

Use Simulis® Thermodynamics to Fill the Gap in UNIFAC Matrices



ProSim

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Praia da Rocha (Portugal)

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1 Simulis® Thermodynamics: a Thermophysical calculation server

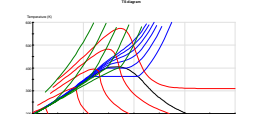
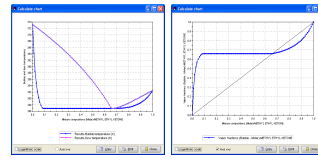
Computes thermophysical properties and phase equilibria on pure components or mixtures:

PROPERTIES CALCULATED

- | | |
|---|--|
| <ul style="list-style-type: none"> 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 | <ul style="list-style-type: none"> 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

- | | |
|---|--|
| <ul style="list-style-type: none"> Equations of State Soave-Redlich-Kwong (SRK) Peng-Robinson (PR) Lee-Kesler-Plöcker (LKP) Predictive Peng-Robinson 78 (PPR78) PC-SAFT (IFF) Nakamura etc... | <ul style="list-style-type: none"> Specific systems Pure Water Amines Sour-Water etc... |
| <ul style="list-style-type: none"> Activity coefficients models NRTL UNIQUAC UNIFAC (Larsen, Dortmund,...) Wilson etc... | <ul style="list-style-type: none"> Electrolytes Edwards UNIQUAC electrolyte ULPDHS etc... |
| <ul style="list-style-type: none"> Combined approach models MHV2 MHV1 PSRK etc... | <p><i>The various available methods can be combined in order to configure a thermodynamic model adapted to a specific system</i></p> |



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

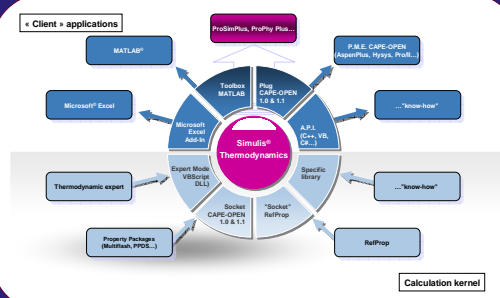
Supplied with a database of over 1 900 components including AIChE's DIPPR® database and access to your "private" databases of pure components properties.



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



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

3 UNIFAC Models Manager

4 Application example: Identification of GIP [CF2H] / [CH2]

R290 (1) - R152a (2)
Equilibrium curve at 293.19K

R290 (Propane)
CC(C)C

R152a (1,1-Difluoroethane)
CC(F)F

R290 (1) - R152a (2)
Bubble and Dew Pressures at 293.19 K

R32 (1) - R290 (2)
Equilibrium curve at 253.15K

R32 (Difluoromethane)
CC(F)F

R32 (1) - R290 (2)
Bubble and Dew Pressures at 253.15 K