



Simulis® Thermodynamics

Mixture properties and fluid phase equilibria calculations

Interoperability, integration, reusability. Simulis Thermodynamics provides any person in industry, engineering or research with high quality thermophysical properties calculations. These calculations can be plugged in any software of wider application range (equipment sizing, system modeling, etc) and properties are available for any kind of fluid.

Simulis Thermodynamics makes open simulation a practical reality.

Simulis Thermodynamics is a calculation server for thermophysical properties and phase equilibria calculations on pure components and mixtures.

It is available as a MS-Excel® add-in, a toolbox in MATLAB® or as a software component which can be easily plugged in any other application requiring reliable and accurate thermophysical properties.

- ◆ **Reliable and accurate thermophysical properties**
- ◆ **Extensive set of services (flash, data regression, phase envelopes, etc)**
- ◆ **Comprehensive pure component and binary interaction databases**
- ◆ **Easy plug in common applications (MS-Excel®, MATLAB®, etc)**
- ◆ **CAPE-OPEN compliant**



SimuLis

Components for Process Simulation



Property calculations in MS-Excel

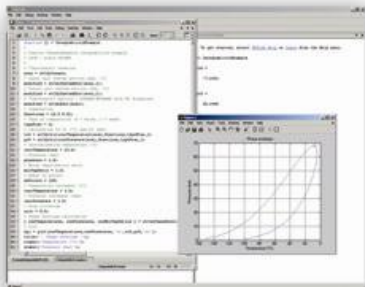
Over 300 robust and validated calculation functions

- Thermophysical properties calculations: transport properties (Cp, viscosity,...), thermodynamic properties (enthalpy, entropy, compressibility factor,...), non-ideality properties (fugacity,...)
- Phase equilibria calculations: liquid-vapor, liquid-liquid, liquid-liquid-vapor (bubble and dew temperatures, bubble and dew pressures, isentropic flash, etc)

Simulis Thermodynamics also provides the derivatives of the properties with respect to temperature, pressure and composition.

Flash algorithms in particular have been developed and validated through many years of intensive use, in order to guarantee a reliable and fast convergence.

One of the richest thermodynamic libraries available on the market



Property calculations in MATLAB

A wide set of thermodynamic models selected for their reliability and robustness:

- Equations of state: Soave-Redlich-Kwong, Peng-Robinson, Lee-Kesler-Plöcker, Benedict Webb Rubin Starling, etc...
- Activity coefficients models : NRTL, UNIQUAC, UNIFAC, etc...
- Combined approach models: MHV2, PSRK, etc...
- Electrolytes: Edwards, UNIQUAC electrolytes, ULPDHS, etc...
- Specific systems: Amines, Sour-Water, Pure Water, etc...

A database of over 1700 components based on AIChE's DIPPR® database, enriched with data from research projects led by ProSim's thermodynamics experts.

With Simulis Thermodynamics the user can configure a model according to each problem by combining the various methods available.

The open architecture of Simulis Thermodynamics allows the integration of your private databases of pure substances, binary interaction coefficients or of your own thermodynamic methods. A specific tool for the management of various UNIFAC models parameters (Dortmund, Larsen,...), according to the groups and sub-groups of decomposition is also provided.

Easy integration in common applications

Thanks to its component oriented architecture, Simulis Thermodynamics can be plugged directly in any application that supports the COM/DCOM technology (MS-Excel®, MATLAB®, C++, Delphi, etc).

Calls to the routines can be automated through the simple adjustment of the API in languages such as Visual Basic, C++, FORTRAN, etc...

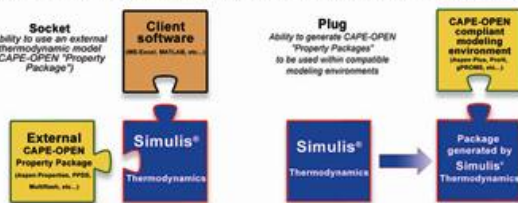
Simulis Thermodynamics makes it possible to use all the power of a validated thermodynamic server in a simple spreadsheet.



The CAPE-OPEN compliance enables you to continue using your usual tools

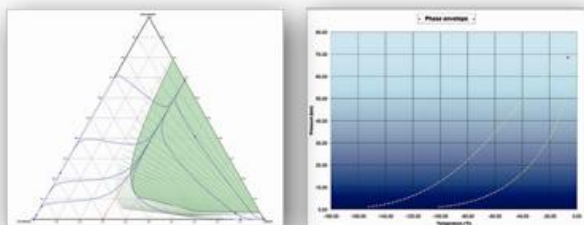
Simulis Thermodynamics implements the standardized CAPE-OPEN interface, making it possible to use external thermodynamics in Simulis Thermodynamics (Socket) or to use Simulis Thermodynamics models in third-party environments that support the CAPE-OPEN standard (Plug).

Any application that integrates Simulis Thermodynamics automatically benefits from its compatibility with the CAPE-OPEN standard.



Corporate thermodynamic experts will generate and automatically dispatch Property Packages throughout their organization, thus putting their expertise to advantage and ensuring that all engineers use properties adapted to each particular system.

A full set of services available



Ternary Diagram

Phase envelope curve

- Graphical display of properties on temperature, pressure or composition ranges
- Generation of property tables
- Data regression of experimental properties
- Estimation of pure component properties
- Plot of phase envelope diagrams
- Calculation of residue curves and plot of ternary diagrams
- Calculation of petroleum fractions properties
- Unit conversion, etc...

These services, and many others, become automatically available in your usual software since it integrates Simulis Thermodynamics.

Other components provided with Simulis Thermodynamics

- **Simulis Properties:** pure substances intrinsic properties (constant or temperature dependant) engine. This component can be plugged in any application that only needs to calculate pure substances properties.
- **Simulis Conversions:** physical units conversion management tool. This component can be plugged in any application that manipulates physical dimension in order to easily manage associated units.



Download the evaluation version on www.prosim.net