ADVANCED PROCESS
MODELLING FORUM 2017
London 25–26 April

Poster abstracts

25-26 April 2017
Chelsea Harbour Hotel
London

PSE Academic

PSE has a strong academic programme, with gPROMS® technology used for research and teaching in some 200 universities around the world.

Every year, PSE Academic invites researchers to submit APM Forum poster presentations that highlight the application of advanced process modelling to a diverse range of research topics.

This year we held a competition for the best poster, with the winner invited to give an oral presentation during the main conference sessions. The winner was:

Numerical simulation of an impact pin mill with DEM-PBM coupling model

by Xizhong Chen*, Lige Wang, Jin Y. Ooi
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We hope that you will find many topics of interest to your business among the poster presentations!

Pieter Schmal
Head of PSE Academic

1. A Framework for the personalised treatment of Acute Myeloid Leukaemia

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Acute Myeloid Leukaemia (AML) is a cancer of the bone marrow and blood which results from mutations causing uncontrolled proliferation, maturation arrest and reduced apoptosis of myeloid blood progenitors. This poster presents a comprehensive mathematical model representing the disease dynamics of cancerous acute myeloid leukaemia cells in bone marrow.

AML cell populations, or "clones", are separated into chemo-sensitive and chemo-resistant subsets and responses of these subpopulations to chemotherapy are captured using a novel population balance model (PBM). Toxicity, a side effect of chemotherapy treatment, can be reduced if normal mature myeloid cells, i.e. neutrophils, can be sustained in peripheral blood within near-normal ranges. Consequently, the AML clonal growth model is combined with a model which captures neutrophil dynamics. Global Sensitivity Analysis was performed to identify critical parameters influencing disease trajectory over time. The predictive power of the proposed modelling framework was validated against retrospective datasets from AML patients treated with a standard combination of chemotherapy involving cytarabine (Ara-C) with or without daunorubicin (DNR) for different drug doses and schedules.

We demonstrate that model predictions are in good agreement with clinical data of leukaemia response and neutrophil recovery in 3 out of 10 heterogeneous patient datasets. The developed model provides the basis for performing optimisation studies in order to determine optimum drug schedules for minimising leukemia tumour burden whilst maintaining an acceptable number of normal cells for reduced treatment toxicity. It is envisaged that the developed gPROMS-based modelling framework would provide a practical decision making tool to explore novel treatment protocols in future combining patient-, leukaemia- and treatment-specific characteristics.

2. Statistical investigation of the composition of simulated intestinal fluid on the equilibrium solubility of oral drugs and in silico prediction using gCOAS

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A statistical design of experiment (DoE) approach was employed to investigate the influence of simulated intestinal fluids (SIF) composition on the equilibrium solubility of BCS class II compounds.

The aim is to enhance understanding of how orally-administered drugs are taken up from the intestinal tract and combine this knowledge with in silico models to predict in the early stages of development the absorption and therefore the performance of these compounds. Method: Using Minitab® 17.2.1 a DoE was constructed in the fasted and in the fed state with 7 and 8 factors respectively and 2 levels (upper and lower limits of factors). Thirteen BCS class II compounds were tested (acids, bases and neutrals). The PSE software gCOAS 1.3.0 was then used to predict the solubility of nine compounds (two acids, four bases and two neutrals) and compared to the experimental data previously generated.

The fasted state experiment proved the feasibility of this systematic approach, simulated the inherent solubility variabilities and determined the key factors controlling solubility. The fed state experiment confirmed the suitability of this approach expanded to the food effect with logically higher solubility values. Similar results were observed for acidic and basic drugs while neutral drugs behaved differently. The simulations were challenging for the correlation of simulated vs experimental solubility values. The results showed a compound specificity; however a refinement of the simulations would certainly improve the correlation.

3. Numerical simulation of an impact pin mill with DEM-PBM coupling model

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Milling is known to be an energy-intensive and highly inefficient process. The design and operation of mills still rely on empirical methods, experience and trial and error rather than sound scientific principles. Population balance models (PBM) have been extensively used to model milling processes. However, the main criticism of PBM is it does not realistically consider the characteristics of a mill environment. On the other hand, the discrete element method (DEM) is a powerful tool to reproduce the microscopic impact events of individual particle inside a mill.

The aim of this project is to perform multiscale analysis of DEM simulation results to inform PBM models in order to obtain more convincing predictions. In this study, a multiscale DEM-PBM coupling approach was proposed to understand and predict the grinding behaviour of alumina particles in an impact pin mill.

DEM was performed to study the particle dynamics and stress events in a centrifugal impact pin mill. The impact information was then passed to PBM to predict the product size distribution under varying operational conditions. Coupled with DEM simulations, the intensification version of gSOLIDS sheds more physical insights and could act as a virtual mill device to predict the material grindability under varying grinding conditions.

4. UREA GRANULATION CIRCUIT SIMULATOR: design, simulation, optimisation and control of UFT granulation plants

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Granular urea is the most-consumed nitrogen-based fertiliser, being critical in the modern agriculture scenario. Industrial urea granulation is mainly performed in fluidised-bed granulators combined with coolers, crushers and screens to constitute granulation circuits. Unfortunately, this process is usually operated by trial and error. Typical dynamic operational problems are undesired plant shutdowns due to the formation of lumps in the granulator and continuous oscillations of product quality due to the cycling nature of the granulation circuits or changes of the desired product granulometry to meet particular market demands. In this context, it becomes critical that an integrated approach is used for the design and control of granulation circuits.

This work presents a simulator for the UFT fluidised-bed granulation technology, which consists of ad-hoc models for the units involved (multichamber granulator, fluidised-bed cooler, double-deck screens and double-roll crushers). These models were integrated in the gPROMS® environment and can be easily adapted to particular plant configurations simply by "dragging-and-dropping" the necessary units from the established model libraries and connecting them to simulate a specific integrated process. Each unit presents a dialog box for the user to set the corresponding design and process variables and parameters.

This simulator can be used, among other tasks, to perform sensitivity analysis and process optimisation, analysis of design changes or flowsheet variations, analysis of different open- or closed-loop operations and as a training tool. Furthermore, all the units are connected by streams characterised by their mass flowrate, particle size and temperature. As a result, variables such as particle size distribution, size guide number and fraction of product on specification can be tracked with time through the units. Finally, using the gPROMS PMLControl library it is possible to customise the desired control loops to maintain plant operation under nominal conditions or turn it to a new operating point.

5. Prediction of pressure drop and blockage boundary in pneumatic transport of cohesive milk powder fines: experimental & multi-scale modelling approach

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Pressure drop and blockage boundary in pneumatic conveying of cohesive dairy powder fines largely depends on the type (i.e. agglomerated fat-filled milk powder - FFMP fines) and properties of the powders (i.e. particle size distribution, densities, adhesive forces); the solids loading; the operating pressure, velocity, and pressure drop of the fluid phase etc.

The dynamics of the pneumatic conveying system is largely influenced by the dynamics of the fluid-particle interaction between the fluid and the solid particle, the particle-particle interactions between the solid particles, and the particle-wall interactions.

In this study, a multi-scale model is developed and validated with lab-scale pneumatic conveying experiment to analyse the influence of conveying parameters on the pressure drop and blockage boundary. During the transport of the FFMP fines in the experimental rig, the pressure drop and the particle volume fraction is measured with the aid of a differential pressure meter and an optical fibre probe respectively.

The multi-scale model is achieved by dynamically coupling computational fluid dynamics (CFD) for modelling the fluid flow field, discrete element method (DEM) for modelling the behaviour of the powder particles, referred to as CFD-DEM. A process model was developed in gSOLIDS® and compared with the validated CFD-DEM in predicting the system pressure drop and particle volume fraction. The validated process model will be used for scale-up to solve industrial scale pneumatic conveying problems associated with highly cohesive dairy powders.

6. Micro-scale process development and optimisation for crystallization processes

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Initial experimental phases of crystallization process development are commonly carried out at very small scales, typically using 1-5 ml vessels. The aims of these early phases of process development are to select a solvent based on solubility and crystal solid state.

These activities are commonly conducted in high throughput reactor systems, such as the Crystal16 and Crystalline, from Technobis Crystallization Systems. However, for the development, validation and optimisation of crystallization process models this data is usually not utilised and the selected solution system is probed experimentally and more quantitatively at much larger scales, typically between 100–1000 ml. A more quantitative usage of the data generated at small scale for the development of process models which may significantly reduce the number of larger scale experiments required, would aid in addressing the increasing constraints on time and materials in pharmaceutical development.

In this work, data from paracetamol and 3-methyl-1-butanol solutions at the micro-scale, 5 ml, was utilised to estimate the crystallization kinetics of the model, including crystal growth and primary nucleation, enabling model development, as well as mechanism discrimination. The final predictions of the developed process model were compared with a previously developed and validated process model, which employed larger scale 1 L scale experiments. A key outcome of this work is an adapted process development workflow for the design, model validation and optimisation of processing models for crystallization systems. This workflow enables crystallization process development with an order of magnitude lower demands for materials, in particular raw API, which may not be available in the early stages of process development. In addition, the design space for the process can be assessed early on, such a process robustness and viability of continuous processing, with less dependence on larger scale, more material intensive experiments.

7. Modelling of waste heat recovery and water-steam power generation systems of integrated metallurgical plants in gPROMS®

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The iron and steel industry is one of the most energy intensive industry sectors and a large contributor to global greenhouse gas emissions. The worldwide adoption of the Paris Agreement to limit global warming leads to an increasing demand for energy efficient production technologies. Modern steel works are therefore equipped with several technological extensions to reduce fuel demand and CO2 emissions. Effective recovery of waste heat and intelligent utilisation of residual chemical energy of process off-gases are key technologies to achieve these goals.

Based on the metallurgical model library created by Primetals Techologies, a waste heat recovery system for the Finex® smelting reduction process was set up using the gPROMS ModelBuilder simulation platform. This energy recovery system is used to produce process steam for further use within a plant at desired temperature and pressure levels. In a second development stage, the system was extended to depict integrated water-steam power generation cycles making use of the combustion energy of excess process gases. Several specific unit operation models were developed to depict the different process steps. These include steam drum, deaerator and injection cooler models as well as gas-water heat exchangers, steam turbine and condensator models. Since all the involved processes are highly dependent on the correct implementation of water-steam conditions, a robust link to water-steam properties is required. This was ensured using IAPWS95 data provided by the Multiflash foreign object interface.

The achieved simulation results were in good accordance with the specific target values. Both waste heat recovery and power generation process models can thus be used to simulate and optimise entire steel plant set-ups within the flow sheeting environment of the gPROMS ModelBuilder.

8. Application of gCRYSTAL® CLD sensor workflow for kinetic parameter estimation

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The particle size distribution (PSD) and particle shape (quantified by an aspect ratio) are two key quality attributes of crystalline particles that determine their performance during drug manufacture. Variations in crystallization process conditions cause particles with different PSDs and aspect ratios to be produced.

The PSD of particles produced in a crystallization process can be predicted to a reasonable degree of accuracy using appropriate theoretical models. The gCRYSTAL software package implements theoretical models for this PSD prediction. The models contain kinetic parameters whose values need to be tuned to capture a particular crystallization process.

This kinetic parameter estimation process may not always be successful due to the wide variation in crystallization process conditions. The degree of accuracy of these parameters can be improved if sensor data collected during the crystallization process is incorporated. The chord length distribution (CLD) data can be used for this purpose. The CLD data contains information about the PSD and aspect ratio of the particles in the slurry.

In this joint project between the University of Strathclyde and PSE, we developed a CLD sensor module for the gCRYSTAL package using gPROMS. We also developed a workflow for the application of this CLD sensor module. This module allows CLD data to be incorporated into the kinetic parameter estimation. Here we illustrate the application of the CLD workflow with data collected during a growth experiment of paracetamol. The experiment was performed at the University of Strathclyde. The predicted aspect ratio from the CLD sensor module agreed well with inline images collected during the process. The predicted PSD also agreed with the measured PSD with offline instruments. However, there is some discrepancies in the tails of the predicted and measured PSD. This could be due to breakage and agglomeration of particles during filtration and drying before offline PSD measurement.

9. Development of a novel continuous filtration unit for pharmaceutical process development and manufacturing: A case study using paracetamol

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The purpose of this work was twofold: to identify the key challenges facing a continuous filter and the key performance indicators of CFD20 and compare its functionality against Biotage manual filtration unit with respect to API filtration, washing and drying; and to understand API slurry chemical and physical interaction with process parameters to design and improve API isolation processes.

The AWL Continuous Filter Drier (CFD20) is a versatile vacuum filtration unit that allows investigation of the process of separation in a fully automated semi-continuous manner. The effect of filtration in both a manual Biotage unit and the continuous CFD20 on crystal size distribution and cake purity were investigated. Key values relating to filtration were also collected allowing evaluation and comparison of the units using Darcy's law. The API selected for this investigation was paracetamol. Two different paracetamol particle size grades were used (granular and micronised) to challenge different aspects of the filtration and washing. Patent Blue V dye was used as impurity for the quantification of wash performance.

The two different paracetamol particle size grades were characterised by determining features such as bulk density, particle size distribution and morphology. Comparing the filtration performance of the units, parameters derived from Darcy's law showed good agreement. Automated data logging facilitates via PharmaMV3 provide consistent data collection and supports improved understanding of filtration process development. Preliminary investigations to evaluate the experimental data using gPROMS were undertaken

to determine which model is most appropriate to describe the experimental data. Conclusions Overall performance of the units was similar, showing that the CFD20 can match best manual lab practice for filtration and washing while allowing continuous processing and real-time data logging. Further filtration fitting on additional data set is required for model implementation.

10. Comparison of dynamic behaviour and energy efficiency of Shell entrained-flow gasifier among three different coal ranks

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The Shell entrained-flow gasifier with a coal drying system can handle various rank coals. A rigorous mathematical model using gPROMS ModelBuilder® was developed to predict the dynamic behaviour and efficiency variation of the Shell coal gasifier. The model includes homogeneous and heterogeneous reactions, slag formation, heat transfer and steam generation in membrane wall structure, syngas quenching and cooling system, which can be applied for a part of an overall integrated gasification combine cycle (IGCC) process simulation.

The amount of syngas and the outlet gas composition were affected by coal rank. The amount of steam generated and energy recovered in membrane wall zone were also predicted in accordance with coal ranks. Under the condition of the same amount of LHV of product gas, the recovered energy in the gasifier was varied depending on the type of coals. It is expected that the simulation results can provide a guideline to operate a coal gasifier according to coal rank.

11. Fixed bed catalytic reactor modelling for TAME synthesis

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TAME (Tert-Amyl-Methyl-Ether) is a gasoline additive used to increase the octane number. The aim of this study is to develop a model in gPROMS ModelBuilder simulating the behaviour of a fixed bed catalytic reactor for TAME synthesis. The reaction is carried out in tubular reactors in the presence of cationic resin catalyst (e.g. Amberlyst 35 wet). The model developed contains three parts: behaviour inside the tubular reactor, behaviour inside the cooling jacket and the connectivity between both parts. Inside the tubular reactor MESH equations (considering time, radial and axial coordinates), with appropriate initial and boundary conditions as well as constitutive equations (UNIQUAC thermodynamic model, LHHW type kinetic model expressed in activities) are used. The cooling jacket is considered as perfectly mixed vessel, so the equations are only time-dependent.

Model simulation results are presented as temperature and composition profiles inside the reactor at steady state. More simulations are performed considering as parameter space velocity (there values for this parameter are considered). Conversion data at the reactor outlet from laboratory pilot plant experiments are compared with simulation results for model validation. Conversion comparison shows good agreement, with a difference between the 2-4%. Molar concentration profiles along the reactor length from gPROMS show decrease of reaction activity as the space velocity is increased, this is supported by the results obtained from the pilot plant. The model developed in gPROMS ModelBuilder proves the possibility to obtain high-fidelity data at an industrial level. Use of KBC Multiflash® for temperature dependent physical properties allows the model to account for the properties dependence on temperature. The model answered reasonably to parameter modification and the comparison with data obtained from the pilot plant show good agreement. A larger parameterisation study of the model should be made in future to improve the model applicability.

12. Modelling of a fluidised bed reactor for thermochemical energy storage applications

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The development of novel thermal energy storage concepts is of great importance to achieve the shift towards sustainable energy systems. Thermochemical energy storage utilising solid-gas reactions is a very promising alternative to latent and sensible thermal energy storage systems, mainly because of the high energy density per volume and the possibility of nearly loss-free storage at ambient temperature.

Fluidised bed reactors offer high heat and mass transfer rates and isothermal operating conditions and are therefore preferred for this application. On the other hand the complex reactor hydrodynamics and reaction kinetics constitute a challenge for precise predictions.

gPROMS® was used to create a model of a fluidised bed reactor for thermochemical energy storage applications. The fluidised bed model is based on the method provided by Kunii and Levenspiel. Also the reaction kinetics of a variety of thermochemical materials are adapted for the operation in such a reactor. Furthermore bubble growth and splitting at the internal heat exchanger tubes was investigated in order to optimise gas-solid interchange. The mass and energy balances are solved to obtain the required amount of the storage material and to calculate the mass-flow and the temperature of the fluidisation gas.

Finally a process utilising three thermochemical storage systems arranged in a cascade of reactors is proposed to efficiently utilise a waste heat source. Three variants of this system that differ in terms of complexity and efficiency are investigated. The results are compared in terms of the converted thermochemical material.

13. N_2O recovery from N_2O generation process by Pressure Swing Adsorption (PSA) process

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Recently, non-CO_2 greenhouse gas (GHG) reduction is considered important as well as CO_2 reduction under United Nations Framework Convention on Climate Change (UNFCCC). A lot of nitrous oxide (N_2O), one of the representative GHGs, is emitted from the N_2O generation process. Since the global warming potential (GWP) of N_2O is almost 300 times the GWP of carbon dioxide, N_2O from chemical process is decomposed by catalytic decomposition in many industrial fields.

On the other hand, there are many industrial applications of N_2O such as medicine (anaesthetic, analgesic), oxidiser (rocket, combustion engine) and aerosol propellant. Especially, high-purity N_2O (99.999%) is used for deposition of an insulating oxide film in the chemical vapour deposition (CVD) process in semiconductor industry. Therefore, the recovery of N_2O is both important in environmental and industrial aspects.

To recover a high purity N_2O from N_2O generation process, a cyclic adsorptive process is studied. To select a proper adsorbent, the adsorption equilibrium of N_2O on two different types of adsorbents was measured up to 1000 kPa and compared with a reference (commercial zeolite 13X, Sinopec, China). Then, the breakthrough behaviours of adsorption bed were evaluated by using a simulated effluent gas mixture to design a pressure swing adsorption (PSA) process.

A rigorous mathematical model including mass, energy, and momentum balances was employed to clarify the dynamic behaviour of the PSA process. The required simulation parameters were obtained from the equilibrium data and breakthrough results and the simulation was carried out by using gPROMS ProcessBuilder.

14. Model-based optimisation of membrane contactors for natural gas sweetening

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Over the past decade, membrane contactor (MBC) for CO_2 absorption has been widely recognised by research groups for its large intensification potential compared to conventional absorption towers [1][2]. MBC technology uses microporous hollow fibre membranes (HFM) to enable effective gas and liquid mass transfer without the two phases mixing into each other.

In this work, gPROMS® ModelBuilder is used to develop a mathematical model that accounts for the effect of membrane pore-size distribution and operating conditions on membrane (partial) wetting for improved understanding of a novel MBC operating at high pressure of 7000 kPa [3]. Then, a model-based optimisation for the design and operation of MBC for natural gas (NG) sweetening is conducted using derivative-free optimisation in MATLAB. This coupling is executed using gO:MATLAB, which enables the entire gPROMS model consisting of partial differential-algebraic equations to be called as a single function in MATLAB.

The optimisation problem involves minimising the MBC's annualised cost, which consists of membrane and solvent regeneration costs, subject to a given CO_2 specification alongside operational constraints and size limitation of the MBC module. In order to assess the intensification potential of MBC, we compare the performance of two optimised industrial-scale modules against a conventional packed column.

15. Water resources management with dynamic optimisation strategies and integrated models of lakes and artificial wetlands

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Eutrophication, associated with high nutrient concentrations and recurrent algae blooms, is the most important environmental problem in surface water bodies. An issue of concern associated with algal blooms is the potential production of toxins by different phytoplankton species within the blooms, which are dangerous for human health. The implementation of short and long term restoration strategies that contribute to health recovery of water bodies requires deep knowledge of the aquatic system, as well as detailed modelling and optimisation

In this work, we propose an integrated mechanistic model for a freshwater eutrophic reservoir and an artificial wetland within a dynamic optimisation framework for determination and planning of water quality restoration strategies. A partial differential equation system results from dynamic mass balances for the main phytoplankton groups; two zooplankton groups and two size classes of zooplanktivorous fish in the reservoir. To account for the most important biogechemical nutrient cycles, the model includes mass balances for organic carbon (dissolved and particulated), phosphorus, nitrogen, nitrite, ammonium, reactive soluble phosphorus, as well as dissolved oxygen. Mass balances for the same nutrient species and dissolved oxygen are formulated for the artificial wetland. To estimate nutrient filtration rates of macrophytes within the wetland, an additional mass balance is included. Algebraic equations stand for forcing functions profiles, such as temperature, solar radiation, river inflows and concentrations, etc. The model is formulated as an optimal control problem within a control vector parameterisation approach in gPROMS.

Two combined restoration strategies are considered: reduction of external discharge of nutrients using an artificial wetland and fish removal as a food chain biomanipulation technique. Optimisation variables are the fraction of nutrient-rich water stream that is derived through the artificial wetland and fish removal rates from the reservoir. The objective function is the minimisation of a weighted sum of

integrals along the entire time horizon: the quadratic difference between phytoplankton concentration and a desired value below eutrophication limits and the quadratic difference between phosphate concentration in the wetland outflows and a desired value. Numerical results provide optimal profiles for restoration actions and their effects on the studied ecosystem.

16. Bayesian Parameter Estimation in gPROMS

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The quantification of uncertainty is a crucial requirement for modelling because a model serves in making a decision with uncertain results. This uncertainty has a multitude of sources - experimental data prone to errors, possibility of choosing from a set of models for the same physical system, disturbances etc. - and it flows from these sources up to the modelled system performance indicators.

The presented work focuses only on parameter uncertainty introduced by experimental measurement errors, and it takes as case study a simple model with non-linear parameter dependence because this dependence makes possible the degeneracy from a normal distribution of parameters and, therefore, a Gaussian spread around MLE may prove unsatisfactory in such situations.

However, a promising solution to this problem is offered by Bayesian inference, which is not limited to a particular type of parameter-dependence and presents also the advantage of including prior knowledge using a clear formulation, i.e. through Bayes theorem. Despite these major advantages, compared to the classical inference approach, the Bayesian inference methods - as Markov chain Monte Carlo (MCMC) sampling used here - are much more expensive computationally. Fortunately, this drawback begins to be less restrictive nowadays due to existence of fast model solvers and exploitation of computer parallel-architecture, as in the case of products based on gPROMS platform.

In order to find how well Bayesian inference with MCMC sampling captures parameter uncertainty and what is its afferent computational effort, a MCMC technique has been implemented in gPROMS and tested. Other, maybe more performant, Bayesian inference techniques will be tested in the near future.

Model-based Innovation Prize 2017

Every year PSE offers prizes totaling €5000 for the best published papers describing the use of our gPROMS® family products in an innovative way or in a novel area of application or technology.

Applications for the 2017 prize will open in June 2017.

Prize overview

We offer three Model-Based Innovation prizes: a winner's prize of €3000 and two runners-up prizes of €1000 each.

The research presented in the submitted papers should make substantial use of gPROMS modelling using gPROMS family products in order to achieve the results described.

The judges will favor novel applications or application in novel technology areas.

Each year the prize is announced at a key academic or industrial conference. This year's award will be presented in November at the AIChE Annual Meeting in Minneapolis, MN

In addition to awarding the prizes, PSE may invite the corresponding authors to present the paper at the next PSE APM Forum and to publish a summary page on the PSE website, depending on copyright and other considerations.

If you feel that you have a paper that will qualify for the prize, you are encouraged to submit an abstract in June 2017.

2016 MBI Prize winners and runners-up

Winner

The winning publication for the €3000 prize:

Combining On-Line Characterization Tools with Modern Software Environments for Optimal Operation of Polymerization Processes

by **Jose A. Romagnoli, Navid Ghadipasha, Aryan Geraili** of Louisiana State University, **Carlos A. Castor, Jr., Wayne F. Reed** of Tulane University and **Michael F. Drenski** of Advanced Polymer Monitoring Technologies, Inc.

Published in Processes 2016, Special Issue Polymer Modeling, Control and Monitoring.

Runners-up

The publications that were joint winners of the €1000 runners-up prizes:

Dynamics of immature mAb glycoform secretion during CHO cell culture: An integrated modelling framework

by **Ioscani Jimenez del Val** of University College Dublin, **Yuzhou Fan** of Technical University of Denmark and **Dietmar Weilguny** of Symphogen A/S, Denmark.

Published in Biotechnology Journal, Wiley-VCH Verlag GmbH & Co.

Dynamic Modelling and Collocation-Based Model Reduction of Cryogenic Air Separation Units

by **Yanan Cao and Christopher L. E. Swartz** of McMaster University and **Jesus Flores-Cerrillo and Jingran Ma** of Advanced Control and Operations Research, Praxair Technology Center, NY.

Published in AIChE Journal.

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