Breaking Modeling Boundaries: the Strategic Advantage of Hybrid Approaches in PSE

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Historically, process modelling based on the system knowledge, i.e. mechanistic modelling, has been the central activity of Process Systems Engineering (PSE). These kinds of models are mostly based on the modeler's knowledge of the system. The advent of Industry 4.0 and the availability of a higher quantity of process data raised interest in data-driven modelling approaches, which can represent the system by retrieving information from the experimental data without including a-priori knowledge in their formulation (Sansana et al., 2021). Hybrid models offer the possibility to merge all available information of the process (i.e., a priori knowledge and experimental data), and leverage the strengths of both modelling approaches while mitigating their respective limitations (Von Stosch et al., 2014).

Mechanistic models generally require less experimental data for their calibration, and due to their strong physical foundation, can be accurate even outside the calibration space. The main weakness of these models lies in the trade-off between the effort required to obtain a certain level of system knowledge (e.g. in terms of experimental costs and time) and the ability to describe complex phenomena. On the other hand, data-driven models are able to capture complex behaviours, but, due to the lack of physical insight, they are mostly reliable only within the calibration space, and need a higher amount of experimental data to provide robust predictions.

These two kinds of models can be combined into a hybrid model structure in which the data-driven component is exploited to learn from the process data the complex phenomena that cannot be described by a-priori knowledge. Hence, the final output of the hybrid model is composed by the combination of the predictions of the two components.

A comprehensive study is proposed to assess the conditions in which it becomes advantageous to use a hybrid model approach instead of a classic mechanistic or data-driven one. The advantages and the limits of the hybrid models are explored, both considering the ability to predict the system behaviour and the quantity of experimental data used to calibrate the model. Different possible hybrid model structures are also explored, to assess in which conditions the two modelling approaches operate most effectively together.

Keywords: Hybrid modelling, mechanistic models, data-driven approaches, process simulation.

References

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