ADVANCED PROCESS MODELLING FORUM

LONDON

20–21 APRIL 2016

agenda

20–21 April 2016
Radisson Blu Hotel
London

Outline programme

Tuesday 19 April – Optional and invited events

Morning	Track 1 – Formulated Products Optional workshops • WS1: Crystallization (gCRYSTAL) • WS2: Spray drying (gSOLIDS) • WS3: Granulation (gSOLIDS)	Track 2 – gPROMS ProcessBuilder Optional workshops • WS6: gPROMS ProcessBuilder – an introduction • WS7: Pressure-swing adsorption
Afternoon	Continuation of morning workshops	• WS8: Whole-plant optimisation • WS9: Batch process optimisation
Afternoon	Advisory boards	Advisory boards
Evening	Welcome drinks at the Radisson Blu Hotel	

Wednesday 20 April – Main conference day 1

Morning	General session Introduction, keynotes & APM applications	
	Track 1 Formulated Products including Life Sciences, Food & Consumer Goods, Specialty Chemicals	Track 2 Advanced Process Modelling
Lunch	Academic poster session	
Afternoon	Track 1 Formulated Products [continued]	Track 2 Chemicals & Petrochemicals and Energy & Environment
Evening	Thames boat cruise & dinner	

Thursday 21 April – Main conference day 2

Morning	Track 1 gPROMS platform & product developments	Track 2 Oil & Gas seminar S1: Best practice pressure relief, blowdown and flare system assessment
Lunch	Academic poster session	
Afternoon	General session Oil & Gas, Refining and Petrochemicals	

Friday 22 April – Meetings by arrangement

All day	One-to-one meetings (PSE offices)

Wednesday 20 April 2016

Morning session – Introduction, keynote and overviews: developments & directions

Chair: Richard Tinsdeall

09:00	**Welcome & introduction**	Richard Tinsdeall Chief Commercial Officer **PSE**
09:10	Advanced Process Modelling – transforming the way the process industries design and operate PSE's mission is continually to drive the development of process modelling and its application within the process industries. Costas Pantelides describes the way that equation-oriented technology is bringing transformational change in sectors from Oil & Gas through to pharmaceuticals, pushing the boundaries of what the process industries should expect from process simulation and modelling tools now and in the future.	Costas Pantelides Managing Director **PSE**
09:40	Keynote: The role of modelling in creating value in a large process organisation Modelling plays a key role in underpinning capital and operating decisions in any large process organisation. DSM have long been expert users of modelling technology to accelerate innovation in its chemicals and, more recently, health, nutrition and materials businesses. Dorus van der Linden provides a perspective of how the technology is used to create value, and where he sees the main impact of future applications.	*Peter Drogt for* Dorus van der Linden Global Competence Manager Modeling & Data Analysis **DSM**
10:10	gPROMS FormulatedProducts: a comprehensive, integrated design tool for formulated products manufacture PSE has focused over the last year on integrating several products – gSOLIDS, gCRYSTAL and gCOAS – into a single platform for the design of formulated products and their manufacturing processes. The resulting integrated platform allows scientists and engineers to screen formulations for end-user attributes, determine whether they can be manufactured efficiently, and use the gPROMS platform's optimisation capabilities to optimise the whole formulation and manufacturing chain. This permits a diverse set of behaviours to be explored within the same flowsheet, leading to powerful new capabilities in the digital design of formulated products.	Sean Bermingham VP Formulated Products **PSE**
10:40	Refreshment break	

Morning Track 1 – Formulated Products (Life Sciences, Food & Consumer Goods, Specialty Chemicals)

Chair: Hassan Mumtaz

11:00	Predicting the output of a fluidised bed opposed jet milling process using population balance modelling In jet milling R&D it is a major challenge to model the process and predict its output using only a small amount of experimental data. Adding to the complexity, jet mills often include a classifier wheel that allows particles smaller than a desired size to exit the mill, therefore controlling the hold-up, residence time and product top size. In this presentation Hellie Tsitsiris reports on Saint-Gobain's ongoing work on jet mill simulation in gSOLIDS using a coupled approach of laboratory scale fragmentation tests and population balance modelling of both the comminution and classification stages of the mill.	Hellie Tsitsiris R&D Engineer **Saint-Gobain**
11:25	Developing and deploying mechanistic model-based solutions for food technologists Chemical engineers are trained in making mass and energy balances and using flowsheeting tools to help them with this. Food technologists have basic knowledge on mass balances. For this audience the learning curve for gPROMS has historically been quite steep. Based on feedback from users, the existing model library has been improved to make the use of gPROMS more intuitive for less experienced users and reduce support requirements from high level users. The approach, improvements and results will be presented.	Martijn van der Hoeven Senior Process Technologist **Danone**
11:50	Multiscale approach for continuous crystallization revamp To increase the capacity of a solid production line, a crystallizer revamp was necessary. A multi-scale approach was followed to design the equipment modifications and to optimise the operating conditions. It required the acquisition of data at lab and industrial scale. A crystallization model was developed coupling Population Balance Modelling and Computational Fluid Dynamics. The kinetics and the kinetic parameters were determined using the experimental data. Finally, this allowed the plant to be debottlenecked.	Mathieu Oullion Senior Scientist Process Engineering **Solvay**
12:15	Lunch	

Morning Track 2 – Advanced Process Modelling

Chair: Bart de Groot

11:00	Integrated steel plant modelling in gPROMS There is an increasing demand for flexible process variations, raw material utilisation, internal by-product and waste material recycling in iron and steel production. This requires new and intelligent tools for mass and energy balancing based on a flow sheeting approach. Primetals has developed a comprehensive metallurgical flowsheet model library for depiction of integrated steel plants using the custom modelling capabilities of gPROMS, to enable the setup of mass and energy balances for plants, development and evaluation of new process concepts, investigations on impacts of raw material changes and trace material distributions.	Bernd Weiss Senior Process Engineer **Primetals**
11:30	Quantifying deactivation mechanisms for a Fischer-Tropsch catalyst in microchannel reactors Velocys Fischer-Tropsch technology offers superior performance over conventional routes for production of high quality diesel fuels and waxes using a catalyst with high activity and a low deactivation rate. Despite its low deactivation rate, there is significant economic advantage to extending the catalyst lifetime to reduce reactivation cycle times and especially to defer catalyst replacement. This presentation describes how gPROMS ModelBuilder is used to model the performance of the Velocys microchannel reactors, including catalyst deactivation, helping to gain understanding of the main deactivation mechanisms and providing optimisation routes for process economics.	Henning Becker Research Engineer **Velocys**
12:00	Tuning of automatic controllers in continuous PLA polymerisation plants through gPROMS simulations Polylactic acid (PLA) has a strong market growth potential as a substitute for fossil-based polymers such as PET, PE and PS. However, the PLA process is very sensitive to impurities and in-line monitoring and automatic control is crucial to maintain product quality and operational safety. Dr Ivano Costa uses a MIMO controller and a validated kinetic model in gPROMS to demonstrate how to develop and implement an automated control strategy that results in a substantial reduction in oscillations on plant safety and the amount of off-spec material produced.	Ivano Costa R&D Project Manager PATC **Sulzer Chemtech**
12:30	Lunch	
13:00	**Academic poster session**	

Afternoon Track 1 – Formulated Products (Life Sciences, Food & Consumer Goods, Specialty Chemicals)

Chair: Frances Pereira

13:30	Introduction to academic collaborations: research partners and CRO providers PSE works closely with a number of academic institutions, research organisations and CRO providers around the world. In this session selected collaboration partners briefly describe their work.	Sean Bermingham, VP Formulated Products **PSE**
13:40	Workflows and technologies for continuous crystallization With the growing interest in continuous manufacturing of pharmaceuticals there is a need to enable the development of robust crystallization processes that control key particle attributes. This presentation describes a systematic approach exploiting targeted experimentation, parallelisation and automation and PAT combined with kinetic and multivariate modelling tools. This approach is applied to design and inform the operation of consistent continuous crystallization processes.	Alastair Florence Centre Director **CMAC** at **University of Strathclyde**
14:05	Model-based analysis of granulation and drying in continuous manufacturing Models only provide real value when they are properly calibrated and validated. This talk shows the application of several powerful modelling methodologies such as global sensitivity analysis, global optimisation and model selection used in the model building framework. Results will be shown for granulation and drying in continuous manufacturing.	Ingmar Nopens Professor Dr. Ir. **University of Gent**
14:30	ERC: C-SOPS capabilities towards continuous manufacturing of solid based drug products The Engineering Research Center for Structured Organic Particulate Systems (C-SOPS) brings together a cross-disciplinary team of engineers and scientists as well as industry leaders to improve the way pharmaceuticals, foods and agriculture products are manufactured. This talk briefly describes the capabilities of the centre to characterise new materials, test new equipment, model the entire production line and facilitate risk assessment and optimisation. The focus is on continuous manufacturing of solid-based drug products, and highlights recent modelling work and demonstrates the application of modelling tools using the on-site pilot plant.	Marianthi Ierapetritou Professor & Chair **Rutgers University**

14:55	Combining mechanistic models and experimentation to drive pharmaceutical innovation The Research Centre Pharmaceutical Engineering (RCPE) is an interdisciplinary research institute focused on pharmaceutical process and product development. Massimo Bresciani describes how RCPE combines model-based approaches with experimentation to drive innovation in the pharma industry through a mechanistic understanding of relevant phenomena at all scales.	Massimo Bresciani Director Scientific Operations **RCPE**
15:15	Refreshment break	
Chair: Sean Bermingham		
11:00	Optimisation of continuous crystallization processes to maintain content uniformity Content uniformity (CU) is a common critical quality attribute of Solid Oral Dosage Forms. In this work, we examine a continuous cascade cooling crystallization process and explore its optimisation, while maintaining the content uniformity of the final dosage form. To predict the CU of the drug product, various models, dependent on the PSD and the dosage level of the API present in final dosage form, are employed. A number of optimisation objectives are then posed, which include increasing throughput of the API and the number of number of crystallizer stages. The trade-offs observed for each optimisation objective are also outlined.	Chris Burcham Senior Engineering Advisor **Eli Lilly**
15:45	Scale-up of fluid bed drying in pharmaceutical manufacture by using a mechanistic model Fluidised bed drying is one of the core processes in pharmaceutical manufacturing of solid products. Roche has been working on implementing a mechanistic model of fluid bed drying in its process development workflow, in order to achieve higher productivity by saving on experimental effort. In this work the single-phase fluidised bed drying model from gSOLIDS was used to scale up the process from laboratory to pilot scale. The equipment and the formulation used were characterised, and practical difficulties in using the model were identified and overcome.	Emmanuela Gavi Scientist **Roche**
16:10	Model based development and manufacture of Drug Product in a Continuous Manufacturing Line Eli Lilly utilises mathematical tools to aid the development of an integrated Powder to Drug Product Continuous Manufacturing Process. In this presentation, a holistic model capable of describing the overall system dynamics is employed to justify the appropriate usage of process analytical technology (PAT) tools to monitor the critical quality attributes (CQAs) and fundamentally increase the observability of the states of the system. The model is next used with state estimation and data reconciliation techniques to help devise a control strategy.	Sal Garcia Engineering Advisor **Eli Lilly**
16:35	Digital Design of Drug Product (D3P): Application of global system analysis to a tablet manufacturing process Traditionally, formulation and process development within the pharmaceutical industry is driven by extensive trial-and-error experimentation. The D3P project integrates qualitative and quantitative tools to facilitate an approach to formulation and process design based on the development of fundamental process and product understanding. A global system analysis approach has been used to realise an in-silico 'design space explorer'. This tool is applied to a roller compaction tablet manufacturing process to understand the impact of raw material and process changes on product quality. The approach can be used to inform risk assessment and to design a robust control strategy for the product.	Gavin Reynolds Principal Scientist **AstraZeneca**
17:00	The utility of the Artificial Stomach Duodenum system in in-vivo oral absorption modelling In vivo drug precipitation has been a major issue facing poorly soluble drugs, especially weak bases. This work aims to provide a framework on how to use the Artificial Stomach Duodenum (ASD) System to assess the extent of precipitation of poorly soluble compounds under biorelevant conditions. The concentration profiles measured in the ASD System are used as inputs in in the gCOAS ASD model to estimate the nucleation and growth kinetic parameters. These crystallization kinetic parameters are then used in the gCOAS GI tract model to simulate in vivo precipitation under human fasted conditions and to calculate the fraction absorbed as a function of dose.	Kaoutar Abbou Oucherif Senior Associate Consultant Engineer **Eli Lilly**
17:50	Close	
18:00	**Thames cruise & dinner**	
23:00	Finish	

Afternoon Track 2 – Chemicals & Petrochemicals

Chair: Marcel Renet

13:45	Development of intrinsic kinetic model for SCR monolith catalysts It is often difficult to determine intrinsic kinetic parameters in fixed-bed reactors as reactor configuration and operating conditions should be chosen such that all internal and external heat- and mass-transfer resistances are negligible. This is not always possible in lab-scale reactors, which will impact the reliability of scale-up and design of pilot and industrial reactors. In this study a kinetic model is developed using gPROMS ModelBuilder by extracting intrinsic kinetic parameters from fixed-bed reactor experiments that simultaneously consider catalytic chemical reactions and all transport phenomena,. The model is then used with CFD for the design of new SCR monolith reactors.	Sang Baek Shin Principal Engineer **Yara International** Stepan Spatenka Principal Consultant Engineer **PSE**
14:15	Optimisation of an acetylene hydrogenation reactor SCG Chemicals is applying detailed catalytic reactor models to optimise the performance of an acetylene hydrogenation reactor, a key component of its olefins plant. Mr Nattawat describes the business motivation for the project, the methodology used in building and applying the reactor model, the key capabilities of the reactor models and software platform being used, and outcome of the project.	Tiensai Nattawat Process Technology Leader Hattachai Aeowjaroenlap Engineer Process Innovation **SCG Chemicals** Stepan Spatenka,**PSE**
14:45	gPROMS Utilities: online utility optimisation for chemical parks Chemical parks are major consumers of energy in the form of electricity, steam and, in some cases, hydrocarbon feedstocks. Given that tariffs and demands are constantly changing, there is much scope for optimising site generation utilities. gPROMS Utilities is an online optimisation framework that can rapidly optimise equipment selection and load allocation to improve overall efficiency and reduce operating costs.	Dorus van der Linden Global Competence Manager Modeling & Data Analysis, **DSM** Penny Stanger Senior Consultant Engineer, **PSE**
15:15	Refreshment break	

Afternoon Track 2 – Energy & Environment

Chair: Mayank Patel

15:45	Advanced process modelling in large-scale optimisation of eco-industrial park design and operation The University of Cambridge is working with Nanyang Technological University, the National University of Singapore and industrial partners to pioneer systematic approaches for multi-level modelling and optimisation within eco-industrial parks (EIPs). The initiative uses innovative technologies, including a four-level – unit, process, plant and industrial network – modelling framework coupled with advanced mathematical modelling and optimisation approaches, to improve energy and resource efficiency throughout the whole EIP system.	Ming Pan Research Associate **University of Cambridge**
16:15	Optimising industrial wastewater systems: from food production to shale gas Industrial wastewater systems are required to clean up process wastewater that ranges from the biological waste typical in food and pharmaceutical production – usually handled by biological treatment – to oil & gas wastewater that requires physico-chemical separation processes. This presentation describes the facilities available in gWATER for dealing with the full range of treatments, illustrated with an example of shale gas water treatment.	Marc Pau Roig Consultant Engineer **PSE**
16:45	Academic poster winner: Simultaneous process design and optimal utility selection Most effective methods for heat and mass network design of industrial processes are based on pinch analysis, and optimal utility selection is also significant when optimising whole system performance and multi-period operation. However, it is difficult to couple pinch analysis directly in an equation-based modelling environment for various reasons related to the system architecture. Ligang Wang describes how this has been done using a gPROMS Foreign Object (FO) for heat and mass integration to consider both the process design and multi-period utility selections.	Ligang Wang Postdoc François Maréchal Professor **EPFL**
17:15	Close	
18:00	**Thames cruise & dinner**	
23:00	Finish	

Thursday 21 April 2016

Morning session – Platform & product developments and applications

Chair: Alejandro Cano

09:00	The gPROMS platform v4.3 preview The current investment in the gPROMS platform that underpins all PSE's products is resulting in substantial new features such as Global System Analysis, new solvers and optimisation technologies, improved performance and rapid advances in usability. PSE MD and gPROMS chief architect Costas Pantelides describes the advances in the forthcoming gPROMS v4.3 and looks ahead to the future evolution of the technology.	Costas Pantelides Managing Director **PSE**
09:30	gPROMS ProcessBuilder v1.1 – full dynamic process modelling The initial release of gPROMS ProcessBuilder v1.0 in July 2015 provided a steady-state flowsheeting capability that could utilise the full modelling and optimisation power of the gPROMS platform. ProcessBuilder v1.1 now brings full dynamics, including dynamic distillation, and opens the potential for applications such as batch process optimisation using high-fidelity models. Bart de Groot describes the latest developments.	Bart de Groot Principal Application Engineer **PSE**
10:10	Global System Analysis – from uncertainty quantification to risk management Global system analysis is a powerful set of mathematical techniques for relating the variability of system outputs – for example, key performance indicators (KPIs) – to the variability in system inputs. By providing quantification of uncertainty at all levels it provides a tool for rapidly exploring the decision space in order to determine the optimal values for input variables, identifying unimportant inputs (thus helping to reduce experimental programme time, cost and use of materials), and providing accurate quantification for risk management. Costas Pantelides describes this major new gPROMS platform technology and its implementation within the equation-oriented framework.	Costas Pantelides Managing Director **PSE**
10:40	Refreshment break	
11:10	gCRACKER online: using state estimation to provide real-time KPIs A key focus of PSE's recent development has been the gPROMS Online Model-based Application (OMBA) tool-kit that enable the real-time application of high-fidelity process models online. Mark Matzopoulos describes how state estimation is being applied to olefins plant cracking furnaces for accurate real-time yield prediction and prediction of the degree of coking.	Mark Matzopoulos VP Chemicals, Petrochemicals & Refining **PSE**
11:40	gSAFT: advances in thermodynamic modelling PSE's next-generation gSAFT physical properties technology provides a unique predictive capability for properties of a large variety of 'difficult' components and mixtures – for example long-chain molecules such as polymers, electrolytes, complex aqueous mixtures and Fischer-Tropsch mixtures, as well as pharmaceutical compounds. gSAFT's SAFT-γ Mie group contribution techniques provide accurate prediction where little or no data is available. gSAFT can be deployed directly within existing gPROMS models with no modification, making modelling of processes containing such mixtures relatively straightforward for the first time. Leader of the gSAFT development Tom Lafitte describes and demonstrates recent developments.	Tom Lafitte Senior Scientist **PSE**
12:10	Lunch **Academic poster session** and refreshments	

Afternoon session – Oil & Gas, Refining and Petrochemicals

Chair: Kevin Wade

14:00	Oil & gas – new capabilities for optimising production and process gPROMS ProcessBuilder now brings new capabilities to the optimisation of production systems and processing facilities. This presentation describes PSE's major new developments in oilfield production optimisation and current activities for the analysis of large-scale distributed processing networks. Two case studies, firstly for an onshore facility with over 100 wells and the second for a 25 well offshore facility are presented showing a significant increase in barrels of oil at the same production cost.	James Marriott VP Oil & Gas **PSE**
14:20	Dynamic modelling of Natural Gas Processing Facilities This talk explains why dynamic process modelling is a critical operational support tool for BP's separation and gas processing facilities, enabling it to minimise plant downtime and production deferrals across its Alaskan Oil & Gas fields. The benefits of detailed facility and flare systems models are described and the requirements for a full field model comprising multiple facilities, connected via a network of pipelines, are discussed.	James Marriott VP Oil & Gas **PSE** Luke Hanzon Process Engineer **BP Exploration Alaska**
14:30	Optimisation of an entire regional gas production network A Shell R&D project is evaluating the feasibility of performing an economic optimisation of the whole of the South Iraq gas production, involving multiple production facilities. The optimisation uses rigorous multicomponent models of all facilities and interconnecting pipelines. Danial Aluma describes the model, which runs to hundreds of thousands of equations, and some of the exciting initial results of its application.	Daniel Aluma Project Manager Basrah Gas **Shell**
15:10	Life cycle economic optimisation as opposed to design heuristics: natural gas dryers Conventional design approaches rely on accepted heuristics in the sizing of industrial units. Those heuristics resemble the culmination of accumulated experiences obtained from operating such units. Life cycle economic optimisation (in which the optimised economic function resembles the life cycle financials of the plant) is rarely considered as a tool for detailed design. This talk presents a methodology of conducting economic life cycle optimisation on temperature swing adsorption systems with natural gas dryers as an example, and shows that life cycle optimisation can lead to substantial cost savings when compared with conventional design approaches.	Yasser Fowad AlWahedi Assistant Professor **Petroleum Institute** Mayank Patel Senior Engineer **PSE**
15:40	Refreshment break	
Chair: Joe Henderson		
16:10	New model-based approach for qualification of ethylene furnace anti-coking technologies SABIC T&I has recently developed a novel model-based approach for qualifying anti-coking technologies for deployment on ethylene furnaces. This approach relies on an in-house gPROMS-based furnace simulation tool that uses superior mechanistic coking kinetics model coupled with SABIC cracking kinetics. Dr Abduljelil Ilyas describes how this has successfully transformed a multi-year anti-coking qualification process into few weeks while ensuring higher chance of success.	Abduljelil Ilyas Chief Scientist Olefins & Aromatics Technology **SABIC**
16:40	Advanced real-time refinery monitoring & optimisation PSE, Bharat Petroleum (BPCL), India's largest state-owned refining company, and Indian SME GyanData are working to implement an online dynamic optimisation of the CDU complex at BPCL's Mumbai refinery. The ground-breaking project features a number of firsts, including state estimation technology that removes the need to wait for 'steady state', dynamic optimisation of the complex transition and online implementation of the system within the plant automation system. This presentation describes the principles and progress to date.	K.S. Kumar Chief Manager Technology **Bharat Petroleum** Charles Brand Senior Consultant Engineer **PSE**
17:10	Concluding remarks	
17:20	Close	