

Simulis[®] Thermodynamics, just one more thermodynamic package?

Application: modeling of formaldehyde-water-methanol system and properties prediction with implemented EoS/G^E models.

Olivier Baudouin, Stéphane Déchelotte, Alain Vacher

ProSim - Stratège Bâtiment A, BP 27210, F-31672 Labège France – www.prosim.net

Simulis[®] Thermodynamics is the name of the thermodynamic package recently proposed by ProSim. Differences with preexisting tools will be highlighted in this presentation and benefits for users and developers of property models will be demonstrated. Its ability to tackle complex systems will be illustrated by modeling of formaldehyde-water-methanol system and implementation of EoS/G^E models.

Simulis[®] Thermodynamics is basically a thermophysical calculation server that generates fluid properties and fluid phase equilibria. But what could be its added value for companies already using well known commercial tools?

The component-oriented approach of its architecture allows seamless plug in any application. Simulis[®] Thermodynamics is provided as an add-in in Microsoft[®] Excel or as a toolbox in MATLAB[®] enabling to run all kind of thermodynamic calculations in these applications. Use of this new tool in conjunction with other commercial packages through its implementation of the CAPE-OPEN standardized interfaces will also be presented here. Benefits of the selected software component approach will be further illustrated with the link developed with DPP (Data Preparation Package – DECHEMA e.V.) to find the property model that better fits the experimental data available in DETHERM. Its capability to embed user codes either as DLL, either as VBScript will be shown.

Besides possibilities offered by this new approach, several examples will be presented to demonstrate some of the property models implemented in Simulis[®] Thermodynamics which are useful in engineering tasks. On one side, modeling of the system formaldehyde-water-methanol will be presented through simulation of a distillation column. On the other side, results obtained with implemented EoS/G^E models (PSRK, MHV2, MHV1,...) will also be presented on some representative systems in order to demonstrate the ability of this tool to embed up-to-date property models able to represent actual systems encountered in the industry.