurrence of operating modes by solving a short-term scheduling model repeatedly. This data can be used to construct a Markov chain from which a large number of long-term schedules can be generated cheaply. These schedules are not necessarily feasible in the original problem but can be used to obtain a good estimate of equipment failure probabilities.

We apply our framework to an integrated planning and scheduling model recently proposed by Biondi et al. [3] with explicit treatment of unit degradation for the state-task-network (STN) originally developed by Kondili et al. [12]. We demonstrate that robust optimization is capable of trading of equipment availability and cost of maintenance for a number of STN instances and we show that Bayesian optimization can be used to optimize the uncertainty set size in a computationally efficient way.

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Hierarchical Frequent Sequence Mining Algorithm for the Improvement of Advanced Alarm Management Solutions

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[2]*Department of Process Engineering, University of Pannonia*

Abstract

Faults and malfunctions on complex chemical production systems generate alarm cascades that hinder the work of the operators and make fault diagnosis a complex and challenging task. The techniques of alarm management aim for the efficient design, implementation, operation and maintenance of industrial process alarms. In chemical production plants, as part of the alarm management system, discrete events, e.g. alarms, warnings, operator actions and system messages, are recorded in alarm management databases providing the opportunity for the development of advanced algorithms for reducing and facilitating the work of the operators.

The high amount of process relevant information carried by these datasets can be conveniently explored by frequent sequence-based Bayes models. We present how these models can be applied for the prediction of the next occurring event by first discovering the frequently reoccurring operational patterns and then assigning probability measures for each event occurrences in the revealed patterns by the Bayes' theorem.

Moreover, as the complexity and the size of the alarm management databases make the application of the traditional sequence mining algorithms almost infeasible, we present how the incorporation of the hierarchical structure of the technology helps to reveal the spreading of the effect of malfunctions over the plant by grouping the large number of variables. The spreading of the effect of malfunctions over the plant is thoroughly traceable on the higher levels of the hierarchy (e.g. units), while the critical elements of the spillover effect can be detected on the lower levels (e.g. sensors/ actuators). Confidence-based goal-oriented measures have been proposed to describe the orientation of fault propagation providing a good insight into the causality on a local level of the process, while the network-based representation yields a global view of causal connections.

The effectiveness of the proposed methodology is presented in terms of the analysis of the alarm and event-log database of an industrial delayed-coker plant, where the complexity of the problem and the size of the event-log database requires a hierarchical constraint-based representation. As an outlook of our presentation, we describe how the tools of advanced data-driven modelling like deep learning and process mining can be incorporated in the analysis of industrial alarm management databases.

Equation-Free Model Reduced Multiparametric Model Predictive Control

Panagiotis Petsagkourakis
University of Manchester

Abstract

Constrained model predictive control (MPC) is a powerful control framework where on-line optimisation and a receding horizon are employed to compute the optimum trajectory for the manipulated variables [1]. The use of MPC for distributed parameter systems, consisting of nonlinear partial differential equations (PDEs) is computationally expensive [2]. The dissipative nature of such systems, expressed as a separation of scales in the eigenvalues of the linearized models [3], has been exploited for model order reduction (MOR) in control of (usually parabolic) PDEs [4], projecting the infinite dimensional states onto a small finite subspace. Nevertheless, the control of PDEs requires the use of high fidelity models. To solve this problem, equation-free methodologies have been proposed [5]–[7] that solves the non-linear dynamic optimization problem; although the computational burden can significantly be dropped with the use of the reduced order gradients, they usually require a considerable amount of CPU-time, which can make them unsuitable for real-time control applications. The on-line computation can be enhanced with the use of multiparametric (mp) optimisation [8] that computes an off-line map of the control law as a function of the states. Therefore, the computational effort is redistributed off-line, overcoming the on-line computational burden of the classic MPC. Even though the majority of computations are performed off-line, the large number of variables of the physical system may produce an intractable computational approach making the use of model reduction necessary. Rivotti et al. [9] combine non-linear model order reduction, based on balancing of empirical gramians to reduce the size of the system with mp approximate non-linear MPC, which can still be prohibitive for complex largescale systems, modelled by a large set of PDEs.

In this work, an equation-free multiparametric MPC is proposed, and only an available black-box simulator (such as COMSOL [10]) is employed, performing inputoutput tasks. An equation-free non-linear dynamic optimisation has been developed based on its static counterpart [11] utilising an equation-free model reductions in direct sequential scheme. The mp-optimization takes advantage of the reduced gradients produced by the non-linear dynamic optimizer together with the implicit function theorem. The multiparametric approach aims to compute an off-line map that approximates the reduced non-linear problem efficiently. First, an initial solution is computed for the non-linear optimisation problem employing the matrix-free Arnoldi iterations [12] for constructing a model reduction orthonormal basis without the use of full gradients. Then, a reduced order multi-linear model is produced as a good approximation of the model and the mp-optimization is solved producing an initial set of critical regions (CR). The CRs are refined using the non-linear dynamic optimisation in order to approximate the non-linear problem within an arbitrary tolerance. The results show that only a small number of CR regions are necessary to sufficiently approximate the problem taking advantage of the good initial solution. The effectiveness of this algorithm is illustrated through a chemical engineering application.

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Global Sensitivity Analysis for Problems with Inequality Constraints

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Abstract

In the presence of uncertainties in mathematical modelling, global sensitivity analysis (GSA) is a method for studying how the variation of model outputs can be apportioned to variations of inputs. GSA enables variable ranking, screening and fixing with direct implications for uncertainty reduction, model calibration, validation and simplification. The most widely adopted method for GSA is based on variance decomposition for the estimation of main and total effects of the input variables, also known as Sobol' indices [1]. In practice, Sobol' indices are computed using Monte Carlo estimators, which rely on (quasi-)random samples of the input distributions [2]. The distinctive advantage of this approach is that it treats mathematical models as black boxes, measures the variability of all inputs simultaneously and comprises the sole method to date for sensitivity analysis on models with dependent inputs [3].

A common issue in complex system models and process engineering is the presence of structural dependencies imposed by inequality constraints that can be explicit (i.e., involving model inputs only) or implicit (i.e., involving model outputs) in nature. Kucherenko et al. addressed this class of problems in the context of GSA, proposing generalised Monte Carlo estimators for constrained GSA (cGSA), which rely on acceptance-rejection sampling [4]. Further findings showed that these dependencies may strongly affect the underlying sensitivities and cGSA can describe accurately the uncertainty propagation in non-rectangular domains [5]. However, the increased computational complexity of cGSA, particularly in estimating marginal probability distributions of subsets of inputs under constraints, adds to the already significant computational costs of GSA. Thus, for higher dimensionality of the input space the existing cGSA estimates may become inefficient.

Addressing the above, this work strives to tackle the challenges in cGSA and investigate the impact of implicit or explicit constraints on a wide class of mathematical models with interest to process systems engineering. The goal is to improve existing methods of cGSA, by applying adaptive sampling and metamodelling, and develop techniques for the identification and description of the feasible input space. These approaches aspire to lead to computationally enhanced cGSA, which can benefit experimental and process design, model validation, robust optimisation and model-predictive control.

Towards the aims of this research, recent work has seen the development of a new method for adaptive sampling within unknown boundaries of the feasible space and techniques for the estimation of the boundary of the feasible domain. cGSA has been effectively applied for input ranking and dimensionality reduction in a test case related to biopharmaceuticals manufacturing, which was further used to describe and interpret the feasible space.

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Unraveling Modularity and Compartmentalization of Biochemical Pathways: Systems Engineering Approaches at the Intersection of Systems and Synthetic Biology

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Abstract

Biological cells use networks of molecular interactions to receive signals, regulate their internal processes, and respond to their external environment. While it is well known that there are large numbers of molecular components, what makes things particularly difficult for understanding and engineering these networks is the non-linearity of interactions, feedback loops at multiple levels, stochastic effects, the intricate spatial organization of components, and the fact that they are subject to evolution. All these present substantial new systems challenges. In this talk, we focus on two aspects which are central to the functioning of cellular information processing networks - the modularity of biochemical pathways and the compartmentalization of molecular components.

These features are also central to engineering such systems, in the field of synthetic biology. Information processing modules form core building blocks for the functioning and organisation of signalling and biochemical pathways. They are central to understanding cellular function and have been the focus of numerous studies in natural biology, and have been engineered in synthetic biology. In systems biology, there is great interest in understanding how these modules behave as part of a network in a wide range of contexts. The current wave in synthetic biology is precisely in going from synthetic modules to systems [1,2,3]. However, there is no systematic framework to address these challenges, which can account for the diversity of modules in terms of their network structure, dynamical systems characteristics and biochemical realisation, and the characteristics of the ambient network.

We have formulated and developed a systems framework, rooted in dynamical systems, to understand how the network environment affects a module, focussing on its network structure, dynamical systems characteristics and biochemical nature [6]. Working within this framework we examine different aspects of interactions between a module and the surrounding network. We perform a comprehensive analysis that reveals the factors that determine the interaction between a module and its network, its ability to maintain its behaviour in the presence of interactions, and its ability to interface with other modules. We discuss a range of insights in the context of modules within natural cellular networks, for whole-cell modelling, and for engineering robust synthetic modules.

Compartmentalization of pathways at the intracellular level plays a critical role in many cellular contexts, including signal transduction and the regulation of metabolic processes. The spatial organization of cellular pathways is being increasingly appreciated and there is significant interest in engineering compartmentalized biochemical pathways - both in manipulating spatial organization within cells, and in building cell-free systems of compartmentalized reactions [4,5]. Compartmental models based on ordinary differential equations (ODEs) are a common choice for modelling in all these contexts. However, it is unclear how reliably such models can be used for design and analysis of such systems. We systematically examine the efficacy of compartmental ODEs as tools for the analysis, elucidation, and design in such contexts [7]. By analysis of a set of basic pathways in both,

natural and engineered contexts, and going from simple to complex pathways, we clearly identify regimes in which such models can be used reliably, when they need to be modified, and in what cases they cannot be used, in each case, explicitly illuminating the reasons why. We reveal surprising consequences of using such models both in natural and synthetic contexts, which we explain analytically. We also extend our framework to examine cell-free synthetic nucleic acid based circuits. Overall, through these studies, we demonstrate how dedicated systems methodologies and frameworks can be used to systematically approach and illuminate contemporary challenges in natural and synthetic biology.

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Refinery Case Study of Optimal Cleaning Scheduling for Fouling Mitigation in the Preheat Train

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Abstract

Refining operations are key in the energy sector for fuels production, but at the same time they are highly energy intensive. During the crude processing large amounts of energy are required and many inefficiencies may be present during the operation. Considering the large amount of crude processed for fuels production, there are great incentives to increase the energy efficiency of refining operations which will lead to a reduction of the operating cost, a reduction of the carbon emissions, and a safer operation. One of the main causes of energy efficiency reduction in refining operations is fouling, the deposition of unwanted material over process surfaces. Fouling decreases the heat transfer rate, increases the pressure drop in pipes, and may limit the throughput of the units in the refinery. The units required more energy for a normal operation as fouling builds up, decreasing their efficiency.

The effects of fouling are more evident in the preheat train, a large network of heat exchangers that preheat the crude before the crude distillation unit (CDU), because of the large flow rates, high temperatures, and composition of the crude. To compensate for the effects of fouling in this network of heat exchangers periodical cleanings are scheduled to remove the deposit and restore the performance of the unit. However, the definition of a cleaning scheduling for the network is a difficult task given the large number of units in the network, the large number of interactions through process streams, and the changes in the operation (e.g. crude types, flow rates). Using an accurate model to predict the behaviour of the exchangers, and mathematical programming tools it is possible to define the optimal cleaning scheduling that minimizes the operating cost and that satisfy all the operating constraints.

Here, the optimal cleaning scheduling and flow control of a heat exchanger network is formulated as a MINLP problem with realistically complex models, with the objective to minimize operational cost over a long horizon (~years). The main decision variables are the sequence and timing of cleanings of the units of the network, and the flow rates (e.g split fraction) within the network. This problem has two main difficulties: i) the combinatorial nature given by the large number of binary variables, and ii) the large size and large number of nonlinearities that arise from the fouling model and the heat exchanger model. To handle these difficulties, we propose to model the discrete decisions as complementarity constraints, relaxing the binary variables and solving a sequence of relaxations of the original problem until the final solution satisfies all the constraints of the original MINLP problem.

This work presents an industrial case study of the hot end of a refinery preheat train for which measurements are available, including a record of the cleanings implemented during the operation period. The exchanger and fouling models are fit against the plant data, and then they are used to solve the optimal cleaning scheduling problem. The optimal results of the model are compared against the refinery operation to show the potential savings and advantages of using this methodology.

Strategic Planning of Supply Chains Considering Extreme Events: Novel Heuristic and Application to the Petrochemical Industry

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Abstract

Chemical supply chains today are a crucial component in the ongoing supply of large population centres. However, episodes of extreme weather in particular have, in recent years, revealed vulnerabilities in global supply networks to high-impact events. And with a possible increase in both frequency and intensity of these events due to climate change, supply chains are at risk of disruption now more than ever, with potentially dire economic, societal, and environmental consequences.

Applying stochastic programming to handle these uncertainties can quickly lead to prohibitively large models that cannot be solved in reasonable time. Numerous methods can be found in literature which attempt to lower the computational effort required to solve large stochastic programs, e.g. by reducing the scenario space. However, these approaches are not designed to handle particularly heavy-tailed extreme event scenario distributions, and hence perform poorly in practice.

To remedy this, we propose a new methodology based on a two-stage stochastic programming framework, to enable flexible planning based on the realisation of uncertain parameters. This is combined with a variant of the sample average approximation method for problem size reduction, along with a scenario selection heuristic based on prior knowledge of the structure of the extreme event scenario distribution. Combined with multiobjective optimisation, this allows for the efficient analysis of the tradeoff between economic performance and disruption risk.

We demonstrate the effectiveness of this methodology using multiple case studies, achieving good solutions in reduced CPU time.

Optimization-Based Analysis of a Thermofluidic Engine for Low-Grade Heat Recovery

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Abstract
The Non-Inertive-Feedback Thermofluidic Engine (NIFTE) is a two-phase thermofluidic oscillator that can convert low-grade heat into useful mechanical work. It consists of one hot and one cold heat exchangers alongside several compartments. The selected working fluid undergoes cyclic condensation and vaporization phases by contacting with the heat exchangers, which induce sustained fluid oscillations.

Most previous mathematical models proposed to analyse the dynamic behaviour of NIFTE have been based on linear descriptions. They provide useful insights to the operation of NIFTE, and give quantitative predictions on the minimum temperature difference required, oscillation frequencies and efficiencies. However, these linear models fail to explain the sustained robust periodic oscillations that have been observed experimentally on a NIFTE prototype. This is known as limitcycle behaviour, which is essentially a nonlinear phenomenon. Markides et al. [1] thus proposed a nonlinear inertive NTP model for NIFTE, and this model has been validated experimentally.

In this work, we adopt an optimisation-based approach to investigate NIFTE under cyclic steady state conditions, based on the NTP model. The cyclic steady states (CSS) are determined via solving a dynamic optimisation problem, and the stability of CSS is subsequently determined by analysing the corresponding monodromy matrix. It is found that multiple CSS are exhibited by NIFTE for certain configurations, which may be either stable or unstable. A parametric sensitivity analysis conducted later reveals that higher system performance could be achieved by controlling the engine at different CSS, including unstable ones.

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Design and Scale-up of an Industrial AACVD under Uncertainty: MINLP Formulation and Solution

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Abstract

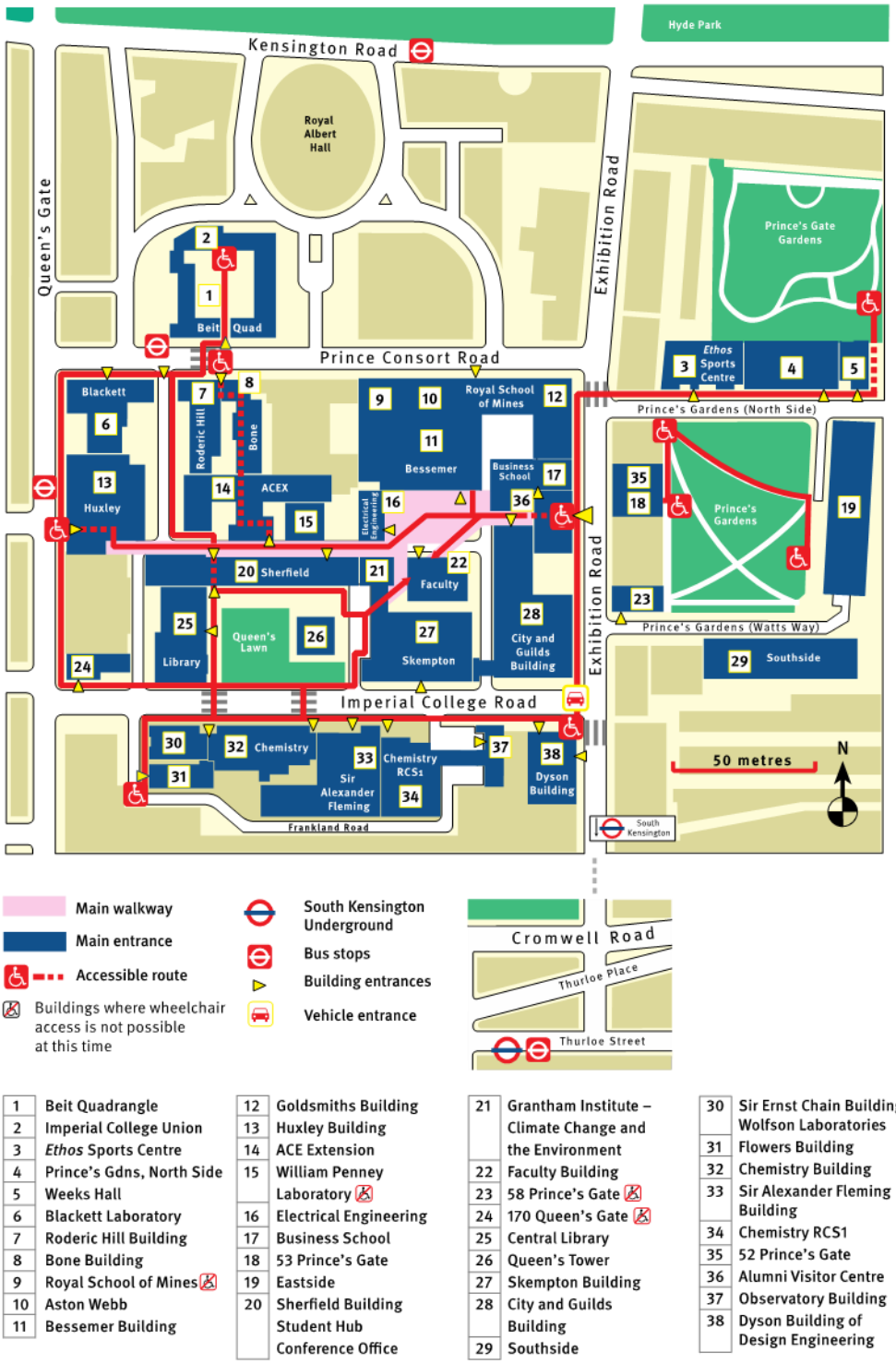
The global energy sector has now sustainability as one of the main objectives. Solar technology is one of the most viable options for a reliable clean energy production. Reducing the cost of solar modules is a key element to increase the potential of such a solution. Solar cells are based on Transparent and Conductive Oxide (TCO) films, which can be produced via a process called Aerosol-Assisted Chemical Vapour Deposition (AACVD). Concisely, this process is based on sequential stages. Firstly, aerosol is generated from a solution containing TCO precursors. Then, the aerosol is transported to a heated chamber, where the solvent evaporates and the precursors deposit, forming the desired film. Not only can TCOs be produced by this process, but also composites, powders, coatings, nanotubes, etc.

Although there is some research available in the literature reporting small scale experimental results from the application of the AACVD technique, there is little about computational modelling. The latter would nevertheless be crucial for the design and scale-up of the AACVD. Consequently, we present an integrated model composed of aerosol generation, transport and delivery. For the aerosol generation, we predict the range of droplet sizes obtained via ultrasonic atomisation of the precursor solution. This is done using probability distributions, which become one of the inputs for the transport model. We can then predict the aerosol loss as a function of the properties of the droplets, the flow and the piping system. The model output shows the fraction of aerosol that reaches the heated chamber as well as its size range. It has been tested for a variety of scenarios, using different combinations of horizontal, inclined and vertical pipes. Finally, the solvent evaporation in the heated chamber is modelled, which depends mainly on the temperature profile of the site and the flow conditions. The precursors are now free to deposit and form the desired products. Uncertainty and sensitivity analyses are performed throughout the process.

The stochastic aspects of aerosol generation, transport and delivery were incorporated using probability distributions. Experimental results were used to validate the model predictions for droplet sizes for the generated aerosol and the loss during transport. Through the formulation of an optimisation problem, the model presented has been used to suggest possible designs for the transport system, minimising the aerosol loss. This approach is suitable for transport distances on the scale of industrial processes. Other applications based on particle atomisation and transport, such as fuel combustion and spray drying or cooling, can also use the models presented here. Finally, the knowledge acquired while handling uncertainties in the modelling of the AACVD process has been used to plan a modelling framework based on Julia, a modern programming language for scientific computing, that will enable us to represent uncertainties and manipulate variables with uncertain values.

Campus Map and Directions

Map of the South Kensington Campus of Imperial College London:



1	Beit Quadrangle	12	Goldsmiths Building	21	Grantham Institute – Climate Change and the Environment	30	Sir Ernst Chain Building · Wolfson Laboratories
2	Imperial College Union	13	Huxley Building	22	Faculty Building	31	Flowers Building
3	*Ethos* Sports Centre	14	ACE Extension	23	58 Prince's Gate	32	Chemistry Building
4	Prince's Gdns, North Side	15	William Penney Laboratory	24	170 Queen's Gate	33	Sir Alexander Fleming Building
5	Weeks Hall	16	Electrical Engineering	25	Central Library	34	Chemistry RCS1
6	Blackett Laboratory	17	Business School	26	Queen's Tower	35	52 Prince's Gate
7	Roderic Hill Building	18	53 Prince's Gate	27	Skempton Building	36	Alumni Visitor Centre
8	Bone Building	19	Eastside	28	City and Guilds Building	37	Observatory Building
9	Royal School of Mines	20	Sherfield Building Student Hub Conference Office	29	Southside	38	Dyson Building of Design Engineering
10	Aston Webb						
11	Bessemer Building						

The PSE@ResearchDayUK will take place in Room 266, Level 4, Roderic Hill Building [7]. Refreshments and lunch will be served in Room 265, Level 4, Roderic Hill Building (next door).

Directions to Room 266, Level 4, Roderic Hill Building:

The easiest way to get to Roderic Hill Building is from the Sherfield walkway.

The entrance to ACEX is adjacent to the Union shop (selling stationery and clothing) and directly opposite a doorway into the senior common room.

Walking with the common rooms on your left hand side, you will eventually reach the entrance to the ACE Extension on your right hand side.

Walk through the ACEX's glass doors main entrance, up the short flight of stairs and zig-zag through to the foyer of Chemical Engineering. Ahead you will see into the control room of the Chemical Engineerig pilot plant (a large pipework system visible beyond the control room).

Turn left, walking around-and-beyond the enclosed staircase, and into a long social area with seating under the windows. Head through towards the whole length of the breakout seating and go through the double doors at the end, into a corridor of offices. Continue along the corridor through to the Department of Aeronautics. Follow the corridor around to the right. At the end, go through the left-hand set of double doors that connect the ACEX to a stairwell of the Roderic Hill Building, marked level 2.

Walk ahead through double doors into the corridor, along to the end and turn right. Room 266 is on the left hand side.

NB: The floor numbers are confusing - stairwell level 4 leads to RODH Building floor 2!

Floor Plan of Level 4, Roderic Hill Building:

Notes

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