

Reliable Process Modeling with Accurate Thermophysical Property Data and Models Using the DETHERM Professional Suite

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Currently available commercial process simulation packages are reliable, valuable tools for a multitude of tasks that arise in the everyday work of chemical engineers. Equipped with real measurement data, thermophysical property models ready for use in a process simulation run can be generated quickly. Nevertheless, the accuracy of such process simulations strongly depends on the thermodynamic models used to describe the physical behavior of the components concerned. Especially in the case of the synthesis, simulation and optimization of separation processes, the phase equilibrium of the system to be separated has to be known exactly. Before simulation results are used for further detailed planning or investments, the engineer does well not simply to use the built-in parameters of the simulator. It is advisable at least to crosscheck the core physical properties of the pure components and mixtures, which are vitally important within a process, against measurement data provided by a sound thermophysical property database. The next step is the comparison of the results of the calculations from the thermodynamic property engine of the process simulator with these experimental data. After thermodynamic consistency checks followed by a regression and optimization run, the evaluated and fitted model parameters can be transferred back to the simulator package. All these features can be handled comfortably by the new DETHERM Professional Suite. This product is an enhancement of the existing DETHERM database and data regression/optimization tools, which are improved, amongst others, by a property-oriented document management system, which can store company's proprietary measurements, reports, regression protocols and process simulation setup files. The complete workflow of the regression and optimization of a separation problem and the final storage of the results will be shown in this paper.