

## Simulis Thermodynamics: Software Presentation.

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Simulis<sup>®</sup> Thermodynamics, marketed by ProSim [1], is a thermophysical calculation server that generates highly accurate pure component and mixture properties (thermodynamic, transport, compressibility...) and fluid phase equilibria (liquid-vapor, liquid-liquid and liquid-liquid-vapor). Based on the AIChE's DIPPR database [2] and enriched by ProSim's thermodynamic experts it provides access to a property database of more than 2000 pure components, and to one of the richest thermodynamic models libraries available on the market: equations of state (SRK, PR, LKP, PPR78, PPC-SAFT...), G<sup>E</sup> models (NRTL, UNIQUAC, UNIFACs...), EoS/G<sup>E</sup> models (MHV2, PSRK, NRTL-PR...), electrolytes models (Edwards, UNIQUAC electrolytes, ULPDHS...) and specific models (Amines, Sour-Water, formaldehyde...). An "expert mode" feature is also available in Simulis<sup>®</sup> Thermodynamics, allowing the user to implement his own models. Simulis<sup>®</sup> Thermodynamics is available as a Microsoft Excel<sup>®</sup> add-in, a MATLAB<sup>®</sup> toolbox or as a software component which can be easily plugged in any other application requiring reliable and accurate thermophysical properties. Simulis<sup>®</sup> Thermodynamics provides also a full set of services such as the generation of property tables, graphical display of properties, data regression of experimental properties, estimation of pure component properties, plot of phase envelope, calculation of petroleum fraction properties, unit conversion... All these services become automatically available in any software as long as it integrates Simulis<sup>®</sup> Thermodynamics. Another benefit of Simulis<sup>®</sup> Thermodynamics is its CAPE-OPEN [3] compliance through its implementation of the CAPE-OPEN standardized interfaces: "thermodynamic plug" and "thermodynamic socket".

### References:

[1] [www.prosim.net](http://www.prosim.net)

[2] ROWLEY R. L., WILDING W. V., OSCARSON J. L., YANG Y., GILES N. F., DIPPR<sup>®</sup> Data Compilation of Pure Chemical Properties, Design Institute for Physical Properties, AIChE, New York, NY (2009)

[3] CAPE-OPEN Lab. Network, [www.co-lan.org/Dissemination.html](http://www.co-lan.org/Dissemination.html)

**Key words:** Thermodynamic calculation server, component architecture, interoperability, integration, reusability.