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SimuLis

An innovative approach for simulation tools

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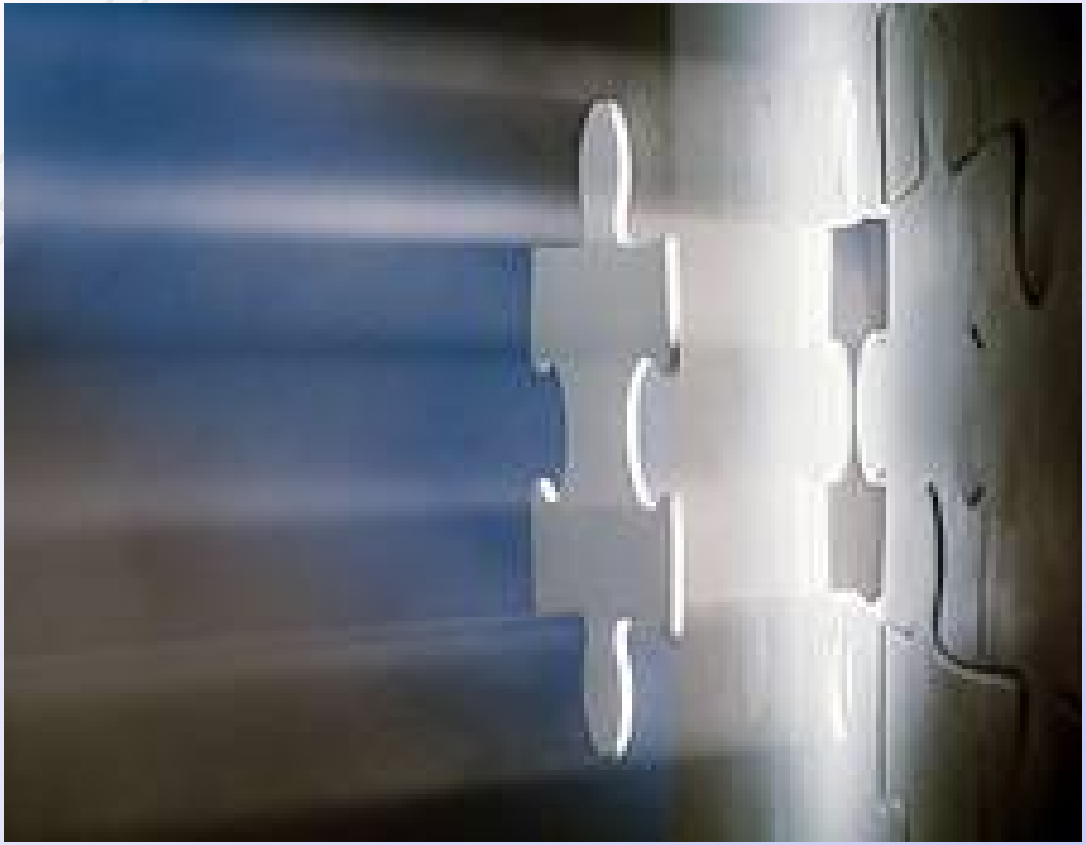
SimuLis



Simulis®?

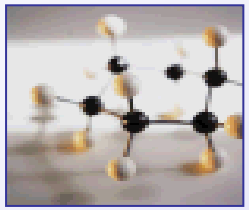
Simulis® software component suite

Simulis® is the name of ProSim new software component suite

- Simulis® Conversions:

Quantities and unit conversion management

- Simulis® Properties (includes Simulis® Conversions):



Pure substance properties server

(constant and temperature dependent).

- Simulis® Thermodynamics (includes Simulis® Properties):

Thermodynamic properties and phase equilibrium calculation server

(pure substances or mixtures).

Simulis® Thermodynamics

Thermodynamic properties and phase equilibrium calculation server for pure substances and mixtures (max. 200 compounds)

- Properties:
  - Transport properties (C_p, μ, λ,…).
  - Thermodynamic properties (H, S, …).
  - Compressibility properties (Z, C_p/C_v, …).
  - Non-ideal properties (γ, ϕ)
  - Pseudo critical properties (T_c, P_c, V_c, Z_c).

- Phase equilibria:
  - Liquid-Vapor (TP, HP, SP, ωT, ωP).
  - Liquid-Vapor phase envelope.
  - Liquid-Liquid (TP).
  - Liquid-Liquid-Vapor (TP, HP, WP).

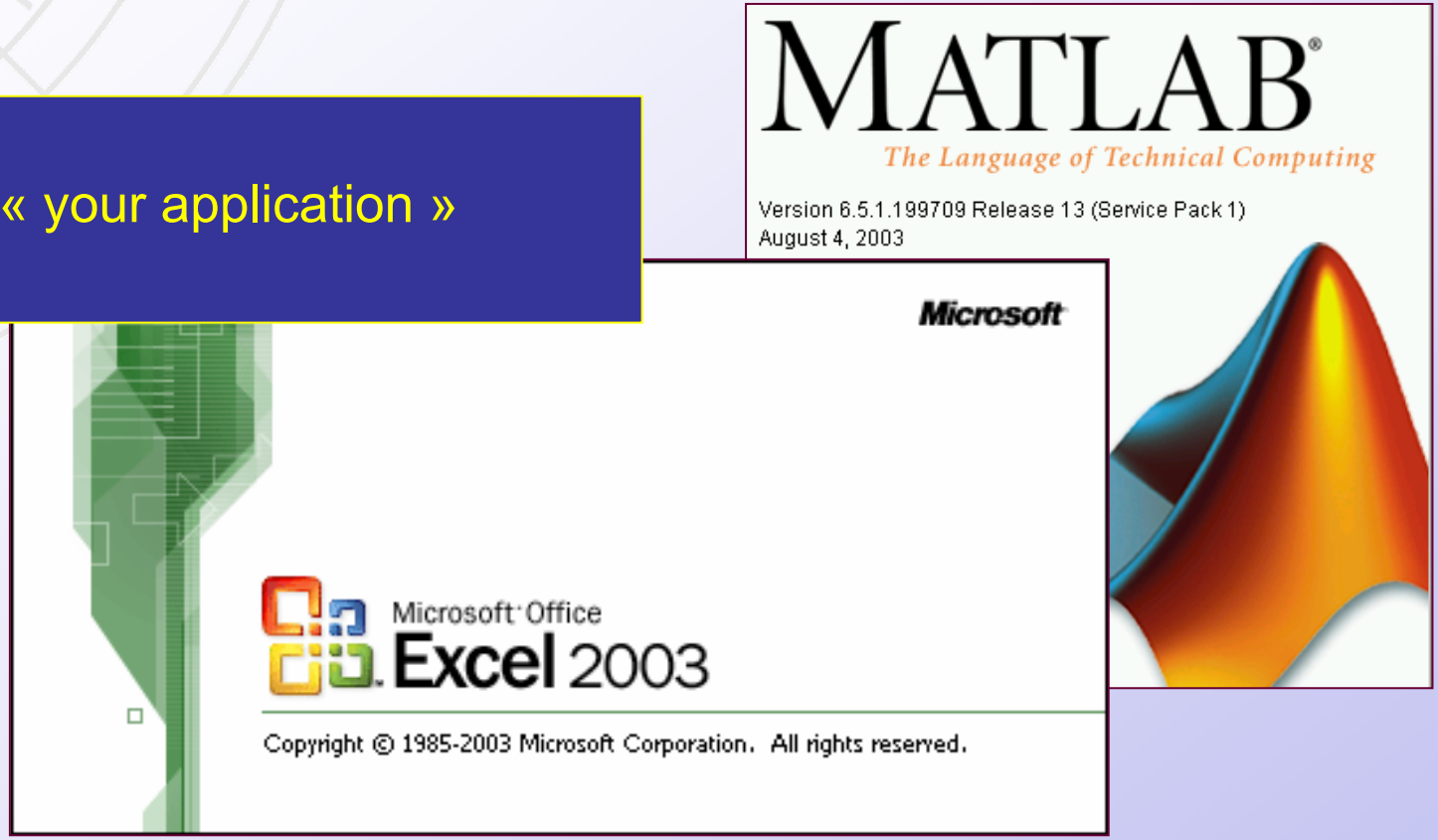
Simulis® Thermodynamics

- Thermodynamic models:
  - Soave-Redlich-Kwong (SRK),
  - Peng-Robinson (PR),
  - Lee-Kesler-Plöcker (LKP),
  - Benedict-Webb-Rubin modified Starling (BWRS),
  - Ideal,
  - Wilson,
  - NRTL,
  - Margules,
  - UNIQUAC,
  - UNIFAC,
  - Engels,
  - Chao-Seader,
  - Sour water,
  - MHV2,
  - ULPDHS, …

SimuLis

Simulis® Thermodynamics integrability

« your application »



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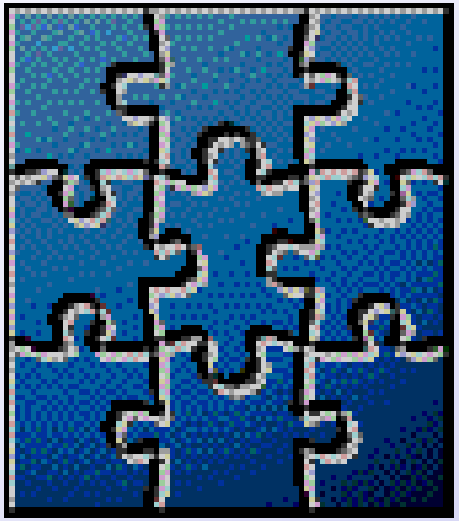
Simulis® Thermodynamics integrability

Benefit of an architecture based on component approach is that any application supporting the COM/DCOM technology (… and others too) can be linked and can interoperate with Simulis® Thermodynamics:



- Visual Basic or VBA (Microsoft® Excel).
- MATLAB®.
- C++.
- Delphi (Object-oriented Pascal).
- FORTRAN.
- …

INTEGRATION is easy.

SimuLis

Simulis® Thermodynamics integrability

TOOLS are better…

Main benefits expected for end users:

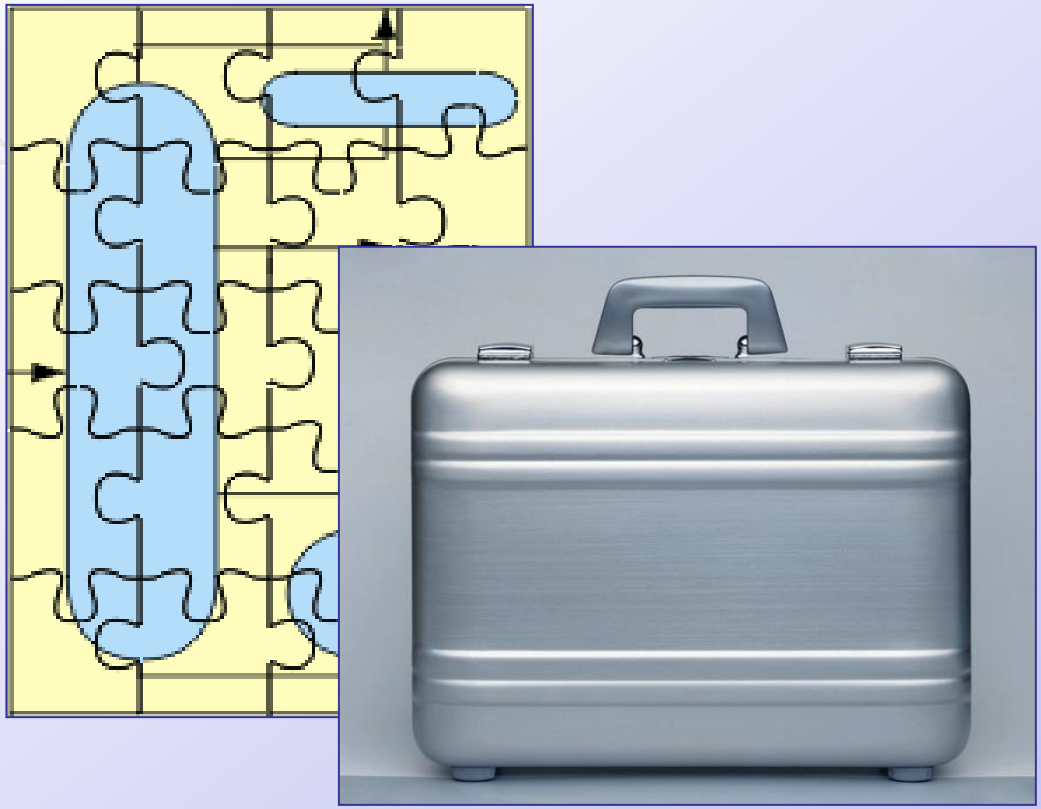
- Quick and easy learning.
- Case-study reusability.
- Data consistency throughout the different applications.
- Interoperability between software components.

Main benefits expected for developers (… and indirectly end users):

- Easier maintainability of smaller codes (Better robustness et reactivity)
- True reusability of components (Development cost reductions)

… and the SERVICE too.

Simulis® Thermodynamics and Packages



Simulis® Thermodynamics and Packages

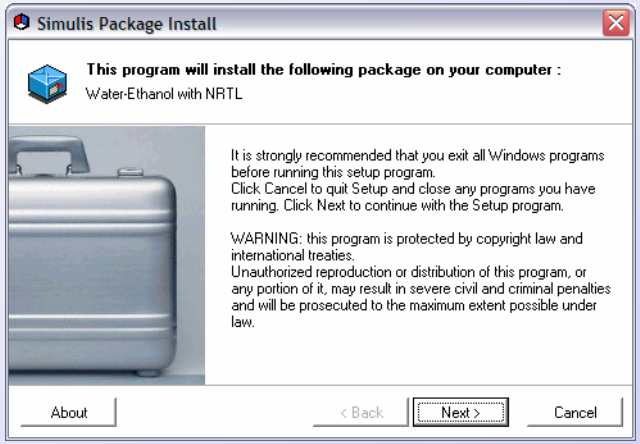
With the help of Simulis® Thermodynamics « data packages » you can build, record and deploy in 4 steps the analysis made by a thermodynamic expert:

1 – **Perform your analysis** focused on the quality of pure substances properties and the pertinence of the thermodynamic model you have retained to fit your system.

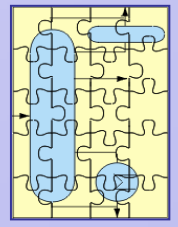
2 – **Perpetuate this « know-how »** throughout a « data package ».

3 – Create automatically an installation script of this « data package » **to deploy it** ….

4 - …**by e-mail** or throughout your company **network** to be used by your colleagues.

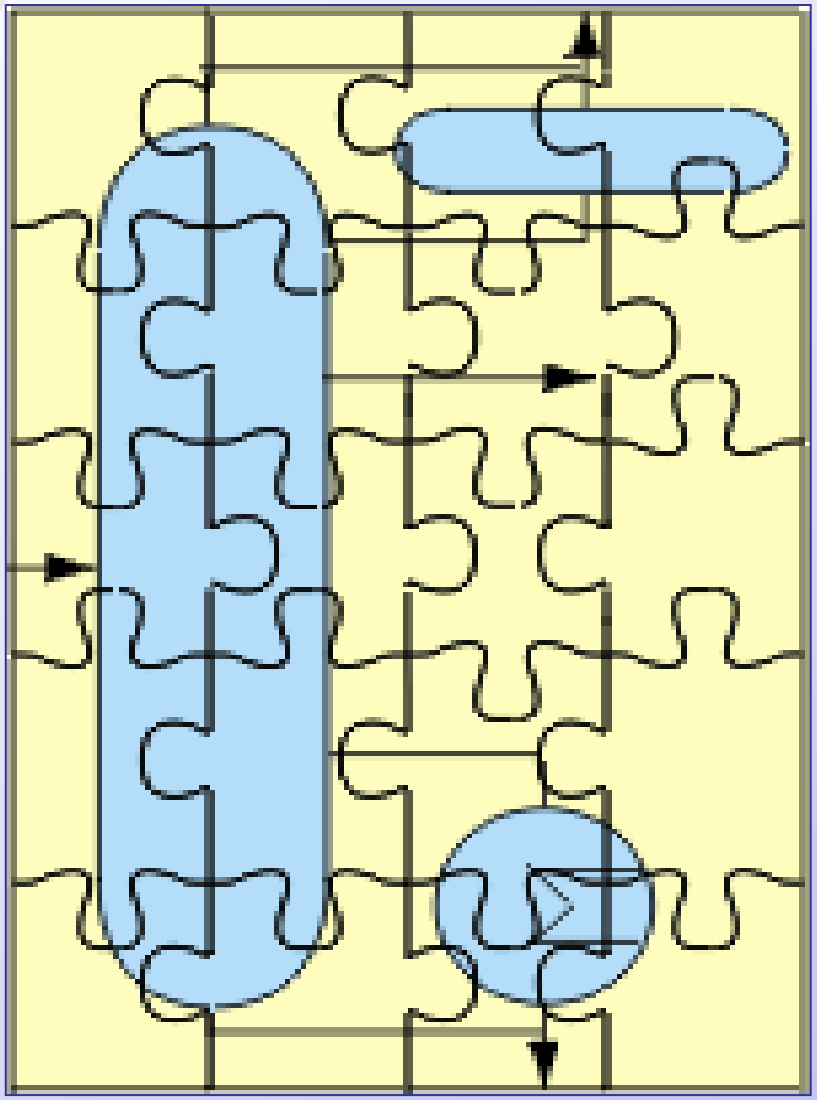


… and « Simulis data packages » are CAPE-OPEN compliant.



SimuLis

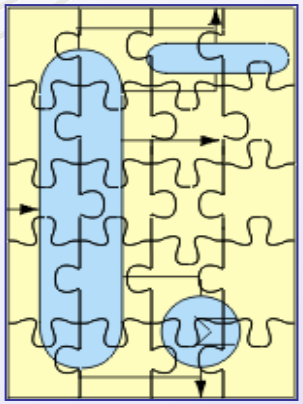
Simulis® Thermodynamics and CAPE-OPEN



Simulis® Thermodynamics and CAPE-OPEN

Simulis® Thermodynamics is based on a proprietary specification …

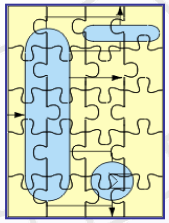
…but implements the CAPE-OPEN standard:



- CAPE-OPEN «thermodynamic socket».
- CAPE-OPEN «thermodynamic plug».

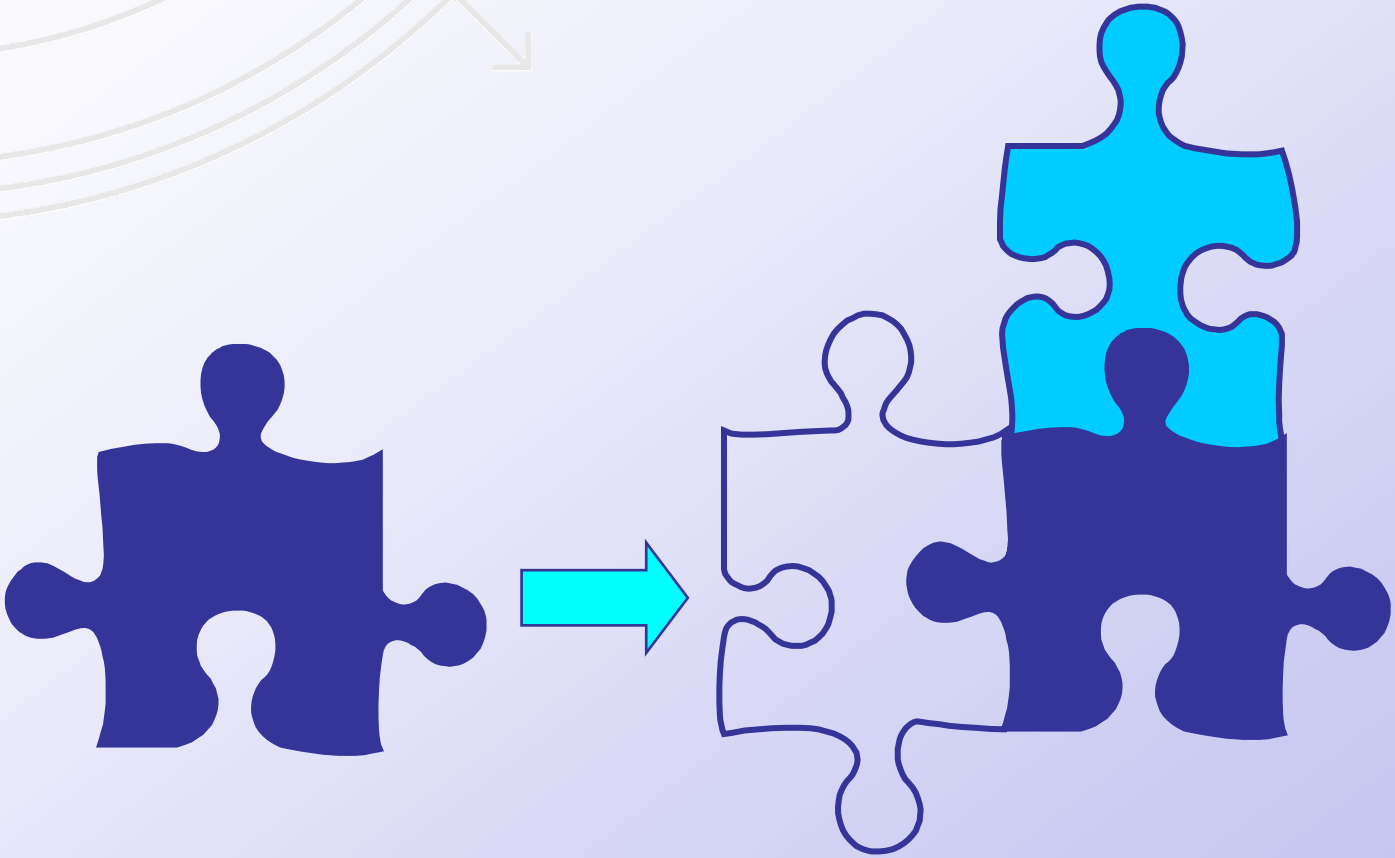
Any application integrating Simulis® Thermodynamics AUTOMATICALLY inherits the CAPE-OPEN thermodynamic compliance (plug and socket).

Simulis® Thermodynamics and CAPE-OPEN



- **CAPE-OPEN «thermodynamic socket»…**

Microsoft® Excel, MATLAB®, « your application », …



Simulis® Thermodynamics

External CO Property Package (Aspen Properties, PPDS,…)

Simulis® Thermodynamics et CAPE-OPEN

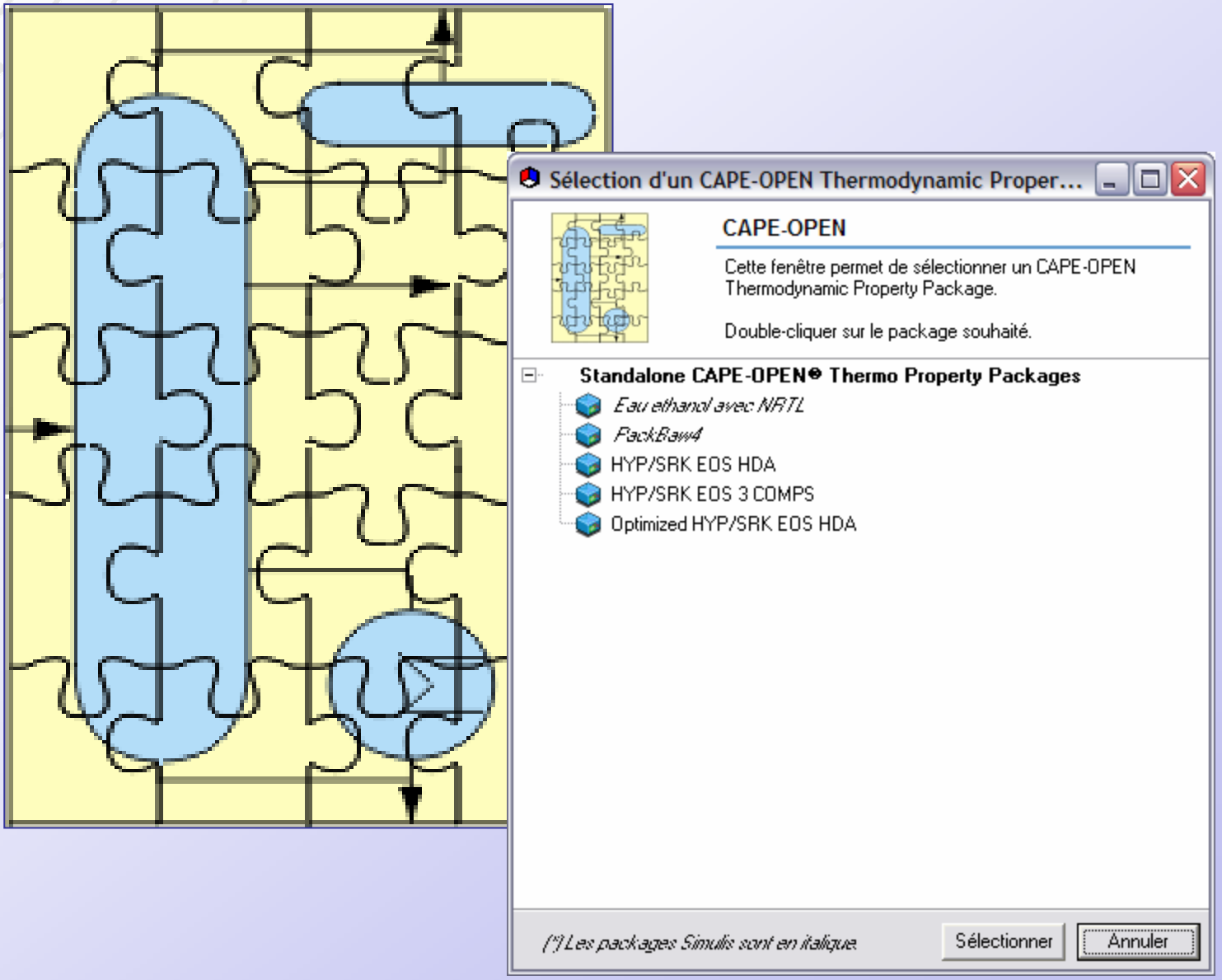
- **CAPE-OPEN « thermodynamic socket »…**

… already successfully tested with:

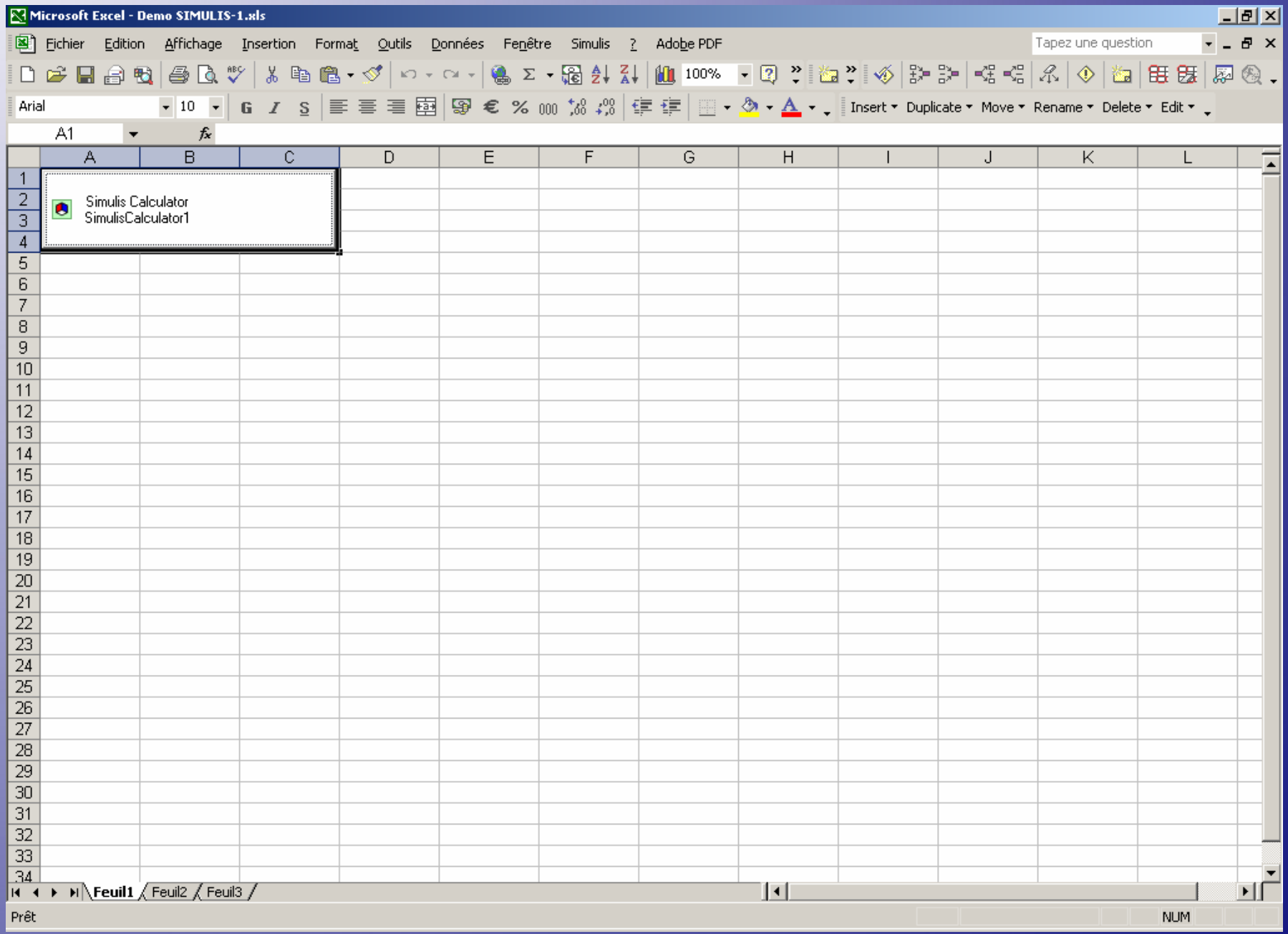
- Aspen Properties (AspenTech)
- MultiFlash (Infochem)
- PPDS (TUV NEL)

SimuLis

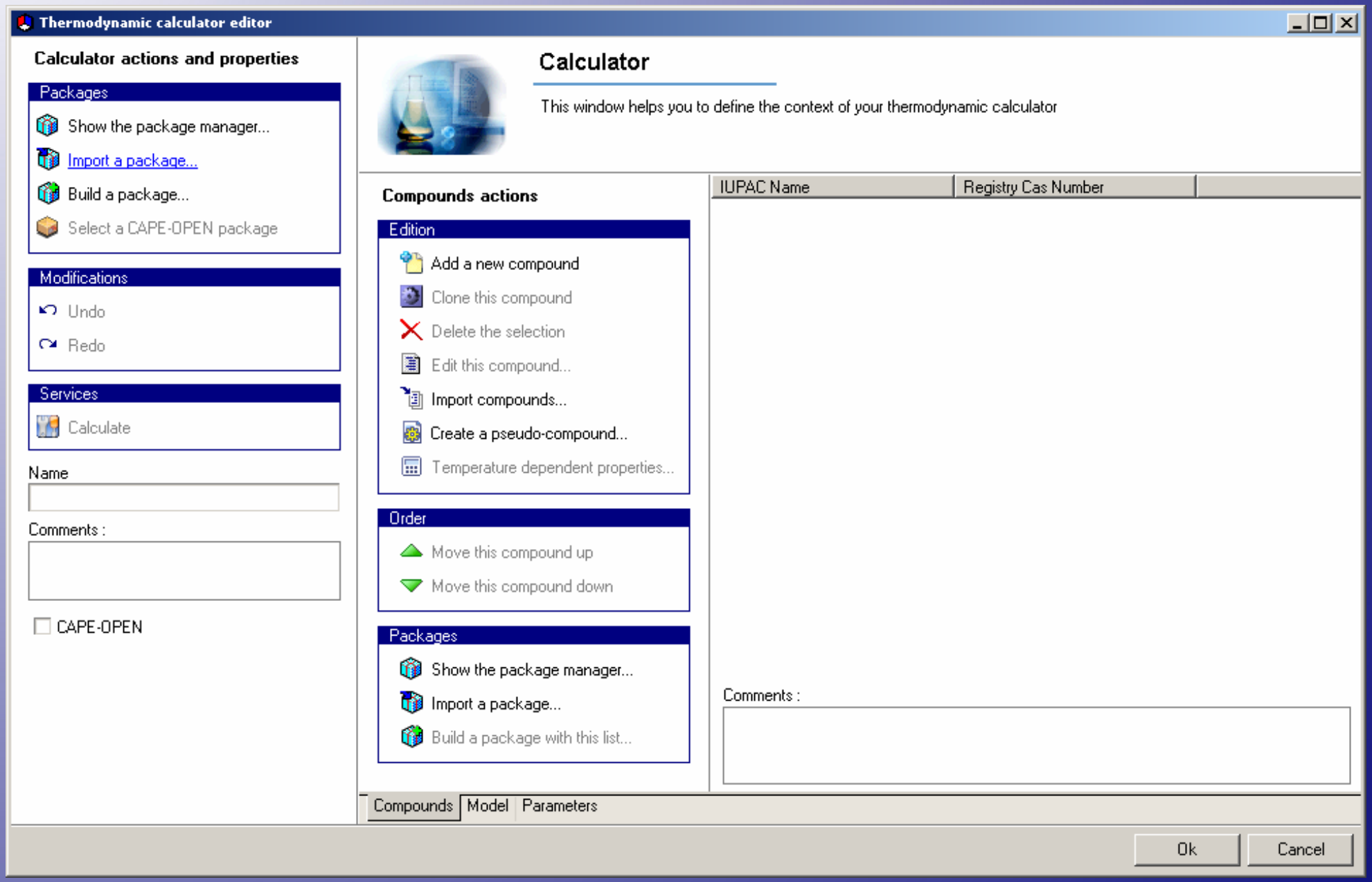
CAPE-OPEN demonstration



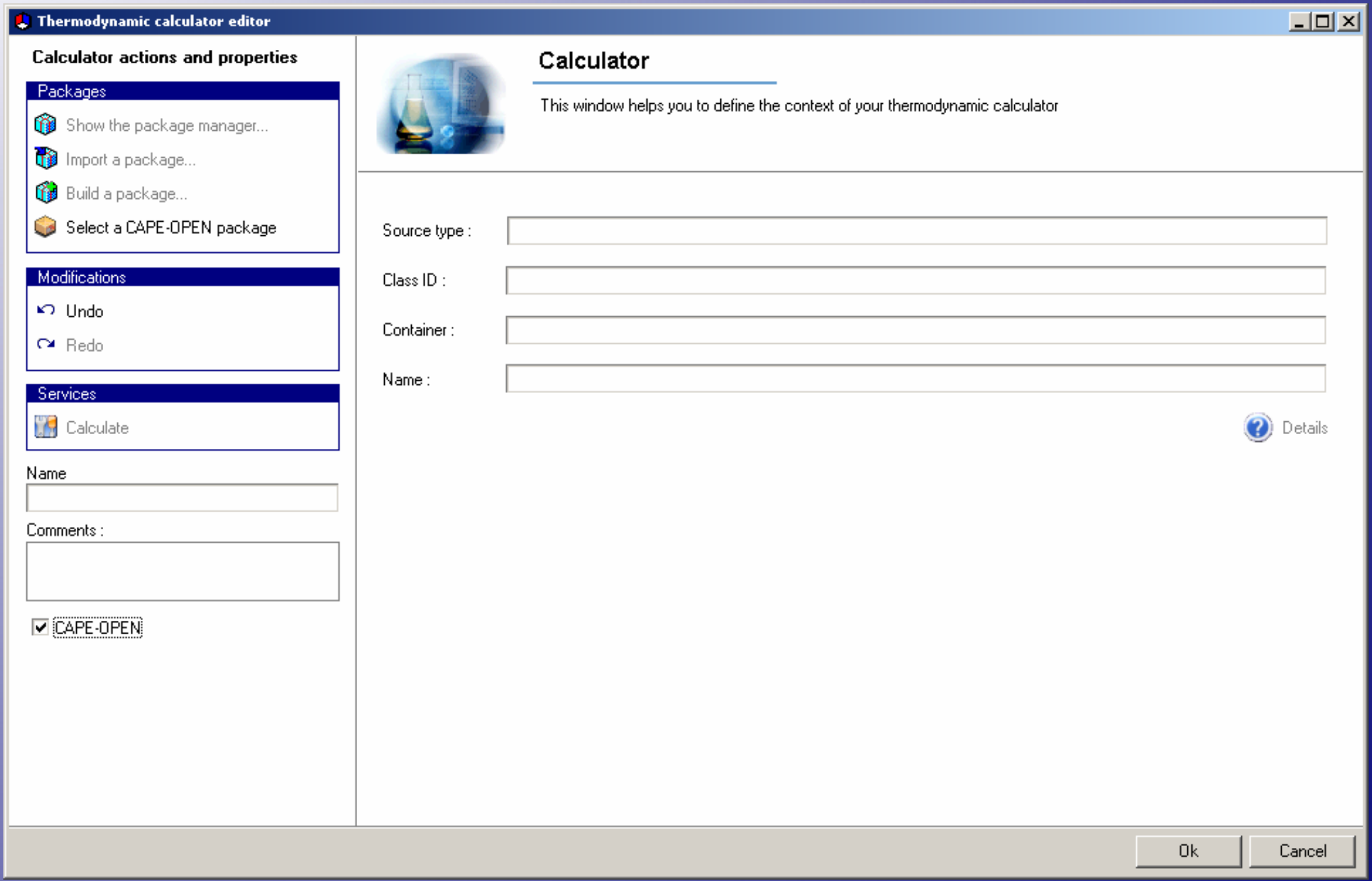
Include SIMULIS Calculator within Excel



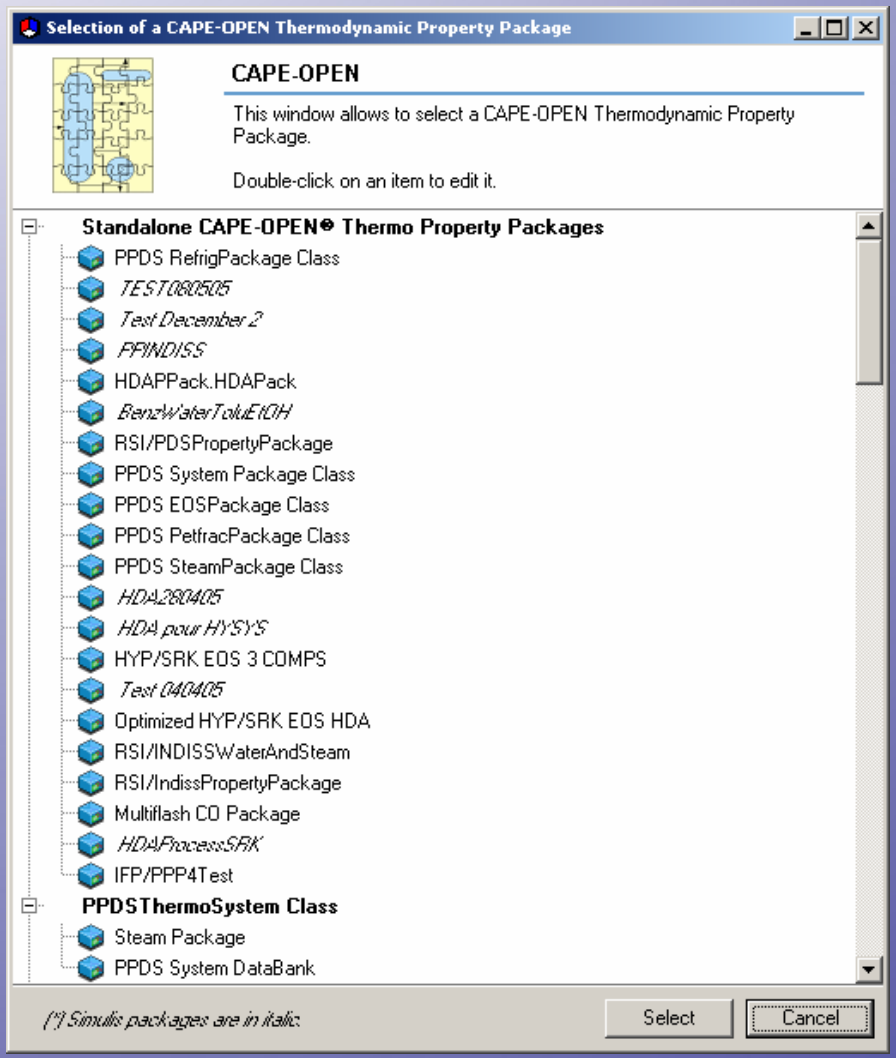
Open SIMULIS Calculator

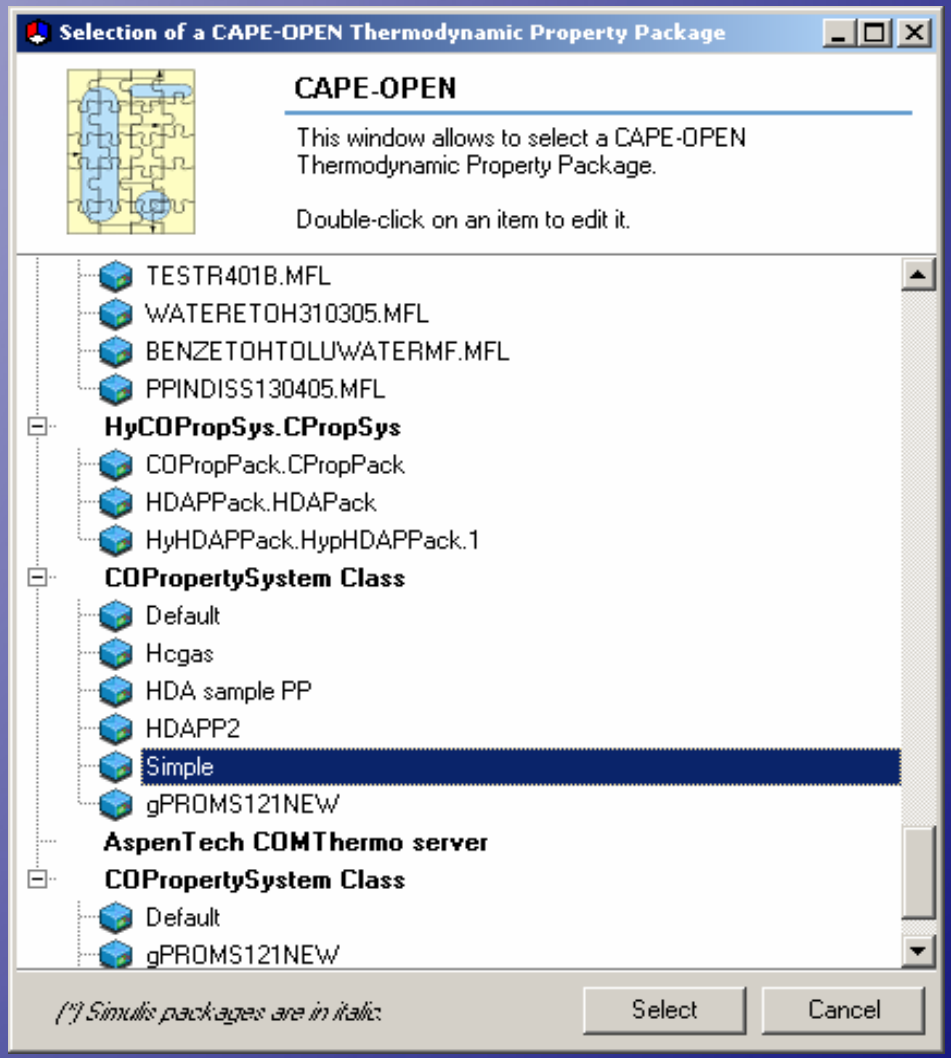


Select CAPE-OPEN

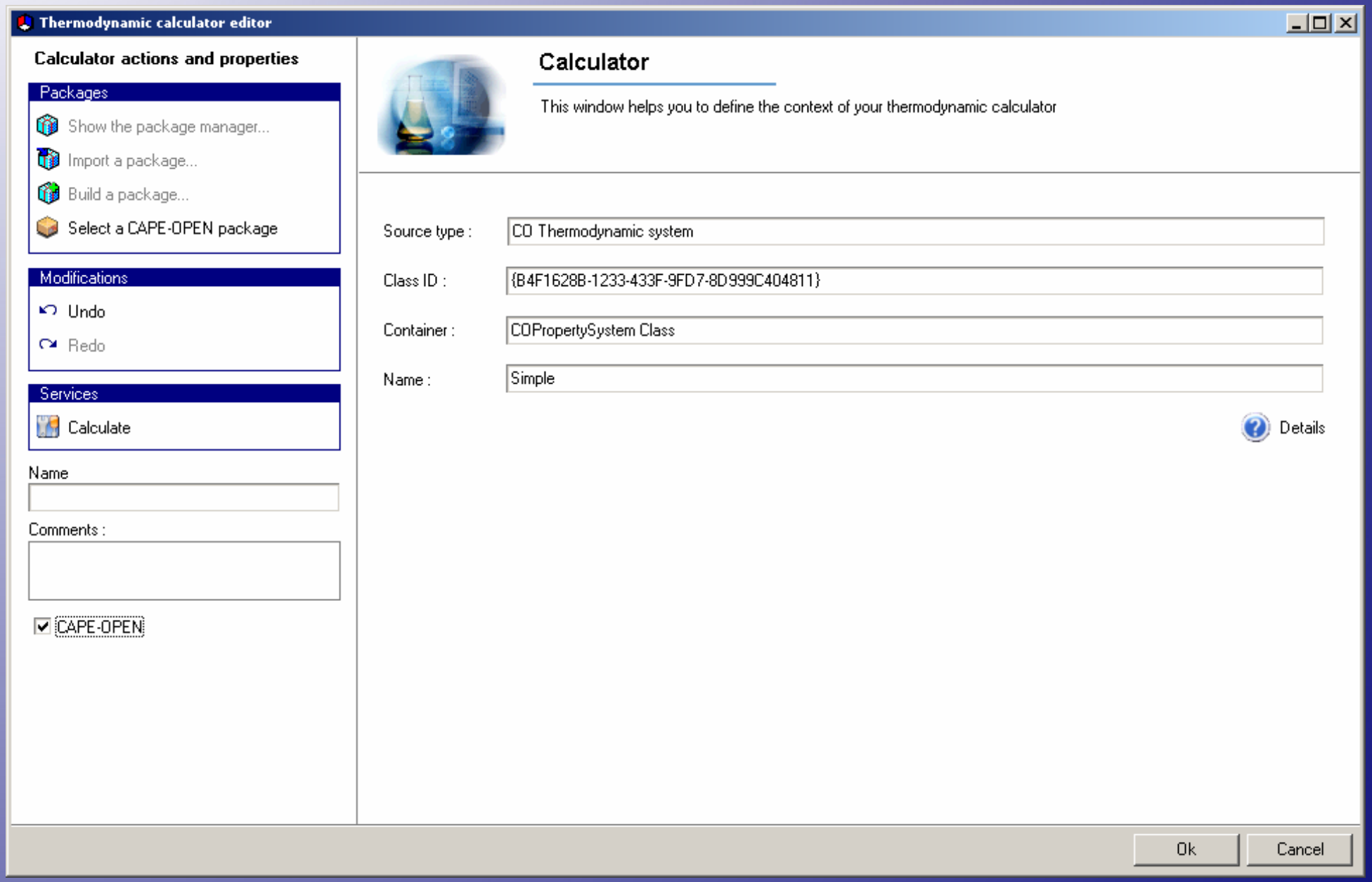


List/select CAPE-OPEN Property Packages

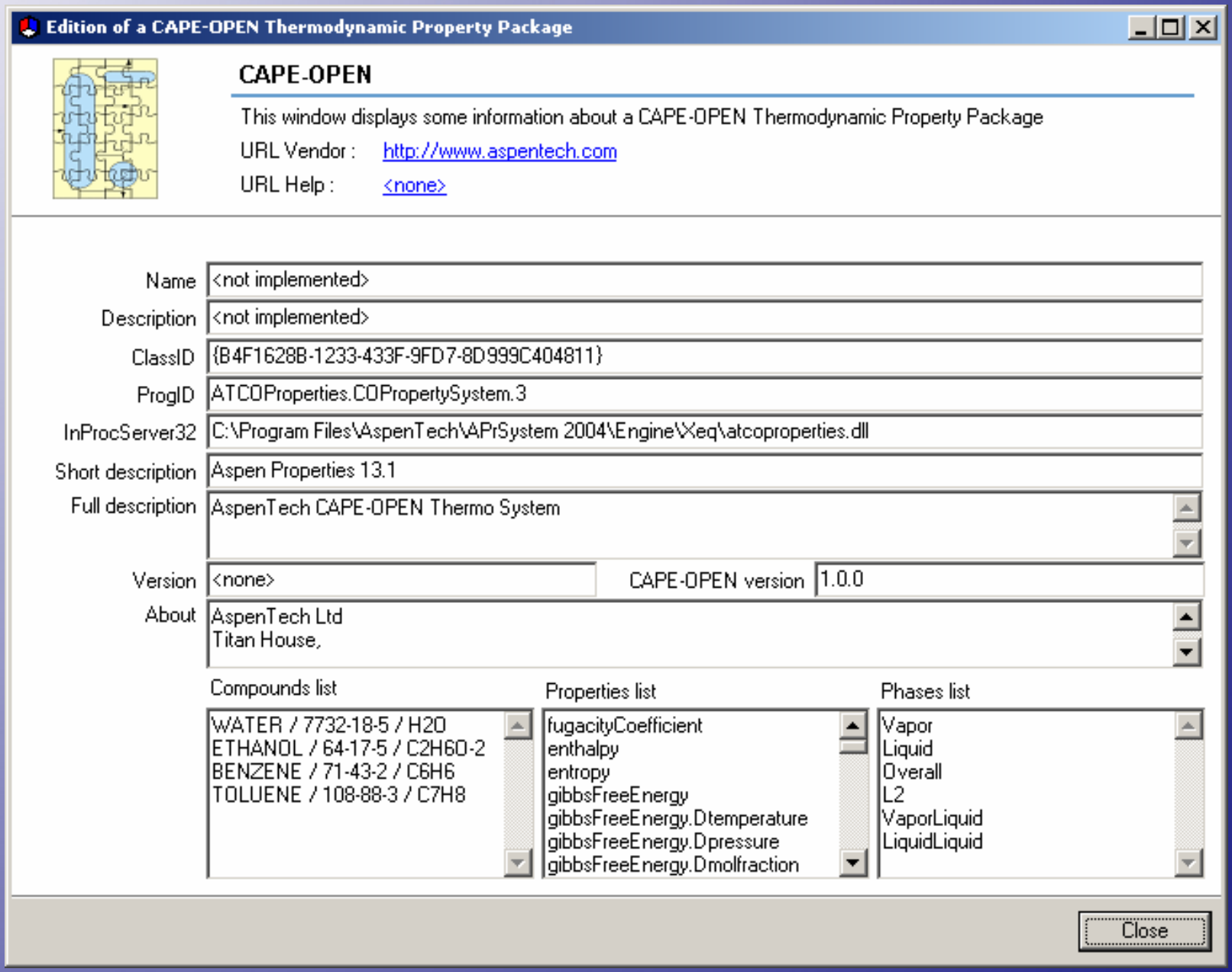




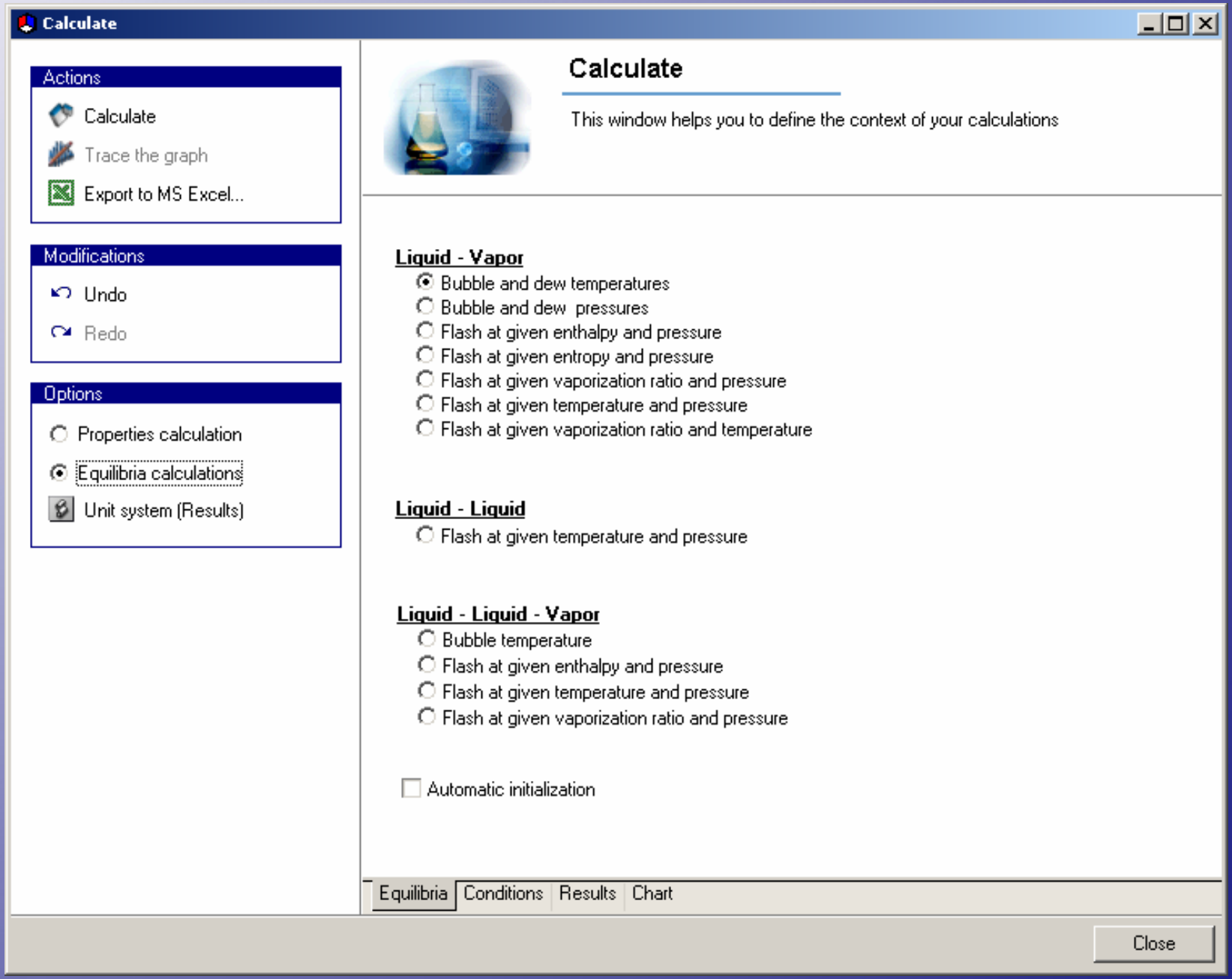
Basic information on PP displayed



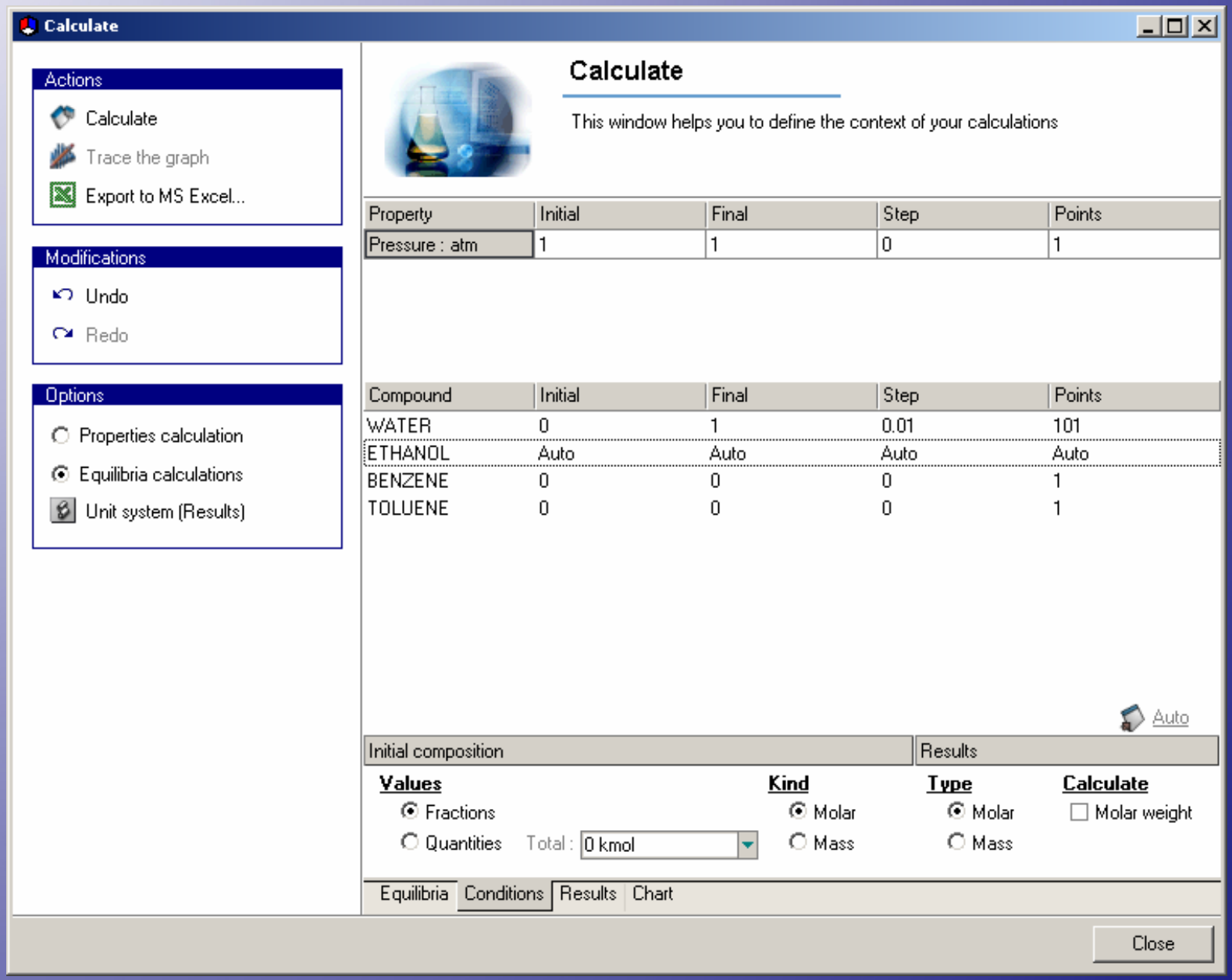
Detailed information displayed



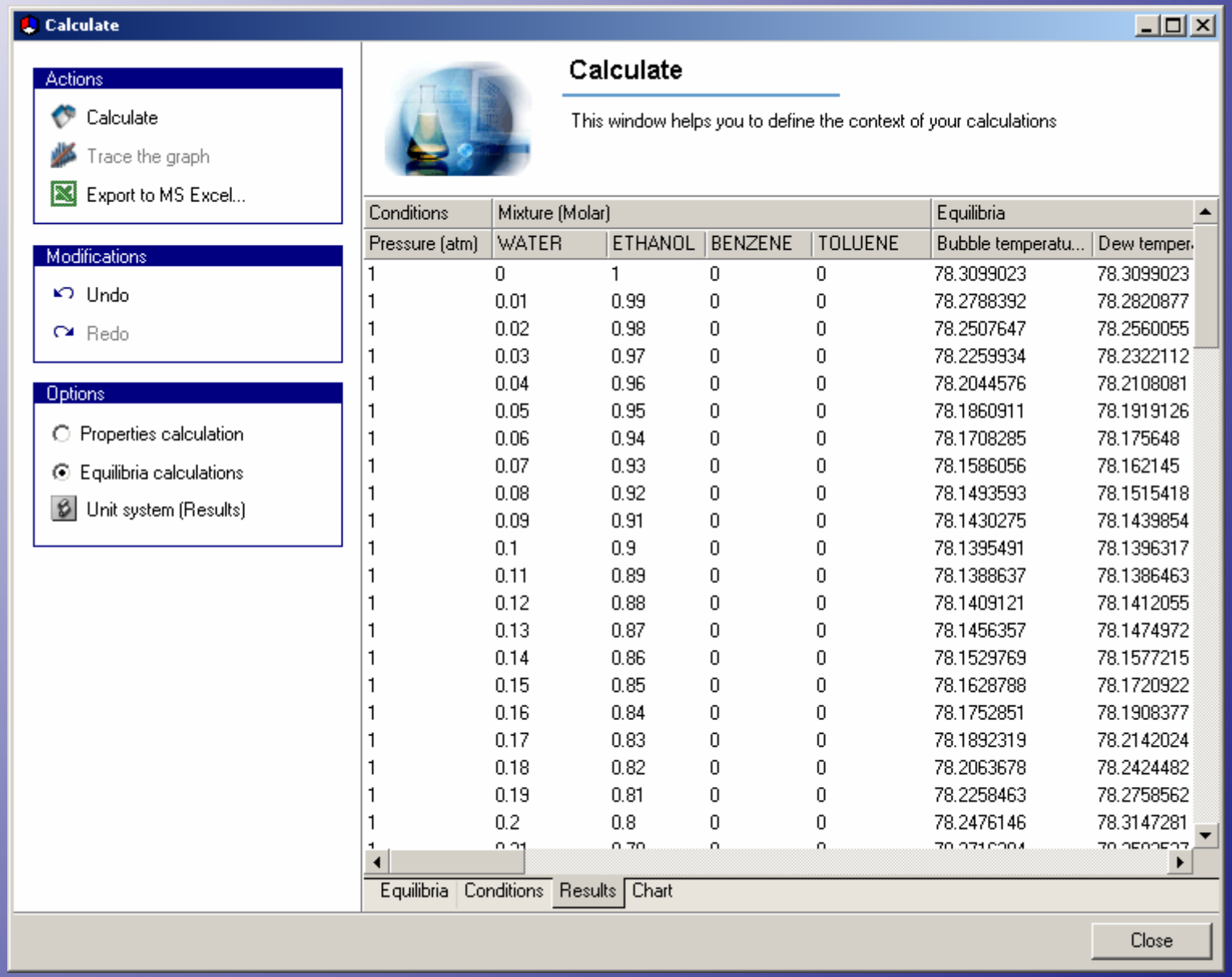
Equilibrium calculation step 1



Equilibrium calculation step 2

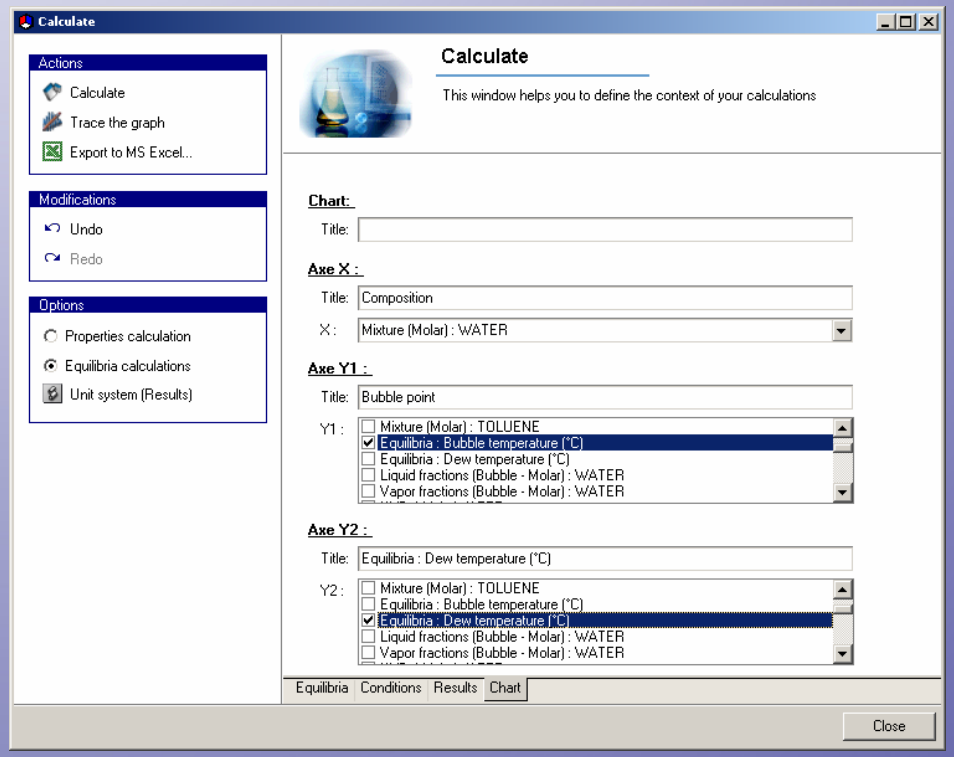


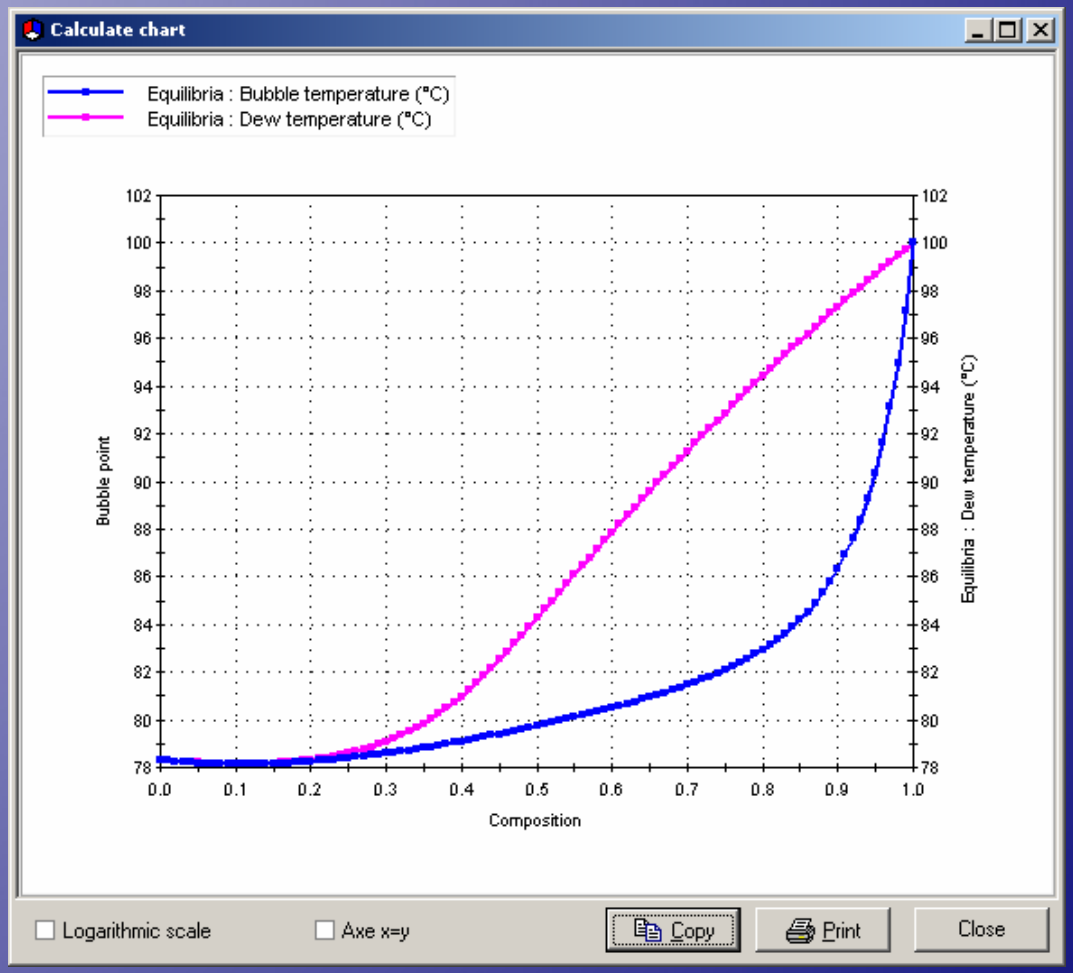
Calculation results tabulated



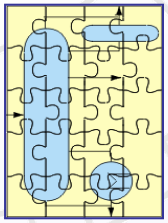
Conditions	Mixture (Molar)				Equilibria	
Pressure (atm)	WATER	ETHANOL	BENZENE	TOLUENE	Bubble temperatu...	Dew temper
1	0	1	0	0	78.3099023	78.3099023
1	0.01	0.99	0	0	78.2788392	78.2820877
1	0.02	0.98	0	0	78.2507647	78.2560055
1	0.03	0.97	0	0	78.2259934	78.2322112
1	0.04	0.96	0	0	78.2044576	78.2108081
1	0.05	0.95	0	0	78.1860911	78.1919126
1	0.06	0.94	0	0	78.1708285	78.175648
1	0.07	0.93	0	0	78.1586056	78.162145
1	0.08	0.92	0	0	78.1493593	78.1515418
1	0.09	0.91	0	0	78.1430275	78.1439854
1	0.1	0.9	0	0	78.1395491	78.1396317
1	0.11	0.89	0	0	78.1388637	78.1386463
1	0.12	0.88	0	0	78.1409121	78.1412055
1	0.13	0.87	0	0	78.1456357	78.1474972
1	0.14	0.86	0	0	78.1529769	78.1577215
1	0.15	0.85	0	0	78.1628788	78.1720922
1	0.16	0.84	0	0	78.1752851	78.1908377
1	0.17	0.83	0	0	78.1892319	78.2142024
1	0.18	0.82	0	0	78.2063678	78.2424482
1	0.19	0.81	0	0	78.2258463	78.2758562
1	0.2	0.8	0	0	78.2476146	78.3147281

Calculation results chart



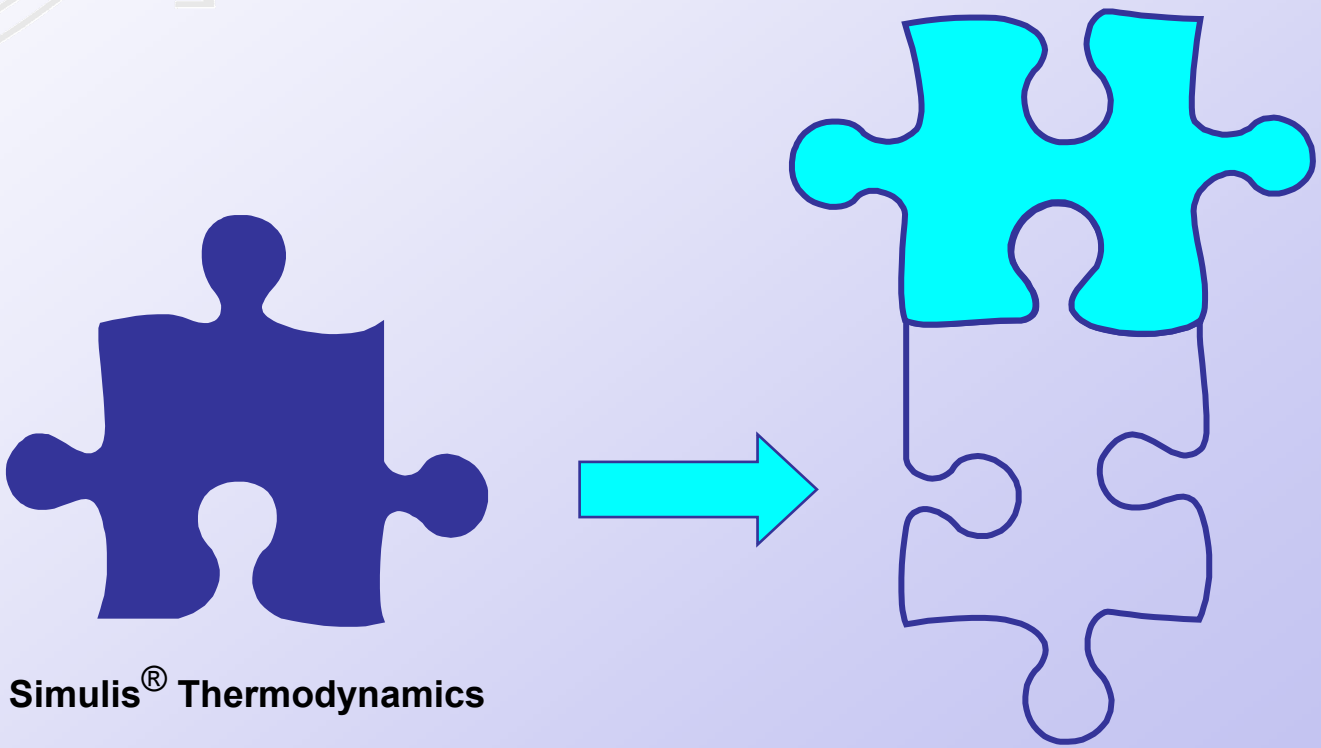


Simulis® Thermodynamics and CAPE-OPEN



- **CAPE-OPEN «thermodynamic plug»…**

Aspen Plus, PRO/II, gPROMS, …



Simulis® Thermodynamics and CAPE-OPEN

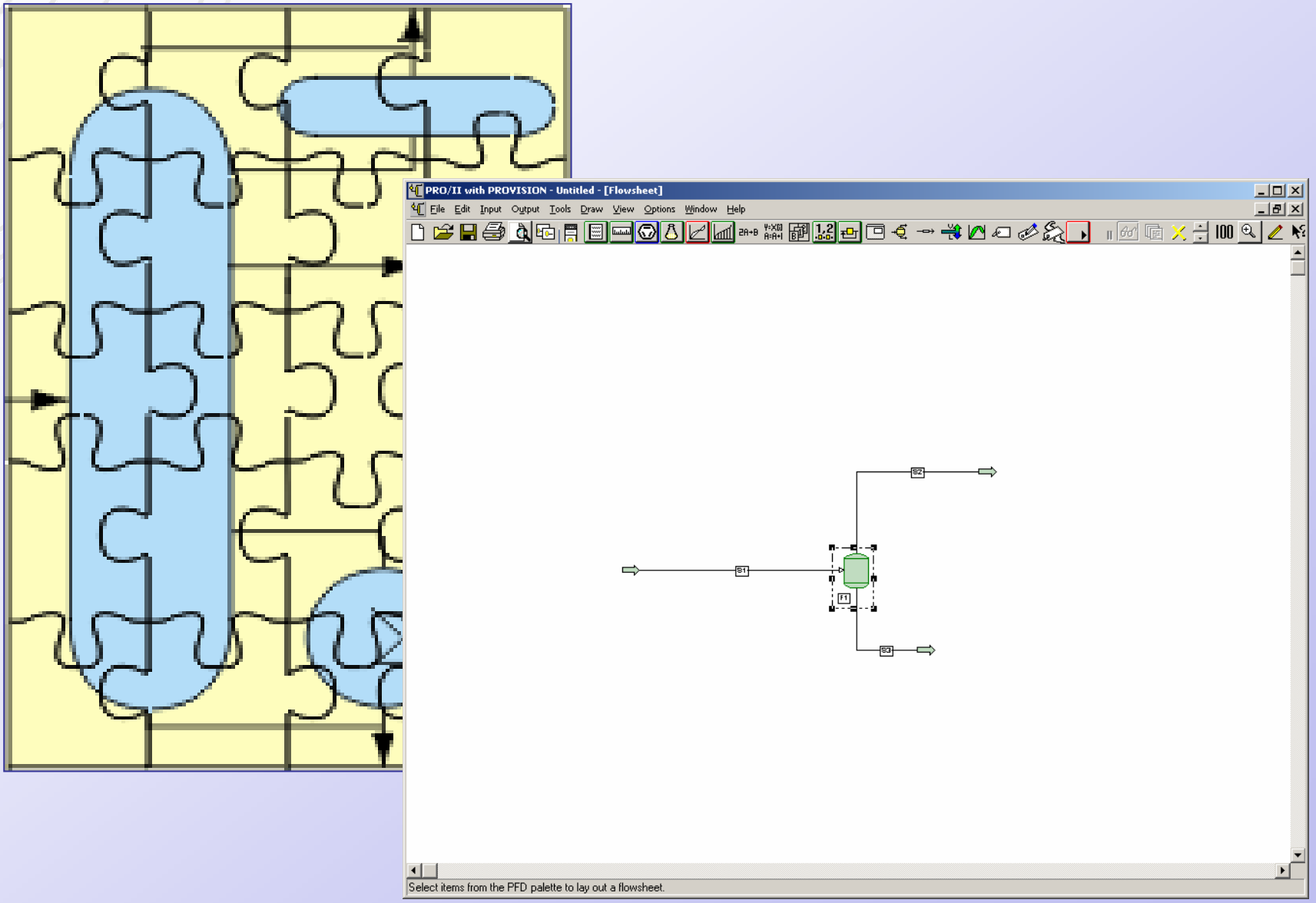
- **CAPE-OPEN Thermodynamic plug**

… already successfully tested in:

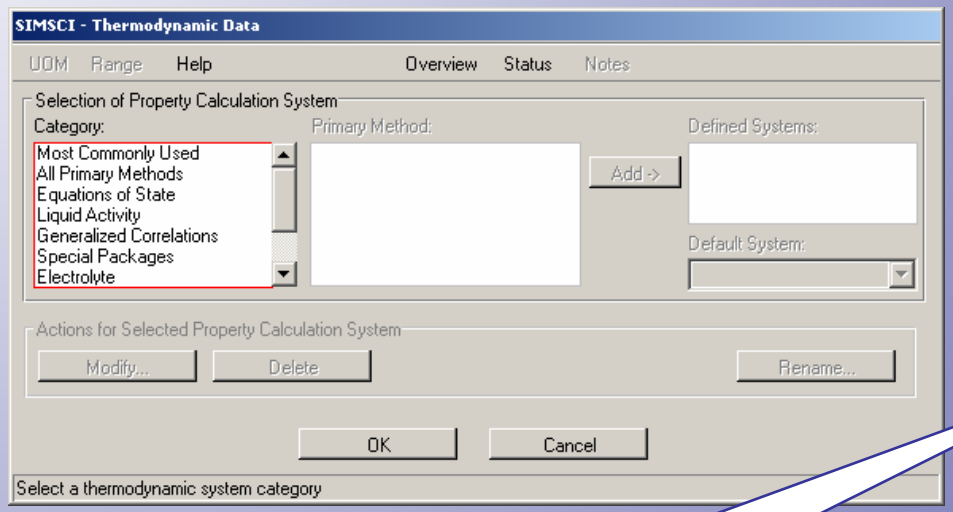
- Aspen Plus 2004 and 12.1 (AspenTech)
- Hysys 2004 and 3.2 (AspenTech)
- PRO/II 7.1 (SimSci)
- gPROMS 3.0 (Process Systems Enterprise)
- XIST (HTRI)
- VALI (BelSim)

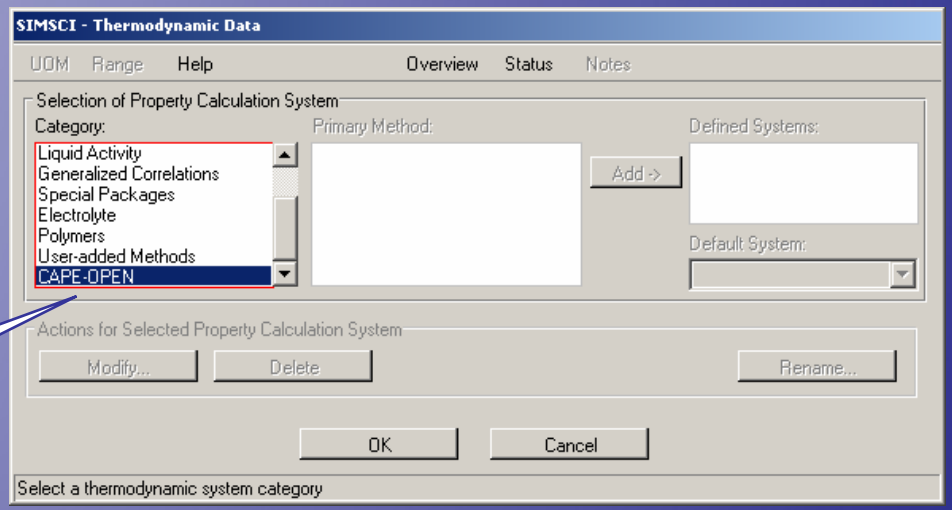
SimuLis

CAPE-OPEN demonstration



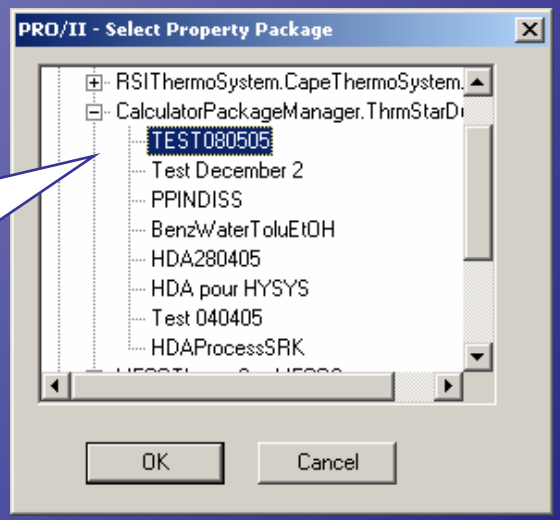
Select SIMULIS PP in PRO/II



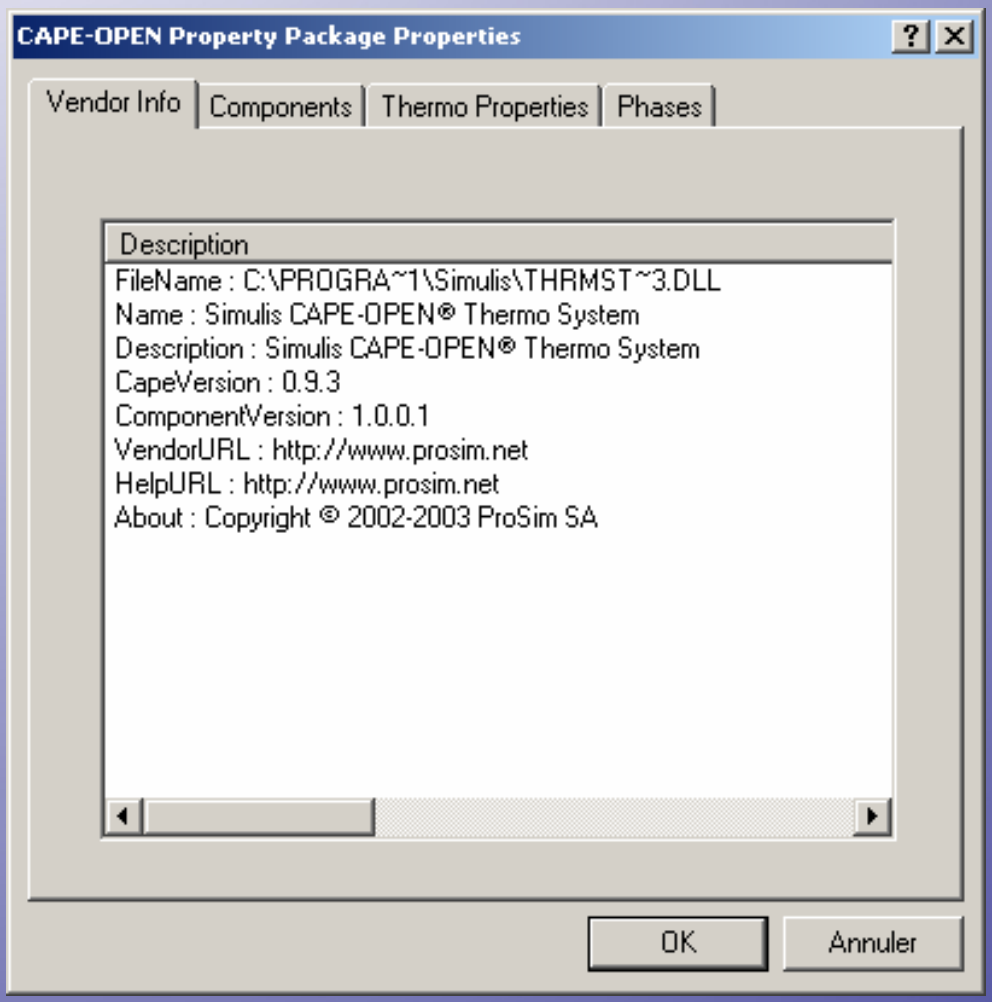


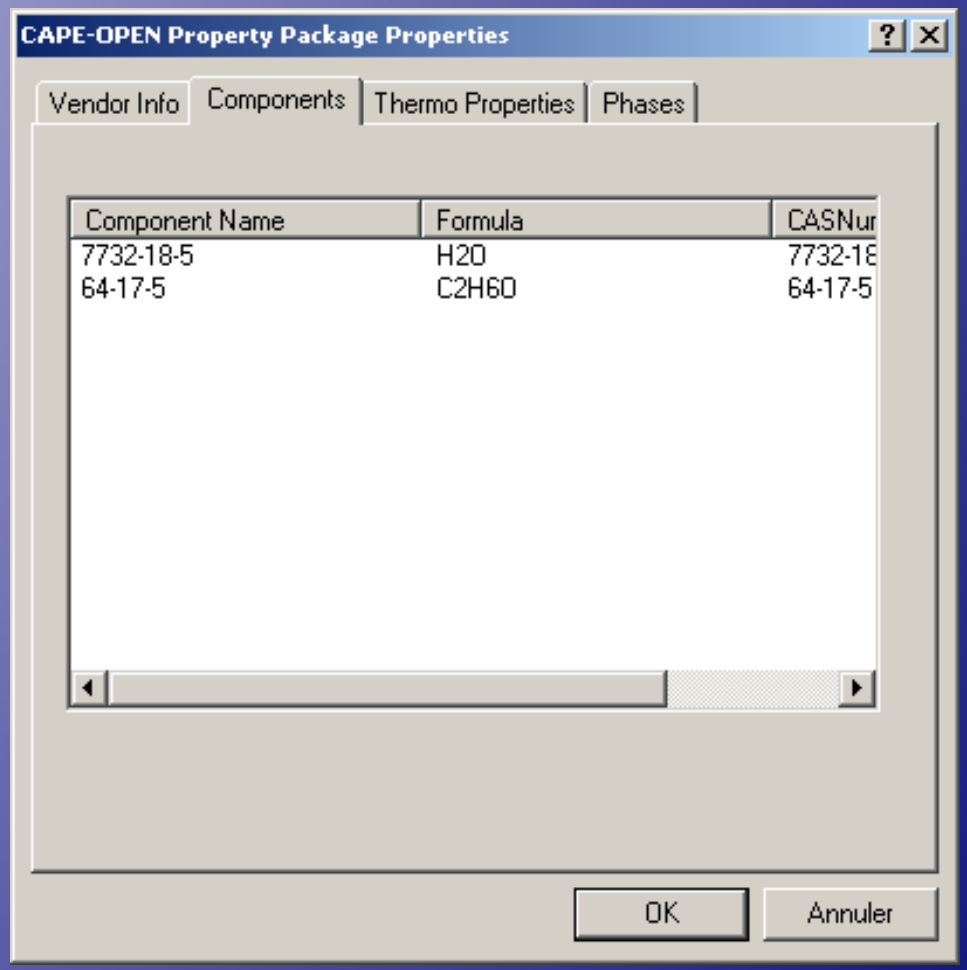
Choose CAPE-OPEN PPs from the list

Select SIMULIS Thermo System and PP

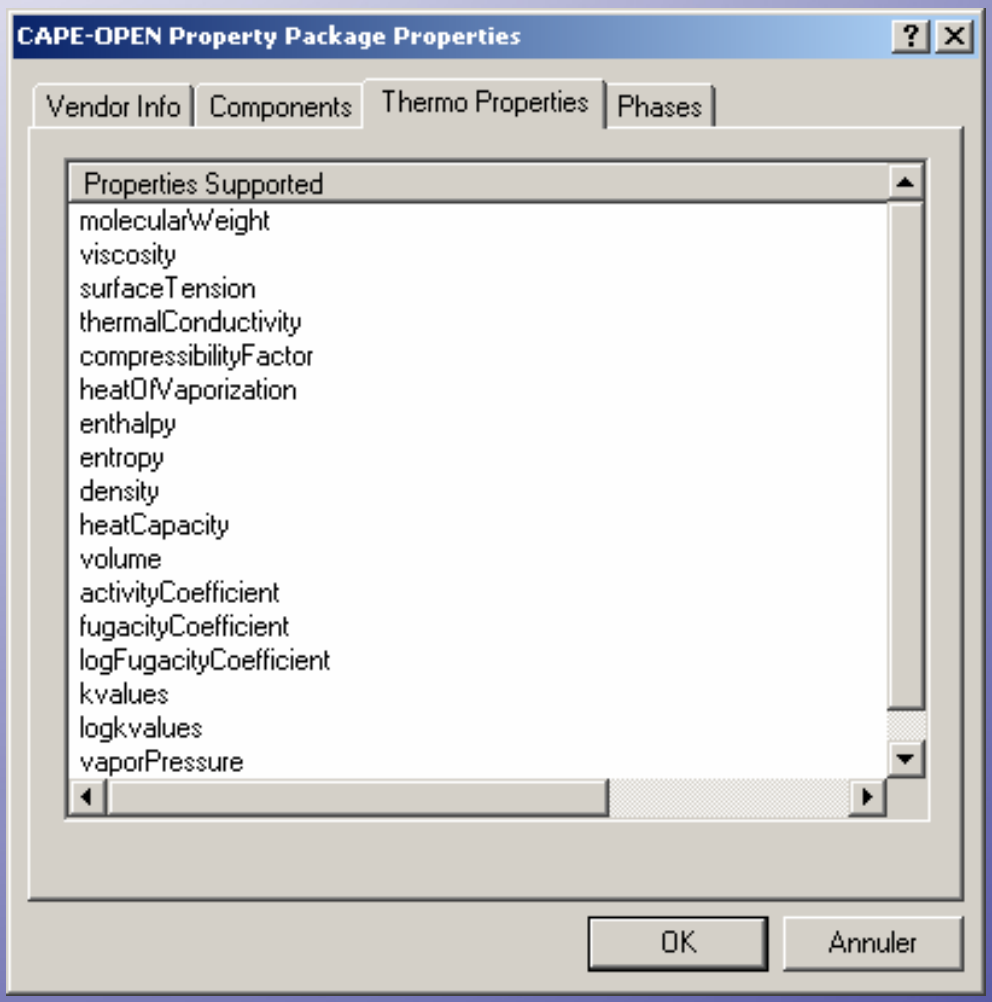


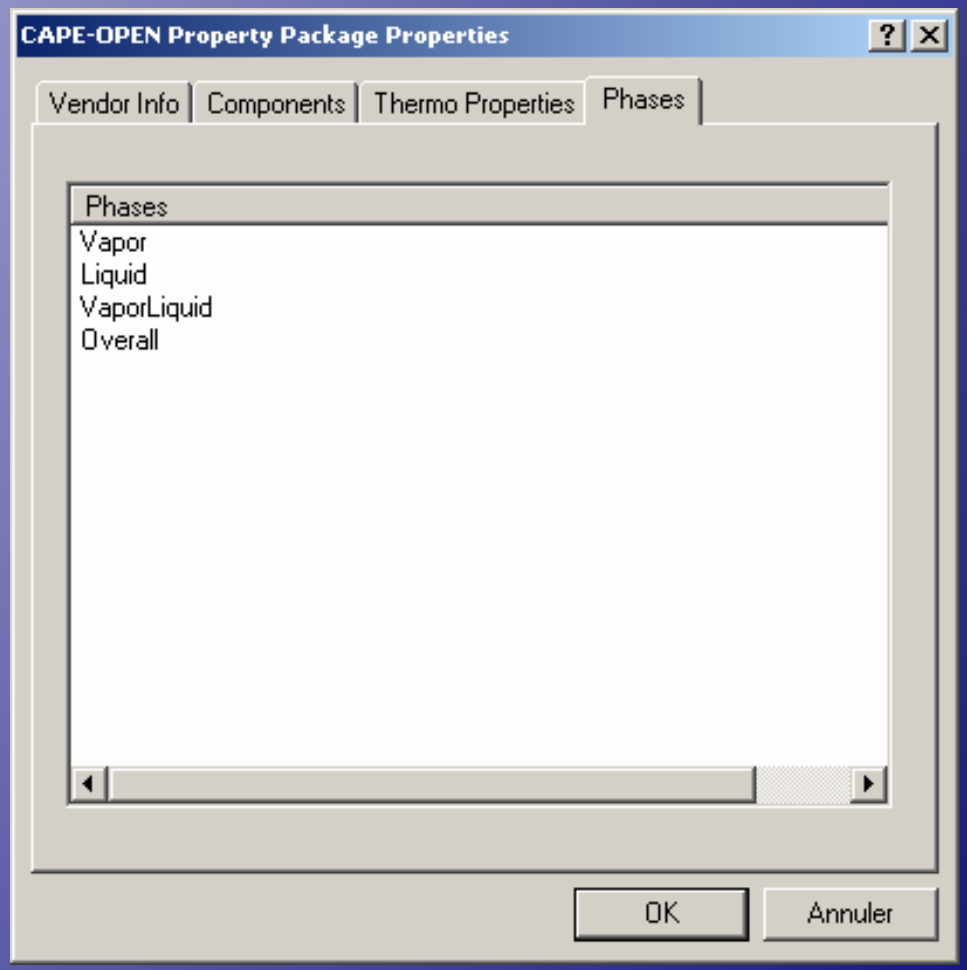
Browse through PP details



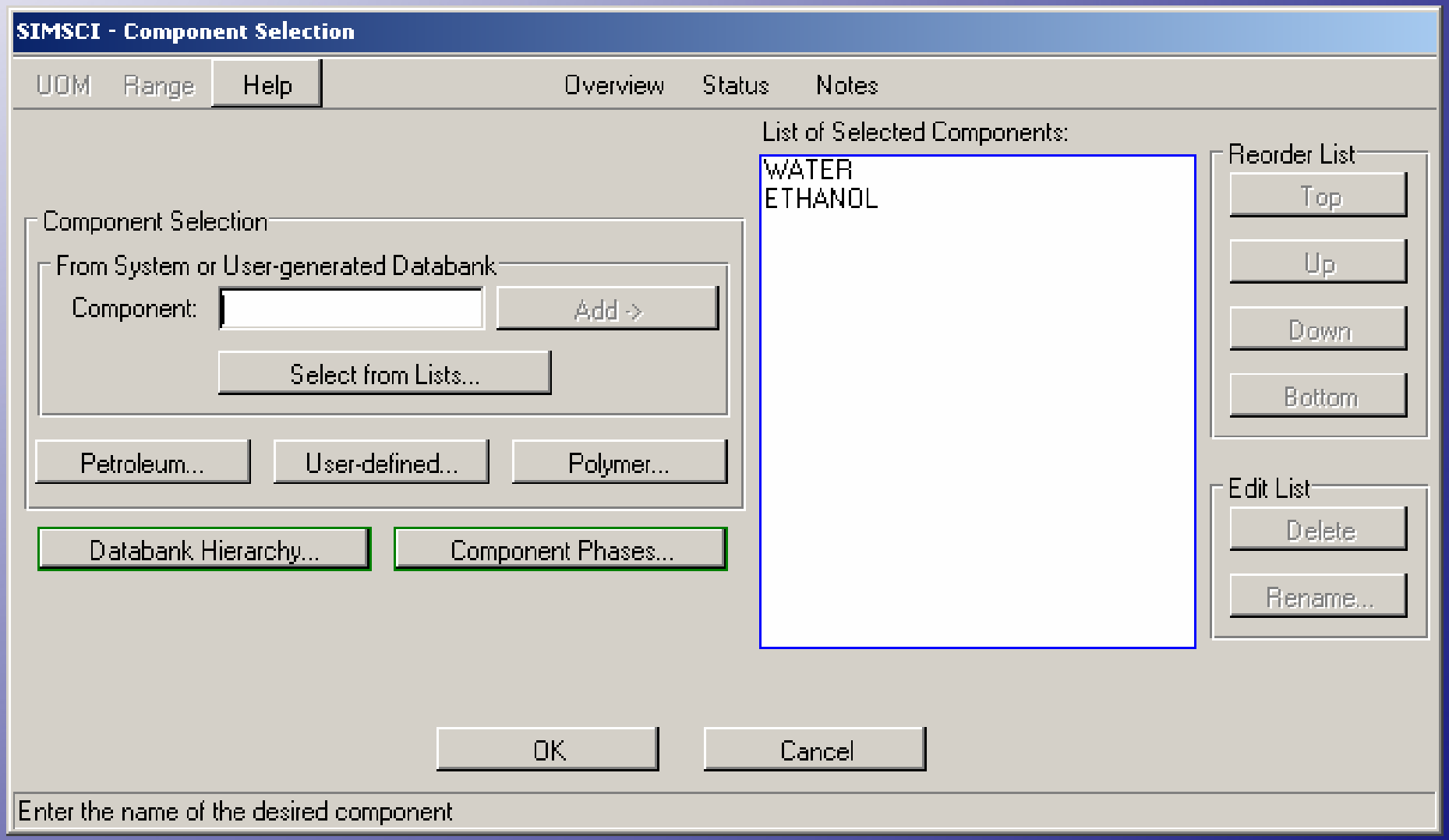


List Properties and Phases

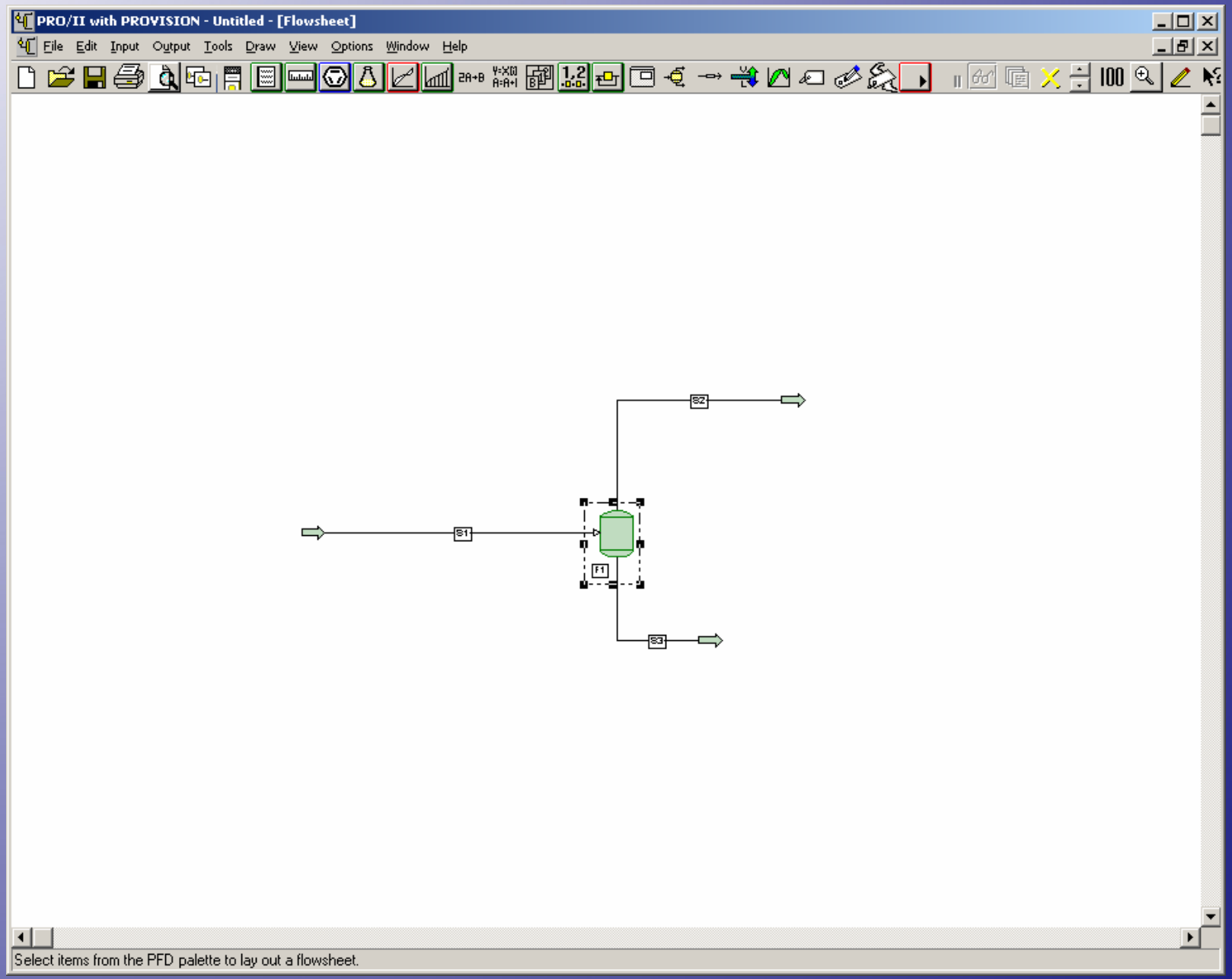




Define compound list



Set up process model



Define inlet stream

Stream Data - Flowrate and Composition

UOM Range Help Tag

Specify flowrate and composition for stream S1

Fluid Flowrate Specification

- (•) Total Fluid Flowrate: 100.00 kg-mol/hr
- ( ) Individual Component Flowrates

Copy Paste

Component	Composition Mole
WATER	0.90000
ETHANOL	0.10000

Clear Compositions Total: 1.0000 [ ] Normalize Component Flowrates Based on Specified Fluid Flowrate

OK Cancel

Push to clear all component composition data

PRO/II - Stream Data

UOM Range Help Tag Overview Status Notes

Stream: S1 Description:

To Unit: F1

Stream Type

- Composition Defined
- Petroleum Assay
- Referenced to Stream
- Solids Only Stream

Flowrate and Composition... | Stream Solids Data... | Stream Polymer Data...

Thermal Condition

First Specification: Temperature 25.00 C

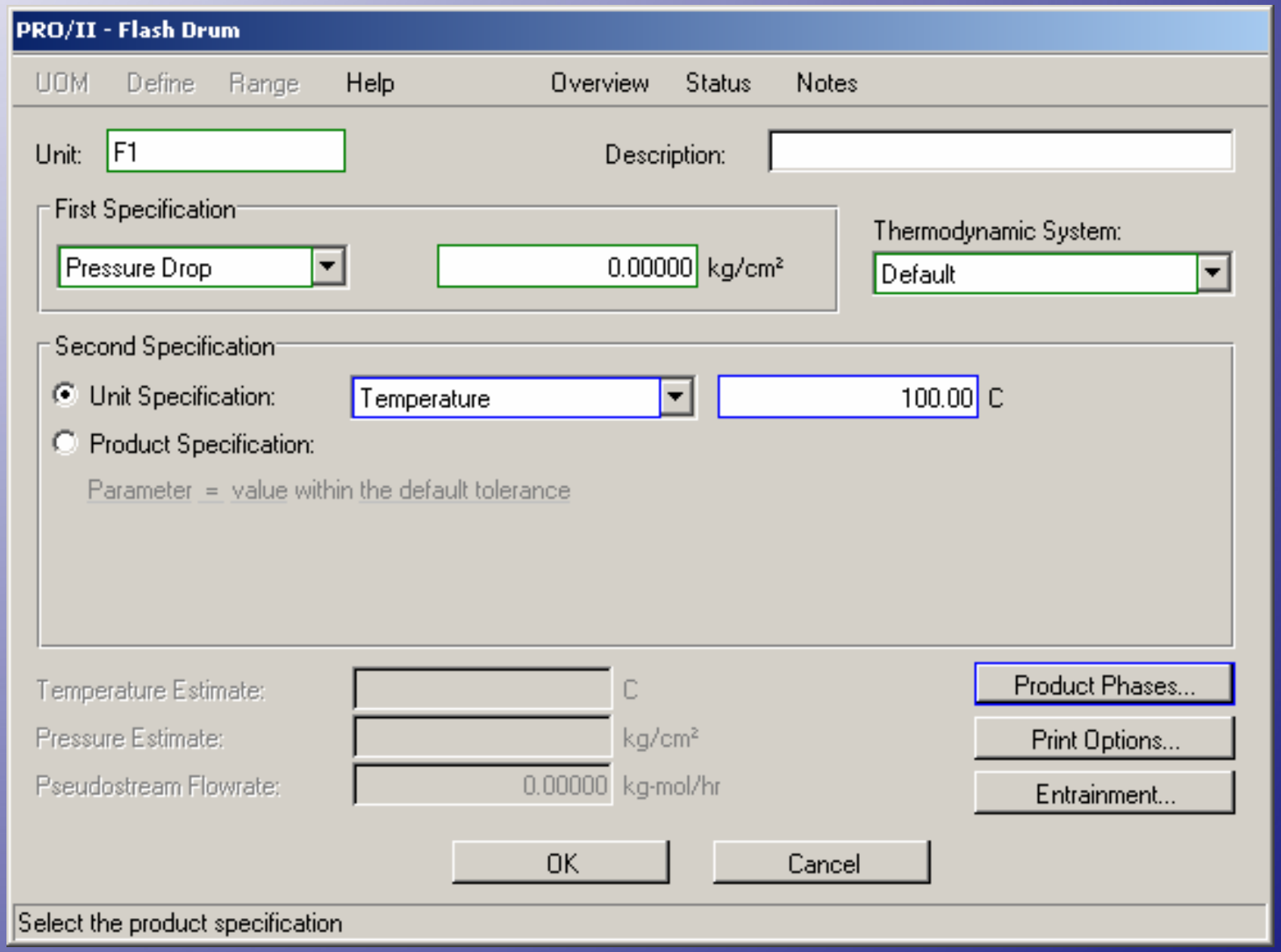
Second Specification: Pressure 1.0000 kg/cm²

Thermodynamic System: Determined From Connectivity

OK Cancel

Select the thermodynamic system

Specify flash parameter



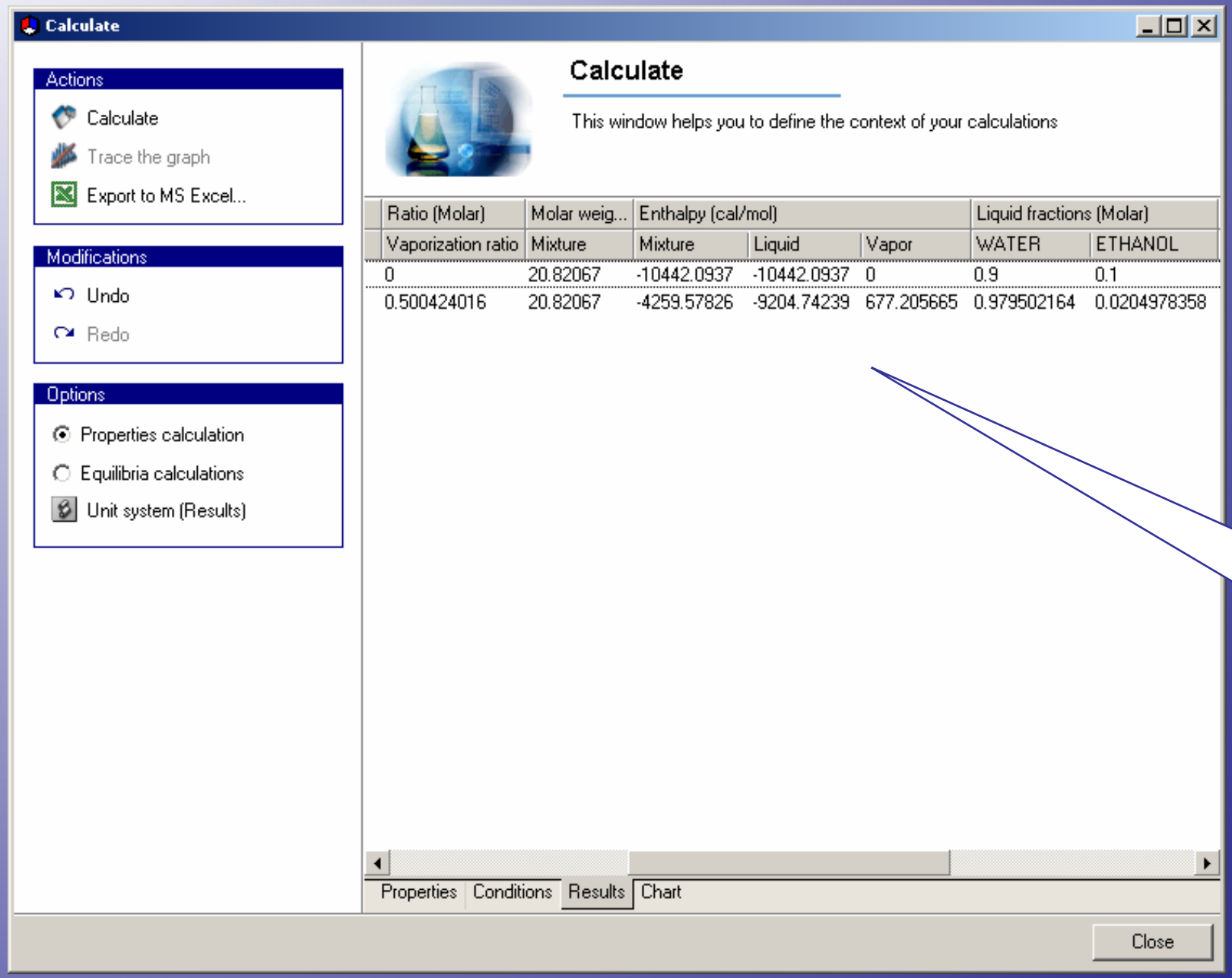
Excerpt of PRO/II input file

```
TITLE
  DIMENSION METRIC, STDTEMP=0, STDPRES=1.03323
  SEQUENCE SIMSCI
  CALCULATION RVPBASIS=APIN, TVP=37.778
COMPONENT DATA
  LIBID 1,WATER/2,ETHANOL, BANK=PROCESS,SIMSCI
THERMODYNAMIC DATA
  METHOD SYSTEM=CO, PID=CalculatorPackageManager.ThrmStarDustPK, &
        PNAME=TEST080505, SET=CO01, DEFAULT
STREAM DATA
  PROPERTY STREAM=S1, TEMPERATURE=25, PRESSURE=1, PHASE=M, &
        RATE(M)=100, COMPOSITION(M)=1,0.9/2,0.1
UNIT OPERATIONS
  FLASH UID=F1
     FEED S1
     PRODUCT  V=S2, W=S3
     ISO  TEMPERATURE=95.1
END
```

PRO/II results

STREAM ID	S1	S2	S3
NAME			
PHASE	LIQUID	VAPOR	LIQUID
FLUID RATES, KG-MOL/HR			
1 WATER	90.0000	41.0664	48.9336
2 ETHANOL	10.0000	8.9760	1.0240
TOTAL RATE, KG-MOL/HR	100.0000	50.0424	49.9576
TEMPERATURE, C	25.0000	95.1000	95.1000
PRESSURE, ATM	1.0000	1.0000	1.0000
ENTHALPY, M*KCAL/HR	-1.0435	0.0339	-0.4595
MOLECULAR WEIGHT	20.8205	23.0472	18.5901
MOLE FRAC VAPOR	0.0000	1.0000	0.0000
MOLE FRAC LIQUID	1.0000	0.0000	1.0000

Verify results in SIMULIS



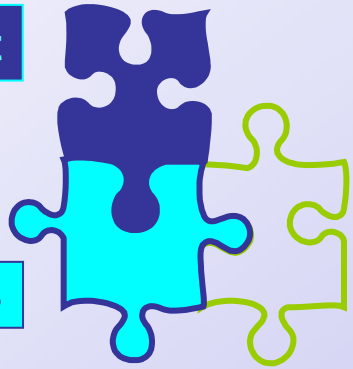
Same vapor ratio, molar weight and enthalpies

Simulis® Thermodynamics follows you in your applications

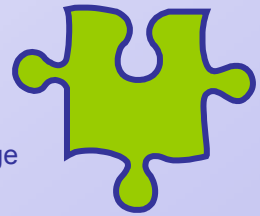
Properties and equilibrium calculations

Client requirement

Simulis® Thermodynamics



CAPE-OPEN Property Package

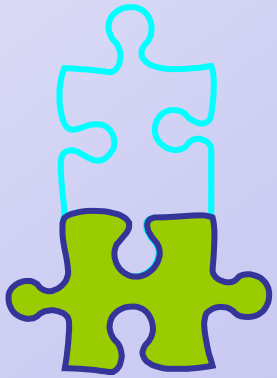


Aspen Properties, PPDS, …

Simulis Package

CAPE-OPEN Property Package

Data and results consistency between the different tools…



Aspen Plus, PRO/II, gPROMS, …

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Thanks you for your attention.

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