Simulis® Thermodynamics

An open framework for users and developers

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ProSim

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)
- PC-SAFT (IFP)
- Nakamura
- etc…

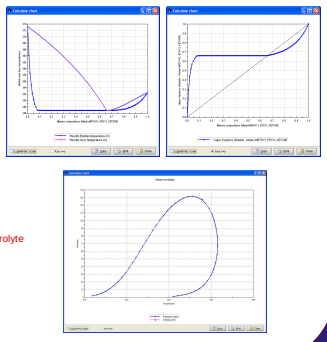
Activity coefficients models
- NRTL
- UNIQUAC
- UNIFAC (Larsen, Dortmund,…)
- Wilson
- etc…

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

Specific systems
- Pure Water
- Amines
- Sour-Water
- 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
- UNIFAC models manager
- etc…

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

Simulis® is the name of the new component oriented software suite of ProSim

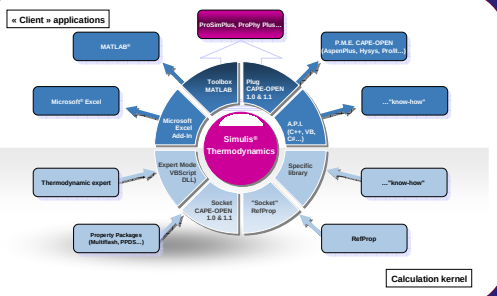
Uses the widely validated thermodynamic library of ProSim:
- **Maturity** of the architecture
- **Reliability** of the results
- **Robustness** of algorithms

Supplied with a database of over 1 900 components including AIChE's DIPPR® database and access to your "private" databases of pure components properties.

DIPPR

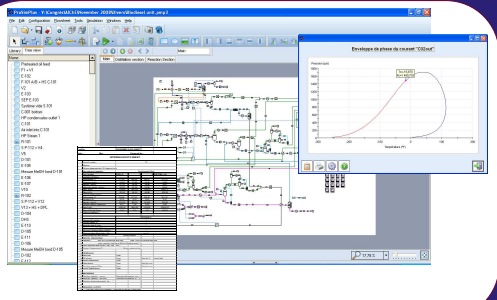
Other software components included:
- **Simulis® Conversions**: physical units conversion management tool
- **Simulis® Properties**: pure substances properties server

② Easy to integrate and to be integrated



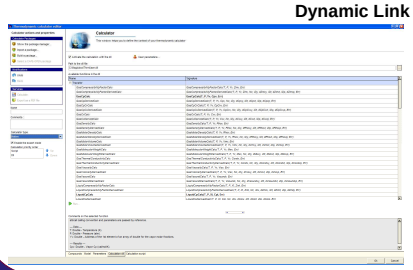
CO-LaN

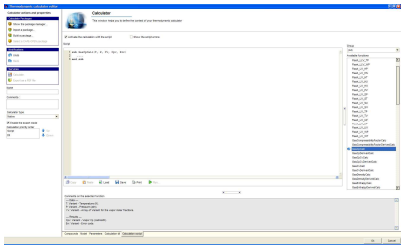
Any application that integrates Simulis® Thermodynamics automatically inherits from its CAPE-OPEN standard compliance



③ Expert mode to add your own thermodynamics models (new or existing ones)

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





Capability to use legacy codes

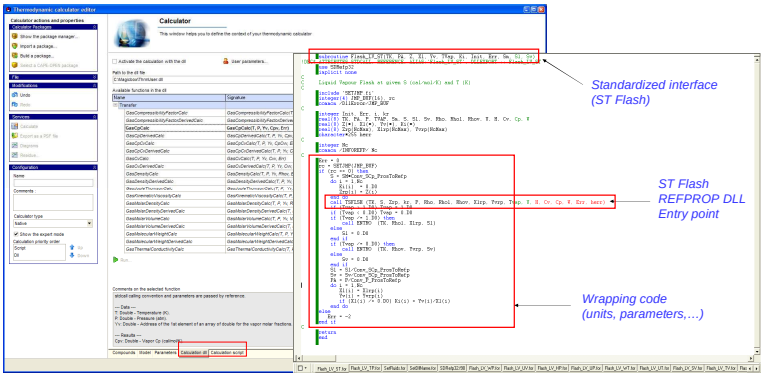
End-users can introduce their own know-how within Simulis® Thermodynamics

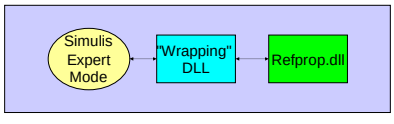
Ability to merge native ProSim codes and legacy codes.

Ability to use native pure compound properties in legacy codes.

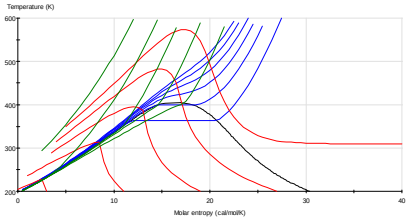
Tests and debugging facilities supplied to developers

④ Expert mode for developers: illustration with REFPROP link implementation





TS diagram



NIST National Institute of Standards and Technology

AIR LIQUIDE

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