From substance data to process models – use cases for machine learning in process engineering

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Using models for the comparison and rating of virtual what-if-scenarios has been an integral part of chemical process design for many years: Integrating physical knowledge and information about measurement data can be sufficiently reliable in order to reveal potential for improvements in the design and the operation of processes that would not have been discovered otherwise. Increasing demands for individualized products and shorter time to market make it necessary to arrive at reliable models efficiently. In this contribution, two widespread problems in setting up models in chemical process engineering are addressed, namely on the one hand the missing availability of reliable thermodynamic data for mixtures and on the other hand the wish to quickly and transparently compare different process designs and operating conditions. For both challenges, the beneficial use of machine learning methods will be demonstrated.

As far as thermodynamic data are concerned, the recent [1] results for the prediction of activity coefficients by matrix completion are used within a flowsheet simulator and compared to the predictions of conventional thermodynamic models for an entrainer distillation. The results are considered especially from the point of view of statistical error estimates for the matrix completion method.

For the comparison of virtual what-if scenarios different schemes to generate model-based scenarios and to train surrogates have been implemented and applied both to complete flowsheets and to single units. Based on this, two different strategies for flowsheet simulation are available: (i) The solution in the flow-sheet simulator, which amounts to solving a large nonlinear system, where the process variables are given implicitly by specifications; (ii) training surrogates for single units and wiring these surrogates, which leads to a much smaller nonlinear system. Examples with an industrial background will illustrate that (ii) can lead to more stable convergence properties. A web-based framework, which has been implemented prototypically, will

be presented that allows for an interactive decision support by comparing different solutions according to different key performance indicators.

[1] F. Jirasek, RAS Alves, J. Damay, RA Vandermeulen, R. Bamler, M. Bortz, S. Mandt, M. Kloft, H. Hasse; The Journal of Physical Chemistry Letters 11 (2020) 981-985