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Editorial

Special Issue on "Process Modelling and Simulation"

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Collecting and highlighting novel developments that address existing as well as forthcoming challenges in the field of process modelling and simulation was the motivation for proposing this special issue on "Process Modelling and Simulation" in the journal *Processes*. Our objective was to provide interested readers with an overview of the current state of research, tools and applications on the use of models for simulation and decision support in the process industry. The special issue brings together fourteen contributions on topics ranging from the process systems [1–3] and (bio)chemical engineering [4,5] fields, to software development [6] and applications in heat and power systems [7,8]. Moreover, the hot topic of data mining and machine learning is also discussed from a process engineering perspective in [9,10]. This conveys the broadness of use and impact that models will have (and already have) for industrial decision support in the approaching digital era.

Process models are the foundation that other applications (sensitivity analysis, predictive simulation, real-time optimization, etc.) build upon. Accordingly, half of the published articles in this special issue focus on model building and parameter estimation and validation. From the chemical and process systems engineering field, we received two contributions [11,12] that model the underlying physical phenomena beyond the classical macro scale, with the aim of having a reliable simulation for predicting the effects of different process operation regimes on product quality, and hence reducing experimentation costs. Also related to this goal, two contributions brought heat and power systems into the scope: [7] proposed a grey-box model of limited complexity that couples the production process with the plant's combined heat and power system in order to reduce operation costs, whereas [8] modeled the hydraulic dynamics in a nuclear reactor cooling pump with respect to different vane structures to ensure safe operation in case of power failures.

Models for decision support must be tailored to the actual process, or the underlying equations should allow the transfer of the lab-scale data to any desired scale. In this sense, [3,4] proposed iterative methods for parameter estimation to progressively improve the plant-model match under realistic conditions, and [5] considered uncertainty in the estimation via robust optimization. Furthermore, a methodology for obtaining physically coherent grey-box models (or plant surrogate ones) from fundamental principles and plant data was proposed in [10], while [1] presented a quantitative validation method based on partial least squares to devise the suitable modelling depth according to the quality of the available experimental data.

Once reliable prediction models are available, they can be used in numerical simulations to analyze the main features of the process or to evaluate the influence of the operating conditions as well as of the external disturbances. Three examples of different applications were published in this regard: [2] developed a 3D simulation that describes the hydration behavior of cereals during cooking; [13] presented a dynamic simulation of a hot-metal steel converter based on thermodynamic and kinetic equations, used to evaluate the influences of different scrap features on the process; and [14] built a 3D model to simulate the fluid dynamics inside the coagulation bath of a spinning process for synthetic fiber production. Nevertheless, the use of models is not limited to offline or real-time predictive simulation, but is likely to extend to process (dynamic and real time) optimization in the near future. Although model-based optimization was not directly within the scope of this special issue, the authors of [5,6] proposed steps in this direction from the application and software viewpoints, respectively.

Although there are almost as many types of models as processes/applications, as well as multiple modelling methodologies to choose from, some key conclusions can be extracted from the received contributions. Plant models in the process industry are no longer just built from very detailed first-principles equations, and their applications often go beyond their classical use in process design to strongly influence the process operation in real time. Therefore, the tradeoff between model complexity and accuracy needs to take account of the decision level where the model is to be used. The increasing computational power, availability of big datasets and improved machine learning algorithms will facilitate model building in the materials, (bio)chemical and process engineering fields [9]. However, the big data that are already available in the process industry are not always complete and informative, and performing further experimental tests on demand may be expensive. Thus, as models are often required to provide reliable predictions outside the plant's current or usual region of operation, data-driven modelling methodologies need to be combined with process physical knowledge derived from first principles, resulting in a hybrid or grey-box model. The characterization of uncertainty from available plant data and its incorporation in process modeling are also important topics that require further research, as they directly affect the quality and reliability of model predictions and the inherent risk in making use of these predictions for decision support.

Finally, the full realization of the benefits of process modeling will depend on being able to deploy detailed first-principle or hybrid models throughout the process lifecycle. Of particular interest in this context is the use of such models, and the calculations based on them, in online decision support and control systems for process operations. This includes many important applications, from equipment condition monitoring, to real-time optimization and nonlinear model-predictive control, all of which would constitute major steps towards the digitalization of the process industries. Achieving this objective on a large scale, however, poses several significant technical challenges. Some of these are computational, arising from the need to perform complex calculations robustly and efficiently in real time. Other challenges are related to devising general software architectures that can support the development of complex digital applications involving multiple model-based computations communicating with each other and with external data servers. Successful advances in these areas will provide process engineers with a complete suite to implement advanced process management systems, boosting the development of virtual plants or digital twins that integrate plant information updated in real time.

We would like to end this editorial note with expressing our sincere gratitude to all the scientific contributors of the papers submitted to this special issue, as well as to the editor-in-chief of *Processes*, Michael A. Henson, the managing editor, Jamie Li, and the rest of the editorial staff for their effort and endless support.

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Guest Editors

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