

# Simulis<sup>®</sup> Thermodynamics: an open framework for users and developers

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## **Abstract**

Simulis<sup>®</sup> Thermodynamics is a thermophysical calculation server that generates highly accurate pure component and mixture properties (thermodynamic, transport, compressibility...) and fluid phase equilibria (liquid-vapor, liquid-liquid and liquid-liquid-vapor). The standard version of Simulis<sup>®</sup> Thermodynamics is provided as an add-in in Microsoft<sup>®</sup> Excel or as a toolbox in MATLAB<sup>®</sup> and enables the user to run complete thermodynamic calculations in these applications, but it can also be plugged in any legacy code. CAPE-OPEN [1] compliance of Simulis<sup>®</sup> Thermodynamics through its implementation of the CAPE-OPEN standardized interfaces, “thermodynamic plug” and “thermodynamic socket”, is presented here. Its capability to embed user codes either as a DLL (Dynamic Link Library) following a standard syntax, either as VBScript (Visual Basic Script) directly written from the Simulis<sup>®</sup> Thermodynamics’ environment is highlighted in this paper. In this case, the user code inherits of all the features of Simulis<sup>®</sup> Thermodynamics: CAPE-OPEN compliance, Microsoft<sup>®</sup> Excel add-in, MATLAB<sup>®</sup> toolbox... Besides description of all these different features, several examples will be presented. Particularly, expert mode of Simulis<sup>®</sup> Thermodynamics (functionality allowing the user to implement his own models in Simulis<sup>®</sup> Thermodynamics) will be highlighted by introducing what has been done with REFPROP code [2], the NIST Reference Fluid Thermodynamic and Transport Properties Database (US Department of Commerce).

## **Introduction**

Throughout their history, process simulation tools underwent periods of change imposing them to adapt to the current hardware and software technologies and to answer a more and more demanding market. Practices are once again disturbed today by networks and co-operative work advent. In addition to the performance and user-friendliness criteria, the various tools must now be able to be substituted and to exchange services. They must be interoperable and integrable. New technologies based on components developed with object-oriented languages should make it possible to meet this new market requirement.

Considering the situation, we undertook to change the architecture of our tools to answer not only our own customers' expectations, but also the whole simulation process software users community. This is Simulis<sup>®</sup> project ambition. Simulis<sup>®</sup> is the name of ProSim's new software suite. The component-oriented approach of its architecture is based on the Microsoft<sup>®</sup>'s COM/DCOM middleware. Today, three components are already available. The first, called Simulis<sup>®</sup> Conversions, allows to manage quantities and unit conversion in an application. The next, Simulis<sup>®</sup> Properties, is a pure substance properties server (properties being constant or temperature dependent). Finally, the last component, called Simulis<sup>®</sup> Thermodynamics, is presented in this paper.

### **Simulis<sup>®</sup> Thermodynamics**

Simulis<sup>®</sup> Thermodynamics is a thermodynamic properties and phase equilibrium calculation server for pure substances and mixtures (up to 200 compounds). It is based on ProSim traditional thermodynamic calculation library which has been validated through many years of intensive industrial use. It is able to calculate the following properties (and their derivatives with respect to temperature, pressure and composition):

- Transport properties ( $C_p$ ,  $\mu$ ,  $\lambda$ , ...).
- Thermodynamic properties ( $H$ ,  $S$ , ...).
- Compressibility properties ( $Z$ ,  $C_p/C_v$ , ...).
- Non-ideal properties ( $\gamma$ ,  $\phi$ ,  $f$ )
- Critical properties ( $T_c$ ,  $P_c$ ,  $V_c$ ,  $Z_c$ ).

And to perform the following phase equilibrium calculations:

- Liquid-Vapor ( $TP$ ,  $\omega T$ ,  $\omega P$ ,  $HP$ ,  $HT$ ,  $HV$ ,  $HU$ ,  $SP$ ,  $ST$ ,  $SV$ ,  $SH$ ,  $SU$ ,  $UP$ ,  $UT$ ,  $UV$ ,  $PV$ ,  $TV$ ).
- Liquid-Vapor phase envelope.

- Liquid-Liquid (TP).
- Liquid-Liquid-Vapor (TP, HP,  $\omega$ P).

Its model library contains the most important ones including:

- Equations of State (RKS, PR, BWRS, LKP, PPR78...)
- Activity coefficient models (Wilson, Margules, NRTL, UNIQUAC, original UNIFAC, mod. Dortmund UNIFAC, mod. Larsen UNIFAC, UNIFAC PSRK...)
- EoS/ $G^E$  models (MHV2, MHV1, PSRK...)
- Specific models (Chao-Seader, Grayson-Streed, NBS/NRC Steam Tables, Formaldehyde, Souers, Carboxylic acids...)
- Electrolytes models (Engels, UNIQUAC electrolytes, Edwards, ULPDHS, Amines and acid gases...).

A pure substance property database, containing more than 1900 compounds, is provided with this software component. Moreover, latest DIPPR<sup>®</sup> [3] database version can be provided with Simulis<sup>®</sup> Thermodynamics and user can manage as many private databases as needed.

### **"Integrability" capability of Simulis<sup>®</sup> Thermodynamics**

Benefit of the architecture based on a component approach is that any application supporting the COM/DCOM technology (... and others too) can be linked and interoperate with Simulis<sup>®</sup> Thermodynamics. So, the standard commercial packaging of Simulis<sup>®</sup> Thermodynamics contains a Microsoft<sup>®</sup> Excel add-in and a MATLAB<sup>®</sup> toolbox and allows to use it in these different environments. A complete API is also provided and it can be easily programmed by using languages such as C#, VB.NET, Visual Basic, C++, Delphi, FORTRAN... This important capability of Simulis<sup>®</sup> Thermodynamics is called "integrability".

### **"Package" concept inside Simulis<sup>®</sup> Thermodynamics**

Another friendly functionality of Simulis<sup>®</sup> Thermodynamics is the "data packages" concept. For example, with the help of Simulis<sup>®</sup> Thermodynamics "data packages", user is able to build, record and deploy in four steps the analysis made by a thermodynamic expert. First, with the standard dialogs available within the component, expert performs his thermodynamic analysis focused on the quality of pure substances properties and the pertinence of the thermodynamic model he has retained to model the studied system. In the second step, he perpetuates this "know-how" throughout an easy creation of a "data package". Then, the two last

steps consist to create automatically an installation script of this "data package" to deploy it by e-mail or throughout his company network in order to be used by his colleagues. For example, this feature interested Air Liquide who adopt Simulis as a thermodynamic standard used at each step of process development (from R&D to Engineering to Plant Operation) within different tools (commercial and in-house).

### Simulis® Thermodynamics and CAPE-OPEN [1]

Even if the architecture of Simulis® Thermodynamics is not based, in native, on CAPE-OPEN standard (mainly due to the requirement to keep validated existing codes), it proposes a nearly total interoperability with other software supporting this standardized interfaces.

On the one hand, Simulis® Thermodynamics allows the client application to calculate properties and phase equilibrium using an external CAPE-OPEN thermodynamic property package (coming from Aspen Properties, Multiflash, PPDS, IVC-SEP packages, COCO TEA...) throughout its "socket" facility (Figure 1).



Figure 1. CAPE-OPEN Thermodynamic "socket" facility.

On the other hand, with Simulis® Thermodynamics, the end-user is able to generate a CAPE-OPEN thermodynamic property package which can be used inside software of other providers (Aspen Plus, PRO/II, gPROMS, Aspen Hysys, HTRI Suite, Unisim Design, COCO COFE, Belsim VALI, INDISS...): this is the thermodynamic "plug" facility (Figure 2).

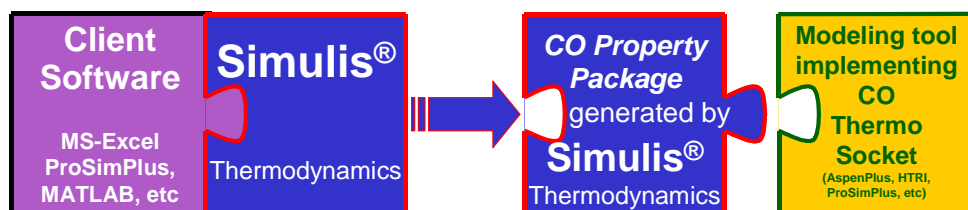


Figure 2. CAPE-OPEN Thermodynamic "plug" facility.

As a consequence, any client application embedding Simulis<sup>®</sup> Thermodynamics automatically inherits its CAPE-OPEN thermodynamic compliance, plug and socket for the two levels of CAPE-OPEN specifications (Version 1.0 and Version 1.1).

### **Expert mode**

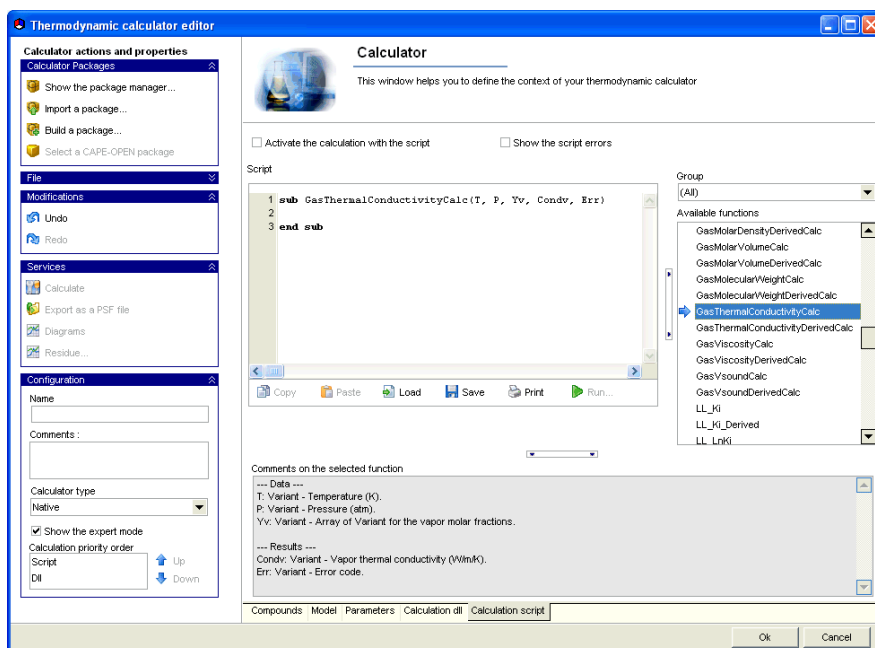
- Scope and objectives

The main objective of the expert mode is to provide thermodynamic experts with a simple and standardized development framework in order to integrate their know-how in Simulis<sup>®</sup> Thermodynamics. Like this they can make their models available in all client applications: Microsoft<sup>®</sup> Excel, MATLAB<sup>®</sup>, all Process Modeling Environment CAPE-OPEN compliant (Aspen Plus, PRO/II, gPROMS, Aspen Hysys, HTRI Suite, Unisim Design, COCO COFE, Belsim VALI, INDISS...) or in any application supporting the COM/DCOM technology (C#, VB.NET, Visual Basic, C++, Delphi, FORTRAN,...). This know-how can be an existing one and then user will benefit from a validated development framework for integration and exploitation of existing codes, or it can be a new one and then user will benefit from the standardized integration structure (entry point definition, user parameters management...). Another strong point of this feature is that pure component properties databases are fully available from the expert mode and release user from pure properties management. Furthermore, this framework supplies developers with tests and debugging facilities. This feature is available from two modes: VBScript or external DLL. For both modes, a predefined syntax has been specified for all properties and equilibrium calculation routines (e.g. vapor thermal conductivity, liquid density, flash at given temperature and pressure,...): required input data and output results are fully described (order, type, units...). Calculation priorities between native, VBScript and user DLL have to be defined by user in the case of multiple implementations of the same calculation.

- VBScript

This mode is an integrated solution as VBScript language is an interpreted one and then doesn't require any external compiler. The main advantage of this mode is that the syntax is close to Visual Basic which is a language well known from most engineers. However, it is not very competitive in term of calculation time. For a short overview, when a user wants to implement for example a new gas thermal conductivity method, he double-clicks on the corresponding property in the supplied list and then a skeleton of the function with the right syntax is automatically built (Figure 3). A test

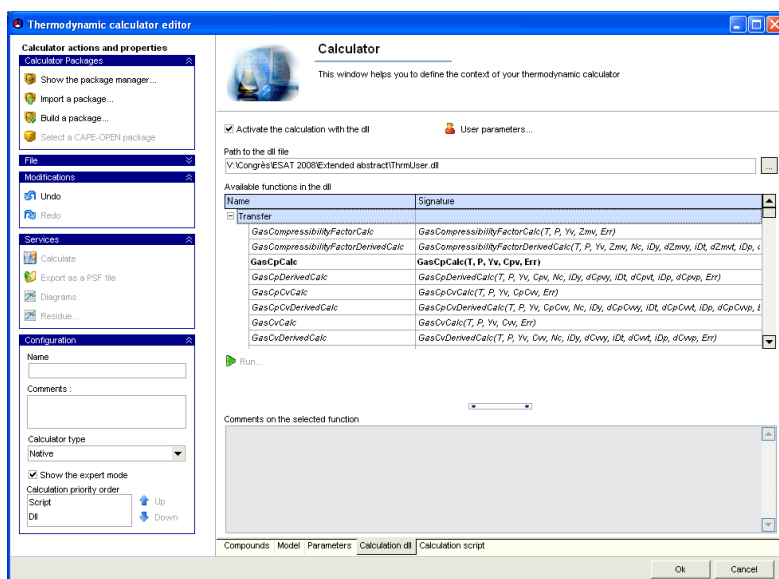
facility is also offered to the developer in order to check the implementation directly from Simulis framework.



**Figure 3.** Expert mode with a VBScript implementation.

- User DLL

Any compiler (C++, Fortran...) can be used to build the user DLL. One of the most advantage with respect to the previous mode is the calculation performance. Moreover, it is very useful when reusing existing codes, which just requires a wrapping to match the predefined syntax of each calculation routine (being in fact an entry point in the DLL). The "stdcall" calling convention shall be used and all routines parameters shall be sent "by reference". If an entry point is effectively implemented inside user library, it appears using a bold font, as shown on the Figure 4 for gas heat capacity.



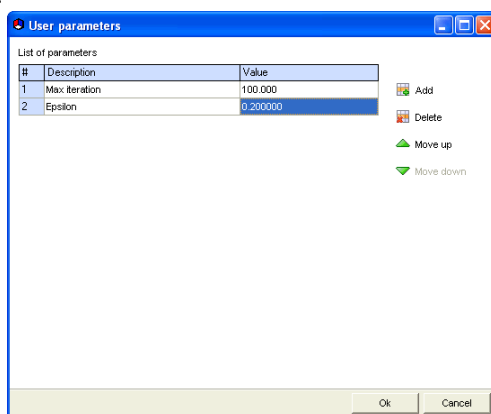
**Figure 4.** Expert mode with an external calculation DLL.

As for the VBScript mode, a test facility is also offered to the developer to validate his implementation directly from the Simulis framework.

Furthermore, some compulsory entry points have to be implemented:

- ✓ To initialize and finalize the DLL.
- ✓ To manage user parameters.
- ✓ To access pure component properties.
- ✓ To access other calculation routines (e.g. native fugacity coefficients...).

User parameters can be interactively described using the following dedicated window:



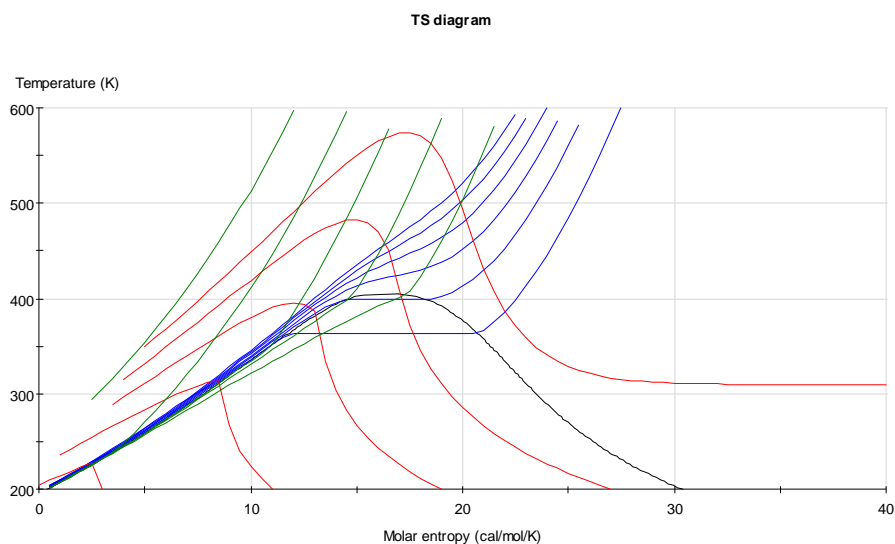
**Figure 5.** User parameters management window.





From now, a user who has a Simulis and a REFPROP user license can benefit from this implementation and then use REFPROP thermodynamics models in all client applications: Microsoft<sup>®</sup> Excel, MATLAB<sup>®</sup>, all Process Modeling Environment CAPE-OPEN compliant (Aspen Plus, PRO/II, gPROMS, Aspen Hysys, HTRI Suite, Unisim Design, COCO COFE, Belsim VALI, INDISS...) or in any application supporting the COM/DCOM technology (C#, VB.NET, Visual Basic, C++, Delphi, FORTRAN,...).

Moreover, all Simulis<sup>®</sup> Thermodynamics services remain available (calculation tool, export as a PSF file, diagrams...). For example, user can calculate and plot a TS diagram using REFPROP models and diagrams service tool available in Simulis<sup>®</sup> Thermodynamics, as shown on Figure 8.

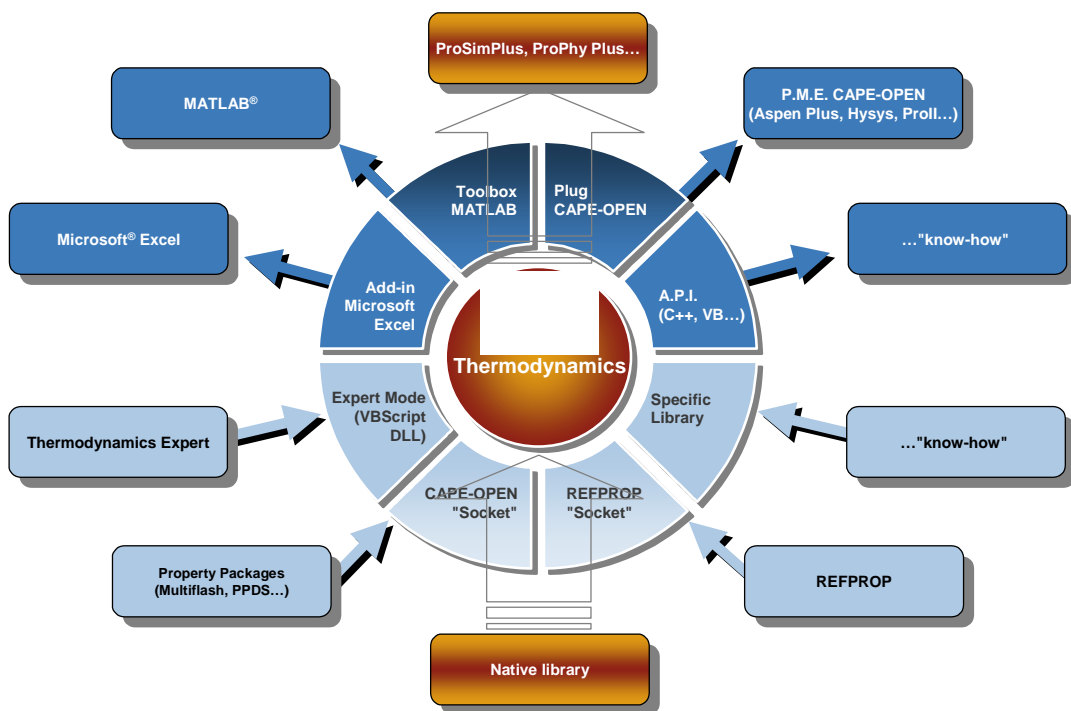


**Figure 8.** Ammonia TS diagram with REFPROP using Simulis diagrams service.

## Conclusion

From now on, components based simulation environments open new horizons to study processes. They allow process engineers, by a judicious assembly of ready to use components, to improve their developments quality while reducing associated times. Thanks to CAPE-OPEN standard, components interchangeability becomes possible. This flexibility makes it possible to select the software component considered to be most powerful for a given application case. The component approach thus incontestably brings gains in productivity to the users as well as to the developers of these systems.

So, as shown on Figure 9, Simulis<sup>®</sup> Thermodynamics is always there where the end-user needs it and guarantees a true data and results consistency throughout the different applications involved.



**Figure 9.** Simulis<sup>®</sup> Thermodynamics: a thermodynamics heart.

## Nomenclature

$C_p$	specific heat
$f$	fugacity
$G$	Gibbs free energy
$H$	enthalpy
$P$	pressure
$S$	entropy
$T$	temperature
$V$	molar volume
$Z$	compressibility factor ( $=PV/RT$ )

## *Greek letters*

$\gamma$	activity coefficient
$\lambda$	thermal conductivity
$\phi$	fugacity coefficient
$\mu$	viscosity
$\omega$	Pitzer acentric factor

## *Sub indexes*

$c$	critical
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## Literature Cited

- [1] The CAPE-OPEN Laboratories Network, <http://www.co-lan.org/Dissemination.html>
- [2] NIST Reference Fluid Thermodynamic and Transport Properties Database (REFPROP), <http://www.nist.gov/srd/nist23.htm>
- [3] Design Institute for Physical Properties, DIPPR<sup>®</sup> 801, <http://dippr.byu.edu/product.asp>

## Acknowledgement

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