Sea Water Modeling with Simulis® Thermodynamics

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ProSim

ensgti PROCÉDÉS PAU

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)
- Nakamura
- etc…

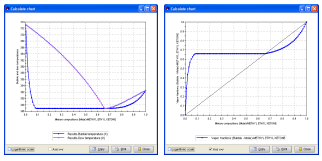
Activity coefficients models
- NRTL
- UNIQUAC
- UNIFAC (Larsen, Dortmund,…)
- Wilson
- etc…

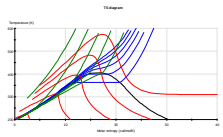
Specific systems
- Pure Water
- Amines
- Sour-Water
- etc…

Combined approach models
- MHV2
- MHV1
- PSRK
- 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





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

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

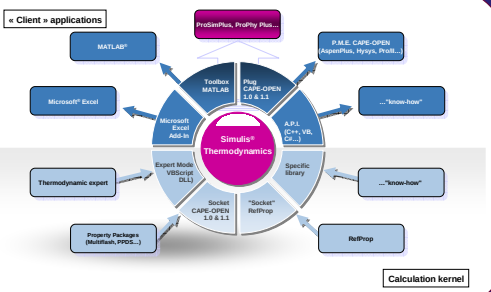
Uses the widely validated thermodynamic library of ProSim:
- **Maturity** of the architecture
- **Reliability** of the results
- **Robustness** of algorithms

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

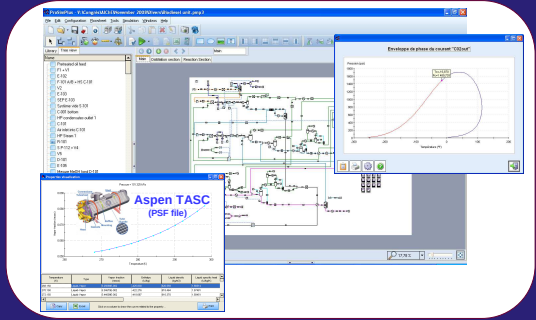
DIPPR

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

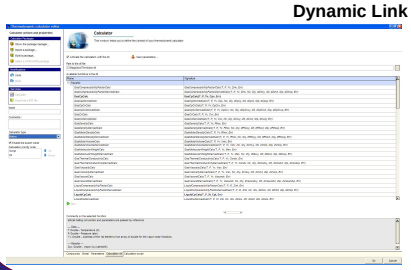


Any application that integrates Simulis® Thermodynamics automatically inherits from its CAPE-OPEN standard compliance

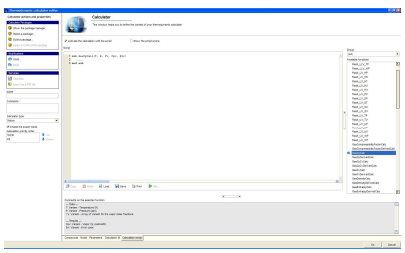


③ Expert mode to add your own thermodynamics models (new or existing ones)

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 Application example: Saline systems and Sea Water Modeling

Inflow (moles)		Outflow (moles of major species)	
H_2O	55.508	**Aqueous Phase**	
NaCl	1.50	H_2O	53.610
$CaSO_4$	1.00	Na^+	1.50
		Cl^-	1.50
		Ca^{2+}	0.051
		SO_4^{2-}	0.051
		Solid phase	
		$CaSO_4,2H_2O$	0.949

Table 4: System Gypsum – Sodium Chloride –Water at 25°C : mass results

Component	Molality (mol.kg^{-1})
NaCl	0.424
MgCl2	0.0553
Na2SO4	0.0291
CaCl2	0.0105
KCl	0.0094

Table 1: artificial seawater composition [1][2]

T(°C)	Ionic strength I	γ_{NaCl} Experiment [1]	γ_{NaCl} Calc.	γ_{Na2SO4} Experiment [2]	γ_{Na2SO4} Calc.
25	0.718	0.672 ± 0.007	0.666	0.378 ± 0.016	0.3735

Table 2: modelled values and measurements in artificial sea water

Reference	Component					
	γ_{Na^+}	$\gamma_{Mg^{2+}}$	$\gamma_{Ca^{2+}}$	γ_{K^+}	γ_{Cl^-}	$\gamma_{SO_4^{2-}}$
Experimental	0.67 [3]	0.26 [4]	0.21 [5]	0.61 [6]	0.68 [1]	0.11 [2]
This work	0.672	0.258	0.212	0.610	0.681	0.114

Table 3: Major Ion Activity coefficients in Seawater (T = 25°C and S $^0/_{00}$ = 35)

[1] R.F. Platford, J. Mar. Res.,23 (1965) 55, [2]R.F Platford and T. Dafoe, J. Mar. Res., 23 (1965) 63, [3]R.F. Platford, J. Fish. Res. Bd. Can., 22 (1965) 885, [4]M.E.Thompson, Science, 153 (1966) 1643, [5]M.E Thompson and J.W .Ross, J. Mar. Res., 23 (1965) 63, [6]P.G. Manglesdorf Jr. and T.R.S. Wilson., J. Phys. Chem., 75 (1971) 1418

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