# Simulis® Thermodynamics: a complete thermodynamic calculation server

ProSim

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## ① Simulis® Thermodynamics: a Thermophysical calculation server

Computes thermophysical properties and phase equilibria on pure components or mixtures:

### PROPERTIES CALCULATED

**Transport properties**
- Isobaric specific heat (Cp)
- Dynamic viscosity
- Thermal conductivity
- Density
- Molar Volume
- Molar density
- Surface tension
- Molecular weight

**Compressibility properties**
- Compressibility factor
- Gamma (Cp/Cv ratio)
- Sound speed

**Thermodynamic properties**
- Enthalpy (H)
- Entropy (S)
- Internal energy (U)
- Isochoric specific heat (Cv)
- Enthalpy of vaporization

**Liquid-Vapor equilibria**
- Bubble and dew temperatures and pressures
- Flash at given temperature (T) and pressure (P)
- Flash at given vaporization ratio and P (or T)
- Flash at given enthalpy (H) and P (or T, or V, or U)
- Flash at given entropy (S) and P (or T, or V, or H, or U)
- Flash at given internal energy (U) and P (or T, or V)
- Flash at given volume (V) and P (or T)
- Phase Envelope

**Liquid-Liquid equilibria**
- Flash at given temperature and pressure

**Liquid-Liquid-Vapor equilibria**
- Bubble temperature
- Flash at given enthalpy and pressure
- Flash at given temperature and pressure
- Flash at given vaporization ratio and pressure

**Non-ideal properties**
- Activity coefficients
- Fugacity coefficients and Fugacity

*Derivatives of the properties with respect to temperature, pressure and number of moles are also provided*

### THERMODYNAMIC MODELS AVAILABLE

**Equations of State**
- Soave-Redlich-Kwong (SRK)
- Peng-Robinson (PR)
- Lee-Kesler-Plöcker (LKP)
- Predictive Peng-Robinson 78 (PPR78)
- NRTL-PR
- PPC-SAFT
- etc…

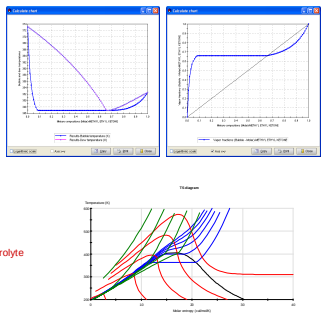
**Activity coefficients models**
- NRTL
- UNIQUAC
- UNIFAC (Larsen, Dortmund,…)
- Wilson
- etc…

**Combined approach models**
- MHV2
- MHV1
- PSRK
- etc…

**Specific systems**
- Pure Water
- Amines
- Sour-Water
- Formaldehyde
- etc…

**Electrolytes**
- Edwards
- UNIQUAC electrolyte
- ULPDHS
- etc…

*The various available methods can be combined in order to configure a thermodynamic model adapted to a specific system*



**A full set of services available:**
- Data regression of experimental properties
- Graphical display of properties on temperature, pressure or composition ranges
- Generation of property tables
- Export of PSF files (HTFS), PVT files (OLGA)
- Estimation of pure component properties
- Plot of phase envelope diagrams
- Residue curves calculation & ternary diagrams
- Calculation of petroleum fractions properties
- Unit conversions
- Predictive models manager (UNIFACs, PPR78, NRTL-PR…)
- etc…

*All these services become automatically available in your usual software since it embeds Simulis® Thermodynamics*

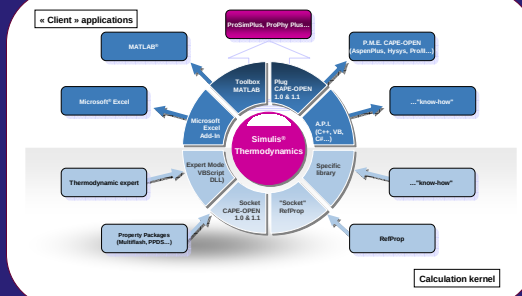
**Uses the widely validated thermodynamic library of ProSim:**
- **Maturity** of the architecture
- **Reliability** of the results
- **Robustness** of algorithms

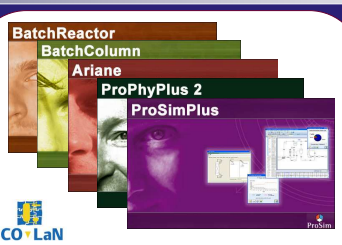
Supplied with a database of over 2 000 components including AIChE's DIPPR® database and access to your "private" databases of pure components properties.

DIPPR

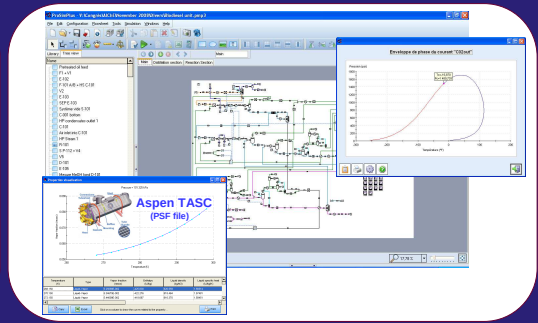
**Other software components included:**
- **Simulis® Conversions**: physical units conversion management tool
- **Simulis® Properties**: pure substances properties server

## ② Easy to embed in your environment



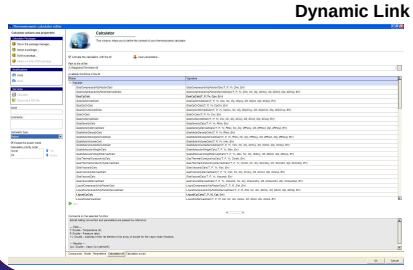



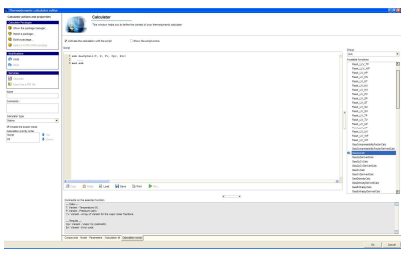

**Any application that integrates Simulis® Thermodynamics automatically inherits from its CAPE-OPEN standard compliance**




## ③ "Expert mode" to add your own thermodynamic models (new or existing ones)

**Dynamic Link Library (DLL)** ⟵ ⟶ **VBScript**





**Capability to use legacy codes**

End-users can introduce their own know-how within Simulis® Thermodynamics

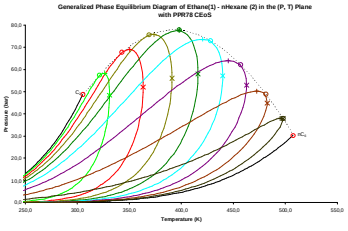
Ability to merge native ProSim codes and legacy codes.

Ability to use native pure compound properties in legacy codes.

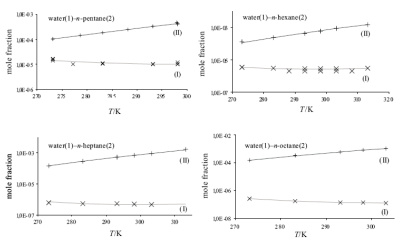
Tests and debugging facilities supplied to developers

## ④ Thermodynamic library enriched every year

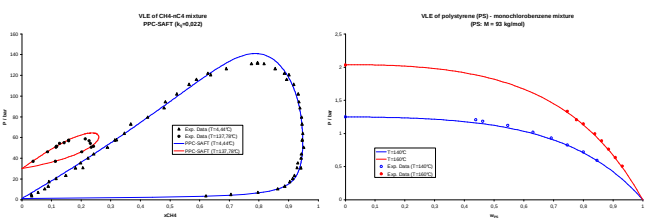
**PPR78 [1 - 4]**




**NRTL-PR [5 - 7]**




**PPC-SAFT [8 - 11]**

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