Reliable process modeling via accurate thermophysical property data and models

Well *simulated*

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The new Detherm Professional Software Suite integrates a thermophysical property database and a data regression package into process simulation. In addition, legacy data collections and internal workflows can be incorporated with ease. Equipped with real measurement data, engineers can quickly generate thermophysical property models ready for use in process simulations.

Currently available process simulation packages, such as Aspen Plus, Prosim, PRO II or Chemcad, are reliable, valuable tools for a multitude of tasks that arise in the everyday work of a chemical engineer. The accuracy of such process simulations strongly depends on the thermodynamic models used to describe the physical behavior of the components concerned. The engineer does well not simply to use the built-in parameters of the simulator. Before simulation results are used for further detailed planning or investments, it is advisable at least to crosscheck the core physical properties of the components and mixtures, which are vitally important within a process, against some measurement data. The thermophysical property database Detherm is one of the prime sources of such measurement data. Currently Detherm contains 6.25 million data sets for 132,000 chemical systems. The database is updated every year and has an annual growth rate of approximately 8 percent. The data stored consist mainly of: phase equilibrium data, like vapor-liquid, liquid-liquid, gas-liquid; PVT data; thermodynamic properties; transport properties; surface tensions; electrolyte data.

Detherm is produced by DECHEMA, in cooperation with DDBST and FIZ Chemie. This team supplies the database with a collection of property-oriented data packages. In addition, Detherm customers can add data packages from the University of Regensburg (electrolyte data), the Technical University of Denmark (solubility data of large complex chemicals) and the American Design Institute for Physical Properties DIPPR (recommended pure-component data).

The new Detherm Professional Software Suite is an enhanced version of the well established Detherm. It enables the user to add and maintain private categories and tags both for private and public data. Electronic documents of any format can also be attached to a data set. The Detherm software can, therefore, be used as a property-oriented document management system. Among other things, it can store measurement reports, regression protocols and process simulation setup files. Due to its modular, open design, Detherm Professional can integrate a com-

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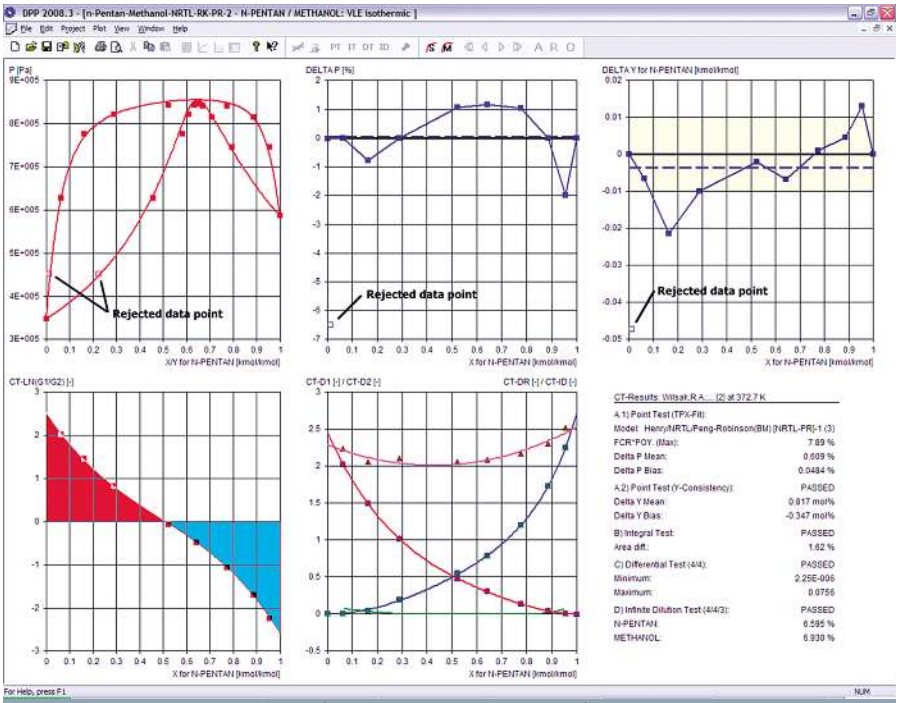

Fig. 1: Example of the extended consistency test of binary VLE data

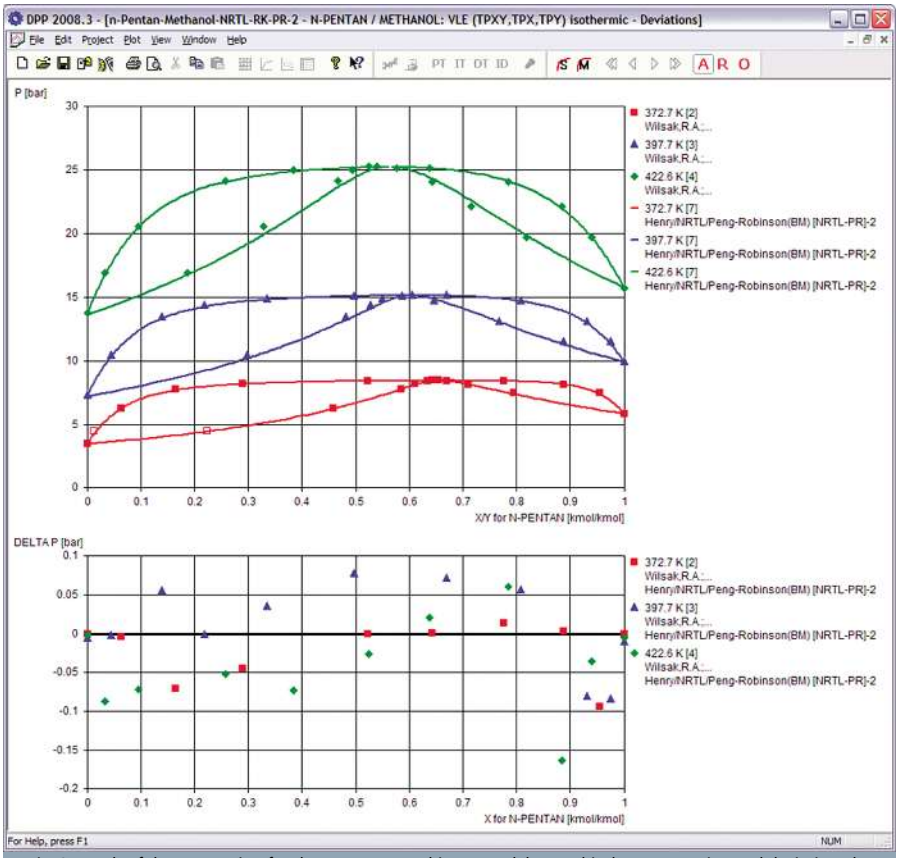

Fig. 2: Result of data regression for the NRTL-Peng-Robinson model – graphical representation and deviation plot

pany's proprietary export modules and even customized dialogs. This permits Detherm data to be exported to any desired kind of format, including individually designed reports as well as legacy data exchange formats.

If measured property data are available, the data have to be compared with the results from the thermodynamic property engine of the process simulator. DECHEMA's Data Preparation Package, a component of the Detherm Software Suite, connects the database to the simulator by interfacing with the simulator's thermo engine. It can easily display measurement plots together with the calculations of the simulator. Especially for mixture properties at higher temperatures or pressures, systematic gaps can frequently be found between the predictions of the simulator's thermo engine and real world data. To fix such issues, once again the Data Preparation Package can be used. Arbitrary thermodynamic models from the simulator can be fitted to data from the Detherm database with just one keystroke. Finally, the generated parameters can be exported ready for use in the simulator.

Using Detherm Professional these parameters and all the project files involved can be stored in the database with just one click. By this means, a proven set of thermophysical property parameters can be instantly shared with other users. For future projects such regression work does not have to be redone, if the same chemical components or mixtures are involved.

Example: separation of n-pentane from methanol

Within a project, the separation of n-pentane from methanol has to be handled. The target temperature is above 400 K. In Detherm you can find a data set measured by R. A. Wilsak et al. reporting three isothermal VLE measurements in the range of 372.7 K to 422.6 K. Other data are available, but not for such high temperatures. The maximum pressure reported in this source is approximately 25 bar. It is decided to model the system using the NRTL activity coefficient model together with the Peng-Robinson equation of state for calculating fugacity coefficients, combined with the Poynting correction (real gas-phase approach). From Detherm the Data Preparation Package can be started with one click. A subsequent comparison of the measurement data with the predictions of the process simulator reveals systematic differences, especially at higher temperatures. The deviations in pressure reach values of 4 bar (15 percent).

Before regression the data are subjected to critical thermodynamic consistency checks (point, area, infinite-dilution and differential tests). At least one data point is found to be unlikely and is removed during these checks (see Fig. 1). All other data can be used for the regression. To achieve more precise modeling one additional binary parameter is activated in the NRTL model and also in the Peng-Robinson model. After regression, a comparison of the model vs. the measurement data shows a significant improvement. Now the errors in pressure are below 0.1 bar (1 percent) (see Fig. 2).

Compared to the initial data the results are now much more accurate and constitute a sound basis for further planning. Future work is simplified since the parameters together with the complete project files and regression reports are stored in the Detherm database. ■