

Simulis® Thermodynamics, Just One More Thermodynamic Package?

Stéphane Déchelotte^{C, S}, Alain Vacher and Olivier Baudouin
ProSim SA, Labege, France

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 use of EoS/G^E models. Simulis® Thermodynamics is basically a thermophysical calculation server that generates fluid properties (thermodynamic, transport, compressibility...) and fluid phase equilibria (liquid-vapor, liquid-liquid and liquid-liquid-vapor). For pure component properties it relies on DIPPR 801 (AIChE database). But what could be its added value for companies already using well known commercial tools? The component-oriented approach of its architecture is based on the Microsoft®'s COM/DCOM middleware, allowing seamless plug in any application. The standard version of 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 be presented here. Its capability to embed user codes either as a DLL (Dynamic Link Library) following a standard syntax, either as VBScript (Visual Basic Script) directly written from the Simulis® Thermodynamics' environment will also be highlighted in this presentation. This feature will be illustrated with the interface developed with Refprop (NIST Standard Reference Database 23). 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. In particular, results obtained with EoS/G^E models (PSRK, MHV2, MHV1,...) will 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.