Simulis® Thermodynamics, Just One More Thermodynamic Package?

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Simulis® Thermodynamics is a thermophysical properties calculation server, proposed by ProSim as the core element of its new component-oriented software architecture. It generates pure component and mixture properties (thermodynamic, transport, compressibility...) and fluid phase equilibria (liquid-vapor, liquid-liquid and liquid-liquid-vapor). This thermodynamic package includes a pure component properties database, based on DIPPR 801 AIChE's database [1] and several thermodynamics models: equations of state, activity coefficient models, specific models... A particular emphasis is on fully predictive models: several versions of UNIFAC models, PPR78, PSRK... The thermodynamic library is continuously enriched. For example, recently, the PPC-SAFT model developed by LIMHP and IFP [2-5] and the NRTL-PR model developed by Pr. Neau et al. [6-8] were implemented.

Simulis® Thermodynamics is based on the Microsoft®’s COM/DCOM middleware. The standard version is provided as an add-in in Microsoft® Excel or as a toolbox in MATLAB® and enables the user to run complete thermodynamic calculations in these applications, but it can also be embedded in any legacy code using the SDK (Software Development Kit). One main benefit of Simulis® Thermodynamics is its CAPE-OPEN [9] compliance through its implementation of the CAPE-OPEN standardized interfaces: “thermodynamic plug” and “thermodynamic socket”. Another main benefit is the capability to welcome existing thermodynamic routines either as a DLL (Dynamic Link Library) following a standard syntax, either as VBScript (Visual Basic Script) directly written from the Simulis® Thermodynamics’ environment. Then, the user code inherits of all the features of Simulis® Thermodynamics: CAPE-OPEN compliance, Microsoft® Excel add-in, MATLAB® toolbox... Differences with similar existing tools will be highlighted in the 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/GE models on some representative systems of industrial interest.