ADVANCED PROCESS
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Poster abstracts

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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 poster presentations from researchers that highlight the application of advanced process modelling to a diverse range of research topics.

This year we also held a competition to choose a poster for oral presentation during the main conference sessions. The winner is:

Simultaneous Process Design and Optimal Utility Selection
by Ligang Wang, François Maréchal of EPFL Switzerland

We hope that you will find many topics of interest to your business among the poster presentations!

Pieter Schmal
Head of PSE Academic

1. Optimisation of biomass supply for iron and steel making industry

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Iron and steel making is one of the most carbon intensive industries, highlighting a need to increase the use of renewables. There is particular opportunity for biomass to either partially substitute coal for primary steelmaking or to produce electricity for secondary steelmaking. However, substituting fossil fuels by biomass is complex as biomass can be produced through various means (i.e. batch, continuous, etc.). In addition, it undergoes seasonal variation and the quality of the fuel can vary. These issues are enhanced further with biomass from waste streams, such as mill, crop or forest residues, which are economically appealing and after fuel pre-processing perfectly suitable for the steelmaking sector. Hence, there is a need to model all stages of the biomass supply chain from waste streams for such a use. This modelling will help to understand the complexities and drawbacks of the supply chain and decrease the steel plants concerns regarding the technical and economic aspects of utilising biomass from waste streams.

Using a gPROMS ModelBuilder environment, a flowsheet describing resource sharing between various biomass waste streams and a steel plant will be created. This flowsheet will model the production process of numerous waste streams, and later the biomass fuels transport, storage and upgrading. The fuel usage in the iron and steel plant over a period of time will also be modelled. This techno-economic approach will aim to optimise this fuel flow between different industries to minimise the cost and hence make the use of biomass in iron and steel making more financially appealing. This work is part of the European SHAREBOX project under Horizon 2020, which is aiming to conduct a flexible management of resources used in the industrial processes by creating a platform that facilitates implementation of industrial symbiosis.

2. Simulation and optimisation of post combustion carbon capture using absorption process

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Coal-fired power plants are one of the main sources of carbon emission. Carbon capture technologies are divided to three main technologies including: (1) Post combustion CO_2 capture; (2) Pre-combustion CO_2 capture and (3) Oxy-fuel combustion capture. Among these technologies, post combustion CO_2 capture by means of chemical absorption seems to be the most suitable technique to reach this goal. The aim of this study is modelling of CO_2 absorption for post combustion capture in coal-fired power plant. In this study, steady state of the CO_2 absorption process from coal-fired power plants is developed in gPROMS and the results are compared with the results obtained from Aspen-Hysys. The effect of solvent, monoethanolamine (MEA) is investigated in this work. Also, the effect liquid to gas ratio, in high and low cases is considered. The preliminary data in literature show that efficiency of the process is more sensitive to liquid-gas ratio than the gas flow rate. However, this needs to be investigated in detail using the available process simulators to further throw light on the all parameters which may effect on the efficiency of the capture process.

3. An integrated multi-scale approach for low carbon energy system design

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The design and optimisation of a low carbon energy system require the application of integrated multi-scale approaches. Such a methodology ideally combines and retrofit the results from high level whole energy system analysis all the way to low level thermophysical properties models.

In the high level, the "System Value" (SV) metric, quantifies the value of a given technology to the electricity system. Through whole-systems modelling, we gain understanding about the market-level importance of a technology's operational characteristics (e.g. flexibility, efficiency, carbon intensity) and their impact on the optimal capacity mix.

In an intermediate level, we model the whole CCS chain, from power (pulverised coal power plant and Combined Cycle Power plant), capture (amine-based post-combustion capture), compression, injection and storage using the gCCS toolkit in gPROMS. Design and operating parameters such as the efficiency and ramp rates, which dictate the power plant's flexible operation, will be given as a input from the results of the SV metric and vice versa. These models are consequently used as a benchmark to re-design the whole CCS chain.

In the lower level, a process-performance indexed aims to design an improved new solvent, by evaluating and optimising the values of the thermophysical properties of an ideal solvent based upon monetised and non-monetised indexes. The process performance of the carbon capture using the newly design solvent will be further integrated with the higher level models, evaluating the effect on the whole CCS chain and the energy system.

We will then re-design the benchmark detailed models to achieve these goals and have the "ideal" decarbonised technologies of the future. This integrated approach then dictate the technical characteristics that the standalone or integrated power and capture model, should have in order to gain a higher value in the energy mix of the future.

4. Optimal design of continuous crystallizers

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Within the project improving process operation via rigorous simulation models (IMPROVISE) in the Institute for Sustainable Process Technology (ISPT) closing the gap between offline and online use of rigorous simulation models has been dealt with. To this end, batch crystallization process operation and modelling were studied, identifying issues such as batch to batch reproducibility, controllability and observability [1]. These pose several problems in the realization and use of online model-based strategies for process control and monitoring which can guarantee the achievement of the desired production targets.

These motivate the research efforts in designing continuous crystallization technology, which may be able to overcome the abovementioned limits of the batch operation. Accordingly, this poster addresses the optimal design of continuous crystallizers. The key process variables (crystallization temperature, number of stages, crystallization volume, residence time) of single stage mixed-suspension mixed-product removal (MSMPR) crystallizers and multiple stages MSMPRs are optimised by minimising a cost function consisting of equipment and utility costs. The constraints for the above mentioned optimisation problem are derived from the definition of production targets (e.g., minimum allowed yield, daily production, relevant particle size distribution attributes of the final product) and upstream operation (e.g., temperature and flow rate of the inlet flow).

The pros and cons of using the proposed configurations are discussed, in the understanding that the effort to propose control strategies for the most convenient configuration will be addressed as future research.

The study has been executed with the gCRYSTAL package.

[1] Systematic observability and detectability analysis of industrial batch crystallizers, M.Porru, L.Ozkan, accepted conference paper, DYCOPS 2016.

5. Estimation of particle size and shape using combined chord length distribution and imaging data

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The efficient manufacture of particulate products depends on the performance of the material during the various steps involved in the process. These properties such as flowability, solubility and filterability (which are important for various downstream processes) are heavily influenced by the size and shape of the particles produced upstream. Hence it is necessary that the particles produced during various upstream processes such as crystallization possess the desired size and shape required for the downstream processes to be successful. However, this cannot be achieved if there is no control mechanism for the upstream processes by which the particles are produced in the first instance. On the other hand, the successful development and implementation of any control mechanism relies on information on size distribution and shape of the particles to be retrieved in situ.

We present methods to obtain information on the size distribution and shape of particles which are applicable in various upstream processes such as crystallization. The methods [1, 2] rely on a chord length distribution (CLD) and imaging data collected by in-line sensors. This CLD and imaging data contain information on the size distribution and shape of the particles in suspension. As the process of retrieving information on the size distribution from the CLD data is not well posed [1], we combine the data from images [2] to make the process more efficient. Our estimates of particle sizes and shape metric agree very well with experimental data.

[1] O. S. Agimelen, P. Hamilton, I. Haley, A. Nordon, M. Vasile, J. Sefcik, A. J. Mulholland, Chemical Engineering Science 123 (2015) 629-640. [2] O. S. Agimelen, A. Jawor-Baczynska, J. McGinty, C. Tachtatzis, J. Dziewierz, I. Haley, J. Sefcik, A. J. Mulholland, Chemical Engineering Science 144 (2016) 87-100.

6. Development of a blast furnace model in gPROMS with thermodynamic process depiction by means of the Rist operating diagram

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The blast furnace can be described as a counter current, multi-phase heat and mass exchange reactor. A variety of mathematical models of this process have been established in the past decades including statistical models, thermodynamic models as well as kinetic-dynamic models. An analogue representation of blast furnace operation is given by the Rist operating diagram which is based on first principle mass and heat balances. In this diagram numerous variables and process parameters of are represented and interrelated, while equilibrium conditions of involved chemical reactions are taken into consideration.

Based on elemental assignments and empirical component distribution correlations, a black box model was created using the gPROMS ModelBuilder simulation platform. The thermodynamic process conditions are analysed in a Rist sub-model enabling the construction of the operating diagram of a blast furnace process. The main system inputs are iron oxides, coke, additives, hot blast and substitute reducing agents in order to produce liquid hot metal, slag and blast furnace gas.

The modelling concept enables the description of interdependencies between the main blast furnace process and the overall thermodynamics described by the Rist operating diagram within a single mathematical model. A detailed analysis of the model behaviour under varying inputs was carried out. The achieved simulation results confirm the applicability of the model for comprehensive simulation of various blast furnace operation scenarios. This allows for further optimisation regarding process efficiency thereby potentially reducing fuel consumption as well as environmental emissions.

7. Preliminary model of a packed bed oxidation reactor

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One-dimensional pseudo-homogeneous model was developed for the partial oxidation reaction of methanol to formaldehyde in an industrial multitubular fixed bed reactor to determine the temperature profiles inside the reactor. A steady-state reactor model was developed in gPROMS® 4.0.0 accounting for the different catalyst layers installed inside the tubes of the reactor. As a preliminary approximation it was assumed that the reactor is isobaric and the overall heat transfer coefficient (Uw) is constant.

The model was developed based on the kinetic equations by Deshmukh et al. (2005) and the resulting temperature profiles compared with data from the industrial reactor. The model predictions presented a considerable deviation from the operational values and new kinetic constants were estimated using the Parameter Estimation tool of gPROMS. The kinetic parameters and the overall heat transfer coefficient were adjusted to four industrial-data sets of temperatures inside the reactor, corresponding to four different operating days; it was assumed that the catalyst had not suffered significant deactivation. The simulation results showed a relative average deviation of 1-2 % from the operational data and the model was able to reproduce the influence of the different catalyst layers in the reactor temperature profile, but presented a considerable difference in the experimental and model hot-spots. Among several future model improvements the next step will be to consider an overall heat transfer coefficient varying with the axial position.

8. Model of a laboratorial tubular reactor by the determination of the residence time distribution

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The analysis of the residence-time distribution (RTD) for a given reactor can bring important information on its flow pattern and give an indication of the degree of deviation to the ideal reactor model.

In the present work the RTD of a laboratorial tubular reactor was experimentally determined for two different flow conditions by the injection of a tracer into the reactor feed through a pulse input and then measuring its concentration in the effluent stream using a spectrophotometer. The mean residence time and the variance were calculated to verify the existence of channeling and dead zones. The experimental RTD was then used to develop a descriptive model of the real reactor. The model calculates the RTD for an association of a piston flow reactor (PFR) with a battery of continuous stirred reactors (CSTR) in series. The RTD dynamic model was built in gPROMS® 4.0.0 and the model parameters (reactor's residence time and number of CSTR's) were estimated using the Parameter Estimation tool by comparing the model predictions to the experimental absorbance values by minimising the deviations.

Finally, a reaction of persulfate with iodide was performed in the same reactor to determine the experimental conversion and compare it to the theoretical conversion given by the ideal PFR model and the RTD model.

9. Modelling and simulation of supercritical fluid extraction of volatile oils from aromatic plants

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Dynamic models are a useful tool for the design, optimisation and scale-up of supercritical fluid extraction processes from laboratory to pilot and industrial scales. In particular, mass balance based models which include mass transfer coefficients in fluid and/or solid phases have a strong physical significance. They take into account the characteristics of the plant matrix, namely the particle size, the bed porosity and also the equilibrium relationships and mass transfer mechanisms. Although several models have been proposed in the literature, their solution is not always trivial and, additionally, the estimation of some parameters using experimental data is required. With this context, the opportunity to use new tools to model, simulate and perform parameter estimation seems promising.

In this work, using gPROMS ModelBuilder, different models are applied to study the extraction of three different volatile oils from aromatic plants: coriander, fennel and savory. The desorption model by Tan and Liou (AIChE J., 35, 1029, 1989) and the model proposed by Sovová (Chem. Eng. Sci., 49, 409, 1994), both with and without axial dispersion, are used. These models consider the variation of the concentration of the supercritical fluid as it flows along the extractor and, thus, include partial differential equations. Parameter estimation is used to determine the desorption rate constant (kd), the internal and external mass transfer coefficients (ks and kf) and the axial dispersion coefficient (Dax). Although some limitations were encountered due to the limited amount of data available for parameter estimation, the results obtained improved the ones previously reported (Grosso et al., Chem. Eng. Sci., 65, 3579, 2010), assessed by the absolute deviation error. gPROMS ModelBuilder appears as a good alternative as it integrates in a single environment features such as model development and parameter estimation.

10. Methyl formate hydrolysis performed in chromatographic reactor. Simulation and experimental results.

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Presented work is focused on modelling process of reactive chromatography, which combines chemical reaction with simultaneous chromatographic separation. In general, different affinity of reagents to fixed adsorptive bed is used to instantaneously separate products. Therefore, high yield is achieved and high purity products leave the chromatographic column one after another. This type of reactor is applied in petrochemical synthesis, pharmacy, optically active ingredients and esters industries, especially when standard separation techniques are inefficient or difficult to implement.

The hydrolysis reaction of methyl formate catalysed by Dowex 50WX8- 200 ion exchange resin was carried out periodically in a fixed bed chromatographic reactor. Several experiments were conducted with different flow rates and temperatures. A number of parameters were calculated with statistical moments method. Based on experiments with non-adsorbing, non-reactive tracers KCl and MgCl2 bed porosity was calculated. Experimental data for adsorption processes with methanol and formic acid were used to evaluate adsorption coefficients for both products of methyl formate hydrolysis.

Mathematical model of chromatographic reaction process was presented and implemented in commercial software “gPROMS ModelBuilder”. For PDE calculations solver SRADAU was chosen. Implemented model was used to estimate all unknown parameters in the process. Bed porosity obtained from simulations was slightly lower in comparison with experimental data. Apparent dispersion coefficient was estimated based on simulations. Simulation carried out for pure methanol and pure formic acid resulted in acquiring adsorption coefficients. Apart from chromatographic process characteristic, reaction parameters were estimated with implemented mathematical model. Arrhenius equation was chosen as model of temperature influence.

Conclusion was that the presented mathematical model with good likelihood can simulate process of methyl formate hydrolysis in fixed-bed chromatographic reactor and can be recommended for obtaining process parameters.

11. Simultaneous process design and optimal utility selection

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Heat and mass integration for better design of heat and mass exchanger networks has been an important issue for process simulation software. Most efficient methods for heat and mass integration are on the basis of pinch analysis. However, it is difficult to couple the pinch analysis directly in an equation-based simulation and optimisation software, since pinch analysis fundamentally features with non-differentiable nature. In addition, heat cascade constraints have to be added for each temperature level (involving array sorting), which is difficult to be handled by mathematical modelling language.

The optimal utility selection can maximise the energetic or the economic benefits from the optimisation of process design, thus is significant from the viewpoint of the whole system. Currently, the optimal utility selection is mostly handled by bi-level algorithms, in which the lower level performs the process simulations by the simulators while the upper level conducts the optimal utility selection and optimisation outside the simulators. It is promising to have an integrate simulation and optimisation environment which could perform simultaneous optimal process design and utility selection.

In this work, we have developed a foreign object (gIntegration) integrated in gPROMS environment for multi-period optimal process design and utility selection. The features of allowing dynamic and zero-dimension arrays largely ensure the flexibility of the heat and mass integration. The gIntegration unit can conceptually connects to any number of heat, power and mass streams from both the processes and the utility. The information collected by the gIntegration is then processed in the foreign object for pinch analysis and mixed integer nonlinear programming for multi-period optimal utility selection. The (grand) composite curves and utility operation for each period thus can be then graphically presented in the report of the gIntegration. An example for process design of CO2 adsorption process and utility selection are given. It is shown that the gIntegration is flexible and efficient.

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2015 MBI Prize winners and runners-up

Winner

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Dynamic modelling of Shell entrained flow gasifier in an integrated gasification combined cycle process

by **Chang-Ha Lee, Hyeon-Hui Lee, Jae-Chul Lee of Yonsei University, Yong-Jin Joo** of KEPRI and **Min Oh** of Hanbat University, Korea.

Published in Applied Energy, Elsevier.

Runners-up

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

Modelling of microreactors for ethylene epoxidation and total oxidation

by **Vincenzo Russo, Martino Di Serio** of University of Naples "Federico II", Italy and **Teuvo Kilpiö, Jose´ Hernandez Carucci**, and **Tapio O. Salmi** of Abo Akademi Unversity, Finland.

Published in Chemical Engineering Science.

Dynamic modelling and control strategies for flexible operation of amine-based post-combustion CO2 capture system

by **Ali Abbas, Minh Tri Luu and Norhuda Abdul Manaf** of The University of Sydney.

Published in International Journal of Greenhouse Gas Control, Elsevier.

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