Process Simulation Software: a Tool for Benchmarking Thermodynamic Models

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When a process simulation software is used for the simulation or optimization of processes, the selection of an appropriate thermodynamic model is essential.

Thermodynamic models share the same objectives: be able to reproduce phase-equilibrium and energetic property data of the largest possible set of pure compounds and related mixtures. Model developers generally test the performances of their models on a limited set of systems. In practice, the accuracy of the results depends on the chemical families of considered compounds and temperature, pressure and composition ranges. The ability of a model to represent real systems containing a large number of components is also limited to the knowledge of the binary interaction parameters.

A comprehensive comparison of model performances on a fair basis is a recurrent expectation of users of process simulation software. For a given model, they want to know:

- The expected errors between experimental data and model calculations for the set of binary systems of interest,

- How errors move with temperature, pressure and composition.

Recently, Jaubert, Privat and coworkers have proposed a methodology to evaluate the capacity of a given model at describing all types of binary interactions. They have developed a reference database containing 200 binary systems sorted in 9 families, according to their “thermodynamic complexity”. Benchmarking all thermodynamic models available in the literature and potentially usable for industrial purposes on this same fair basis would greatly help users of commercial process simulation software.

To initiate this study, the performances of the well-established PSRK predictive model was evaluated using this methodology. Performing phase-equilibrium and energetic property calculations on 200 binary mixtures represents a tedious work which could be generalized and simplified by the use of a software dedicated to this kind of tasks. Thus, a calculation methodology was established using Simulis Thermodynamics, the ProSim thermodynamic calculation server based on a software component approach.