Simulis® Thermodynamics

Mixture Properties and Fluid Phase Equilibria Calculations

Interoperability, integration, reusability. **Simulis Thermodynamics allows anyone in industry, engineering or research to run high quality thermophysical properties calculations. These calculations can be plugged in any software of wider application range (equipment sizing, system modeling...) 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 Microsoft® 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** (flashes, transport and thermodynamic properties, data regression, phase envelopes...).
- **Comprehensive pure component and binary interaction parameters databases.**
- **Easy plug-in to common applications** (Microsoft® Excel, MATLAB®...).
- **Flexible and CAPE-OPEN compliant solution.**

ProSim

Software & Services In Process Simulation

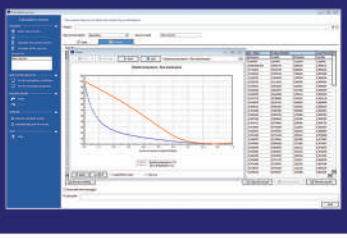
We guide You to efficiency

More information:
www.prosim.net
info@prosim.net

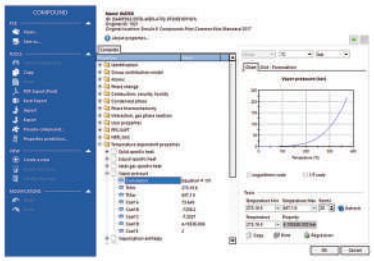
Robust and validated calculation functions

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

Simulis Thermodynamics also provides the derivatives of the properties with respect to temperature, pressure and composition.
Flash algorithms in particular are continuously developed and validated thanks to many years of intensive use to guarantee a reliable and fast convergence.



One of the largest thermodynamic library available on the market



Editing the compound properties

- A **property database for more than 2300 pure components**, based on the AIChE's DIPPR® database and enriched by ProSim's thermodynamic experts. In addition, you can generate properties from experimental data directly in Simulis Thermodynamics or use its built-in predictive methods.
- A **binary interaction parameters database**.
- Numerous predictive methods based on molecule structure (group contribution) and COSMO.
- An **extensive library of property models** selected for their reliability and efficiency and validated through intensive industrial applications. Included mathematical algorithms can be applied to tackle complicated mixtures, such as highly non–ideal, two-liquid phase, electrolyte or petroleum systems.
  - o Equations of state: RKS, PR, LKP, BWRS, PPR78, GC-PPC-SAFT…
  - o Activity coefficient models: NRTL, UNIQUAC, UNIFACs, COSMO-SAC-dsp…
  - o Combined approach models: MHV2, PSRK, NRTL-PR, VTPR…
  - o Electrolytes: Pitzer, Edwards, e-NRTL, UNIQUAC electrolytes, ULPDHS…
  - o Specific systems: Amines, Pure Water, HF, isotopes H2…

Furthermore, the combination of different methods allows users to adapt the model precisely to the problem to be solved.

Easy integration in common applications

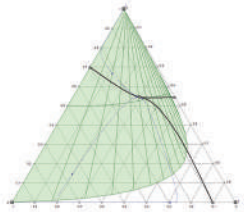
Thanks to its component-oriented architecture, Simulis Thermodynamics can be plugged directly in any 32- or 64-bit applications that support the COM/DCOM technology (Microsoft® Excel, MATLAB®, C++, Delphi...).
Calls to the routines can be automated easily thanks to the supplied API in languages such as Visual Basic, C++, C#...

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

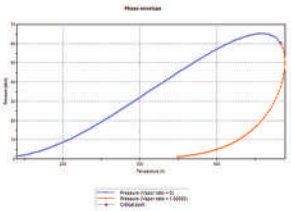
MATLAB

Microsoft Office Excel

A full set of services available



Ternary Diagram



Phase envelope curve

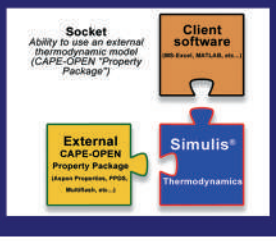
- Graphical display of properties on temperature, pressure or composition ranges
- Generation of property tables
- Data regression of experimental properties
- Prediction of pure component properties
- Plot of phase envelope diagrams
- Calculation of residue curves and plot of ternary diagrams
- Calculation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

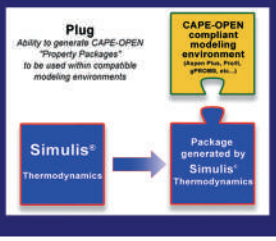
These services, and many others, become automatically available in your favorite tools since Simulis Thermodynamics is fully operational in Excel, MATLAB…

A flexible and CAPE-OPEN compliant solution

The open architecture of Simulis Thermodynamics allows users to easily integrate their own private databases for pure substances or their own thermodynamic methods. A specific tool for the management of parameters of various predictive models based on group contribution (UNIFACs, PPR78, GC-PPC-SAFT…) is also provided.
Simulis Thermodynamics implements the standardized CAPE-OPEN interface, making it possible to use external thermodynamic models (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, to share their expertise and ensure that all engineers in their organization use properties adapted specifically for each particular system.

Other components provided with Simulis Thermodynamics

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

ProPhyPlus Option

Based on Simulis Thermodynamics, ProPhyPlus is a stand-alone calculation software to run all the calculations, without any programming. ProPhyPlus software performs fast, interactive, fluid phase equilibria and fluid properties directly from its own user-friendly graphical interface.

www.prosim.net | info@prosim.net
Immeuble Stratège A - 51, rue Ampère - 31670 Labège - FRANCE - Tel: +33 (0)5 62 88 24 30
325 Chestnut Street, Suite 800 - Philadelphia, PA 19106 - USA - Tel: +1 215 600 3759