Interoperability between Modelling Tools (MoT) and Process Simulators (ProSim) through CAPE-OPEN Standards

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06AIChE Annual Meeting, San Francisco, CA

Outline

- Objective
- Computer Aided Process Engineering Tools
  - MoT
  - ProSim & CO Interface (SIMULIS & Wrapper)
- Integration of MoT-ProSim
- Case Study
  - Thermo-Interface (External-Model:PC-SAFT)
  - Unit-Interface (Model:Short-Path Evaporator)
- Conclusions

Objective

Highlight aspects of interoperability of software tools through the application of Computer-Aided Modelling tools (for generation and use of Modelling Objects) in CAPE-OPEN compliant process simulators

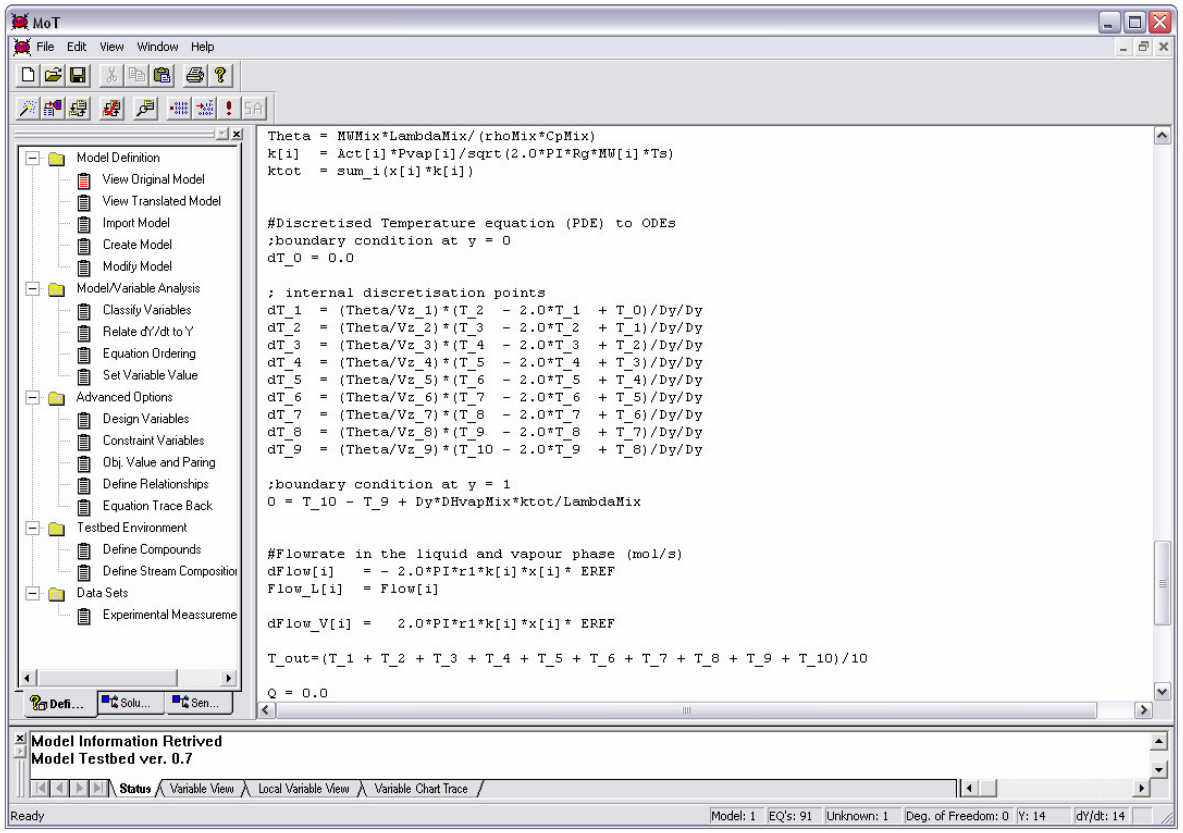
more specifically, uses of CO- interfaces for thermo-models and unit operations are demonstrated

Computer Aided Process Engineering Tools

1. MoT

2. ProSim
   - Simulis thermodynamics
   - CO-wrapper
   - ProSimPlus

1. MoT


MoT
File Edit View Window Help
Model Definition
View Original Model
View Translated Model
Import Model
Create Model
Modify Model
Model/Variable Analysis
Classify Variables
Relate dY/dt to Y
Equation Ordering
Set Variable Value
Advanced Options
Design Variables
Constraint Variables
Obj. Value and Paring
Define Relationships
Equation Trace Back
Testbed Environment
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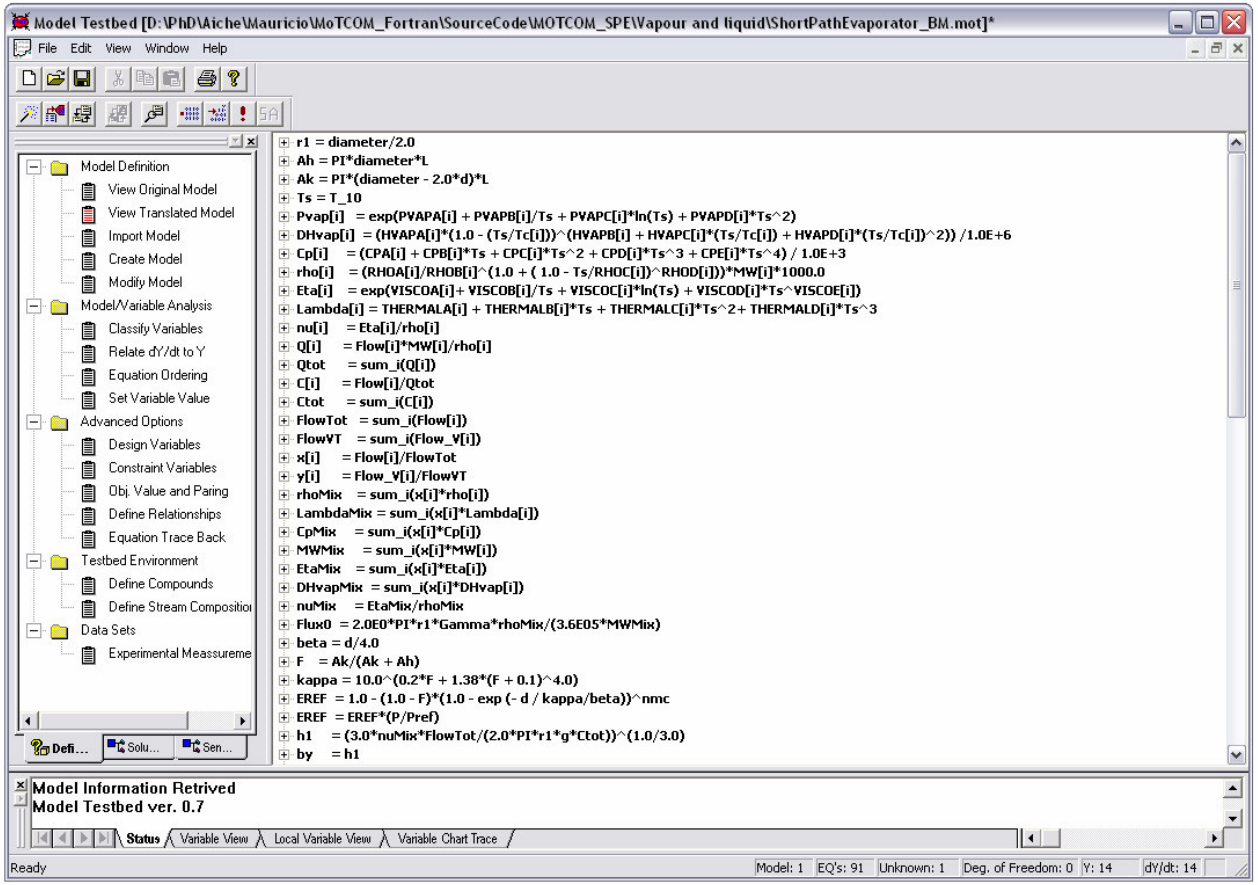
Data Sets
Experimental Meassureme
Theta = MWMix*LambdaMix/(rhoMix*CpMix)
k[i] = Act[i]*Pvap[i]/sqrt(2.0*PI*Rg*MW[i]*Ts)
ktot = sum_i(x[i]*k[i])
#Discretised Temperature equation (PDE) to ODEs
;boundary condition at y = 0
dT_0 = 0.0
; internal discretisation points
dT_1 = (Theta/Vz_1)*(T_2 - 2.0*T_1 + T_0)/Dy/Dy
dT_2 = (Theta/Vz_2)*(T_3 - 2.0*T_2 + T_1)/Dy/Dy
dT_3 = (Theta/Vz_3)*(T_4 - 2.0*T_3 + T_2)/Dy/Dy
dT_4 = (Theta/Vz_4)*(T_5 - 2.0*T_4 + T_3)/Dy/Dy
dT_5 = (Theta/Vz_5)*(T_6 - 2.0*T_5 + T_4)/Dy/Dy
dT_6 = (Theta/Vz_6)*(T_7 - 2.0*T_6 + T_5)/Dy/Dy
dT_7 = (Theta/Vz_7)*(T_8 - 2.0*T_7 + T_6)/Dy/Dy
dT_8 = (Theta/Vz_8)*(T_9 - 2.0*T_8 + T_7)/Dy/Dy
dT_9 = (Theta/Vz_9)*(T_10 - 2.0*T_9 + T_8)/Dy/Dy
;boundary condition at y = 1
0 = T_10 - T_9 + Dy*DHvapMix*ktot/LambdaMix
#Flowrate in the liquid and vapour phase (mol/s)
dFlow[i] = - 2.0*PI*r1*k[i]*x[i]* EREF
Flow_L[i] = Flow[i]
dFlow_V[i] = 2.0*PI*r1*k[i]*x[i]* EREF
T_out=(T_1 + T_2 + T_3 + T_4 + T_5 + T_6 + T_7 + T_8 + T_9 + T_10)/10
Q = 0.0
Model Information Retrived
Model Testbed ver. 0.7
Status
Variable View
Local Variable View
Variable Chart Trace
Ready
Model: 1
EQ's: 91
Unknown: 1
Deg. of Freedom: 0
Y: 14
dY/dt: 14

1. MoT


Model Testbed [D:\PhD\Aiche\Mauricio\MoTCOM_Fortran\SourceCode\MOTCOM_SPE\Vapour and liquid\ShortPathEvaporator_BM.mot]*
File Edit View Window Help
Model Definition
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Data Sets
Experimental Meassureme
r1 = diameter/2.0
Ah = PI*diameter*L
Ak = PI*(diameter - 2.0*d)*L
Ts = T_10
Pvap[i] = exp(PVAPA[i] + PVAPB[i]/Ts + PVAPC[i]*ln(Ts) + PVAPD[i]*Ts^2)
DHvap[i] = (HVAPA[i]*(1.0 - (Ts/Tc[i]))^(HVAPB[i] + HVAPC[i]*(Ts/Tc[i]) + HVAPD[i]*(Ts/Tc[i])^2)) /1.0E+6
Cp[i] = (CPA[i] + CPB[i]*Ts + CPC[i]*Ts^2 + CPD[i]*Ts^3 + CPE[i]*Ts^4) / 1.0E+3
rho[i] = (RHOA[i]/RHOB[i]^(1.0 + (1.0 - Ts/RHOC[i])^RHOD[i]))*MW[i]*1000.0
Eta[i] = exp(VISCOA[i]+ VISCOB[i]/Ts + VISCOC[i]*ln(Ts) + VISCOD[i]*Ts^VISCOE[i])
Lambda[i] = THERMALA[i] + THERMALB[i]*Ts + THERMALC[i]*Ts^2+ THERMALD[i]*Ts^3
nu[i] = Eta[i]/rho[i]
Q[i] = Flow[i]*MW[i]/rho[i]
Qtot = sum_i(Q[i])
C[i] = Flow[i]/Qtot
Ctot = sum_i(C[i])
FlowTot = sum_i(Flow[i])
FlowVT = sum_i(Flow_V[i])
x[i] = Flow[i]/FlowTot
y[i] = Flow_V[i]/FlowVT
rhoMix = sum_i(x[i]*rho[i])
LambdaMix = sum_i(x[i]*Lambda[i])
CpMix = sum_i(x[i]*Cp[i])
MWMix = sum_i(x[i]*MW[i])
EtaMix = sum_i(x[i]*Eta[i])
DHvapMix = sum_i(x[i]*DHvap[i])
nuMix = EtaMix/rhoMix
Flux0 = 2.0E0*PI*r1*Gamma*rhoMix/(3.6E05*MWMix)
beta = d/4.0
F = Ak/(Ak + Ah)
kappa = 10.0^(0.2*F + 1.38*(F + 0.1)^4.0)
EREF = 1.0 - (1.0 - F)*(1.0 - exp (- d / kappa/beta))^nmc
EREF = EREF*(P/Pref)
h1 = (3.0*nuMix*FlowTot/(2.0*PI*r1*g*Ctot))^(1.0/3.0)
by = h1
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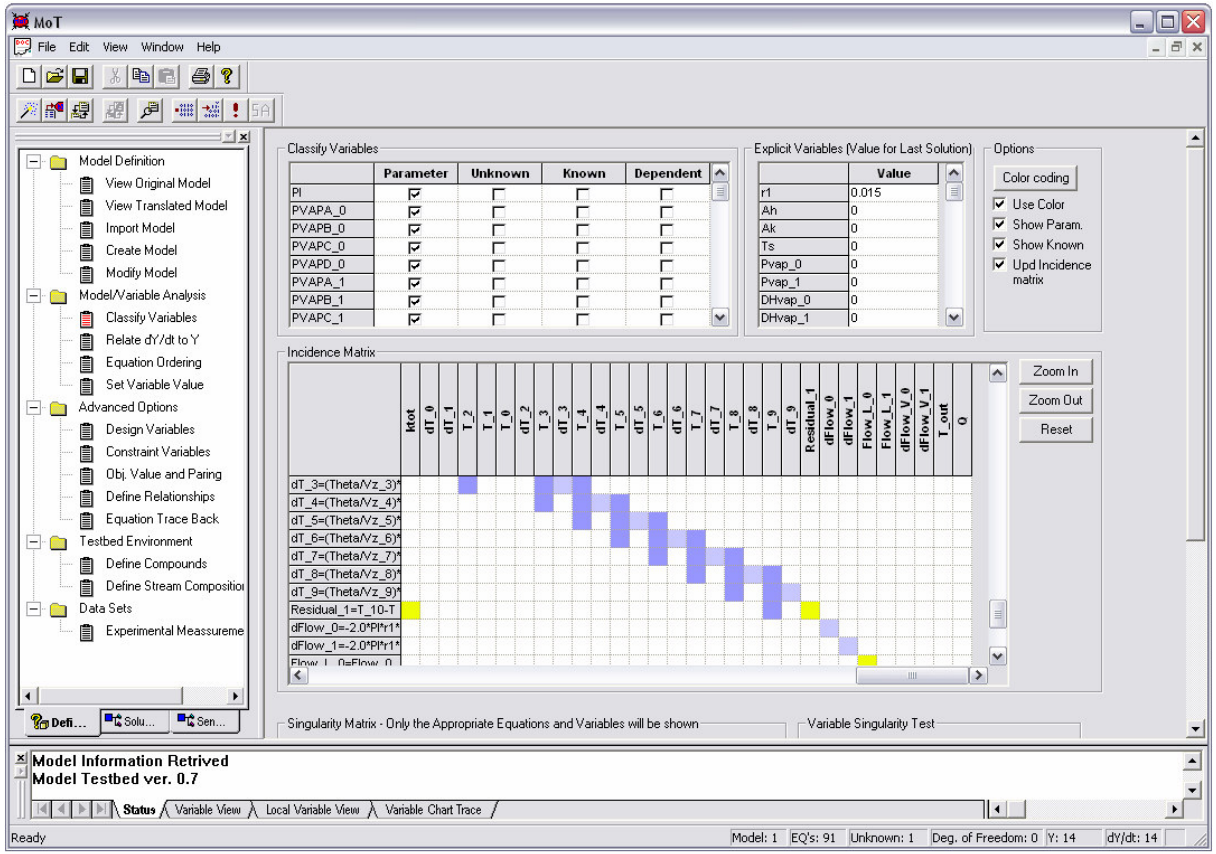
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Data Sets
Experimental Meassureme
Classify Variables
Parameter
Unknown
Known
Dependent
PI
PVAPA_0
PVAPB_0
PVAPC_0
PVAPD_0
PVAPA_1
PVAPB_1
PVAPC_1
Explicit Variables (Value for Last Solution)
Value
r1 0.015
Ah 0
Ak 0
Ts 0
Pvap_0 0
Pvap_1 0
DHvap_0 0
DHvap_1 0
Options
Color coding
Use Color
Show Param.
Show Known
Upd Incidence matrix
Incidence Matrix
Zoom In
Zoom Out
Reset
Singularity Matrix - Only the Appropriate Equations and Variables will be shown
Variable Singularity Test
Model Information Retrived
Model Testbed ver. 0.7
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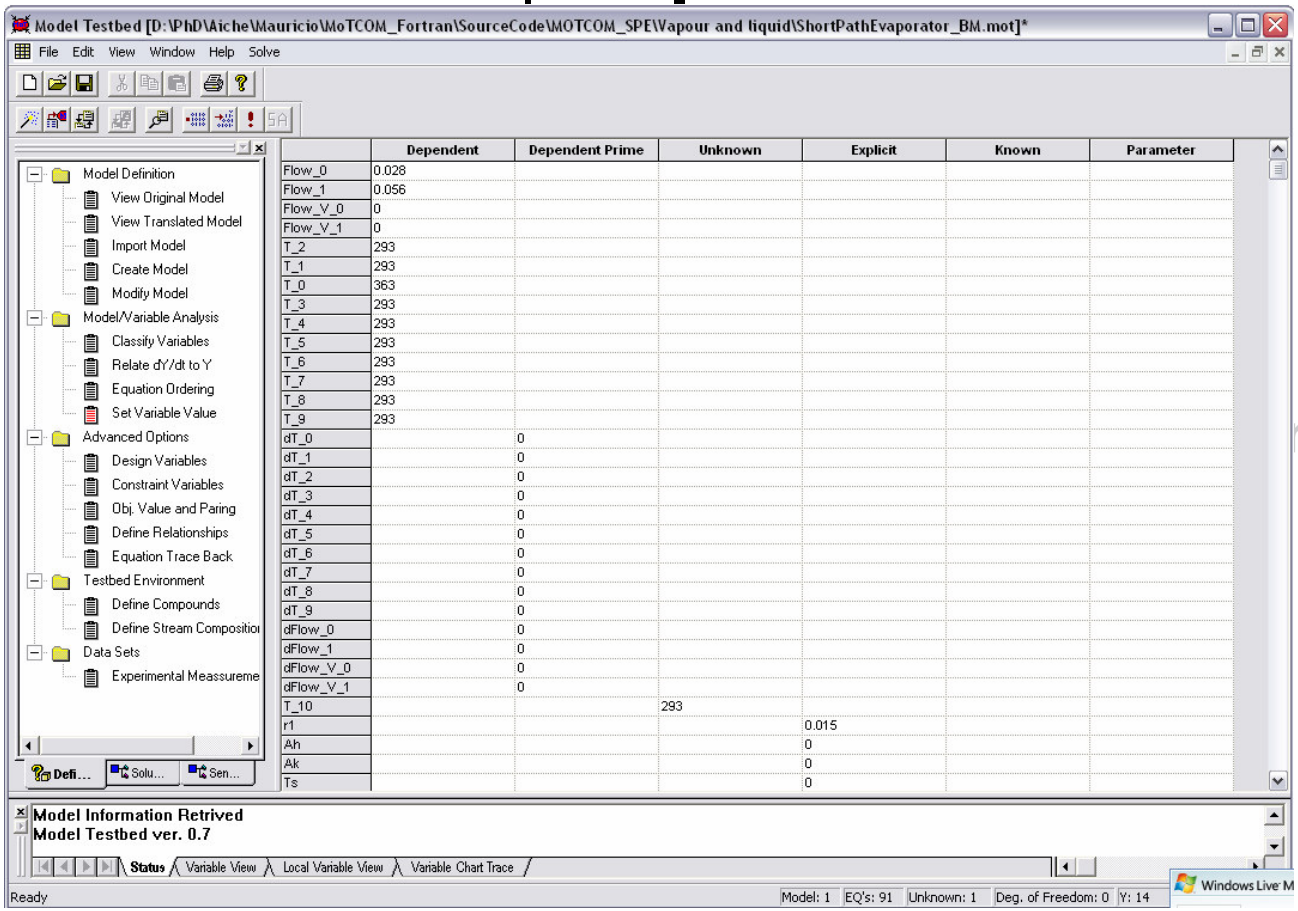
Model Testbed [D:\PhD\Aiche\Mauricio\MoTCOM_Fortran\SourceCode\MOTCOM_SPE\Vapour and liquid\ShortPathEvaporator_BM.mot]*
File Edit View Window Help Solve
Model Definition
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Data Sets
Experimental Meassureme
Defi...
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Dependent
Dependent Prime
Unknown
Explicit
Known
Parameter
Flow_0 0.028
Flow_1 0.056
Flow_V_0 0
Flow_V_1 0
T_2 293
T_1 293
T_0 363
T_3 293
T_4 293
T_5 293
T_6 293
T_7 293
T_8 293
T_9 293
dT_0 0
dT_1 0
dT_2 0
dT_3 0
dT_4 0
dT_5 0
dT_6 0
dT_7 0
dT_8 0
dT_9 0
dFlow_0 0
dFlow_1 0
dFlow_V_0 0
dFlow_V_1 0
T_10 293
r1 0.015
Ah 0
Ak 0
Ts 0
Model Information Retrived
Model Testbed ver. 0.7
Status
Variable View
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Ready
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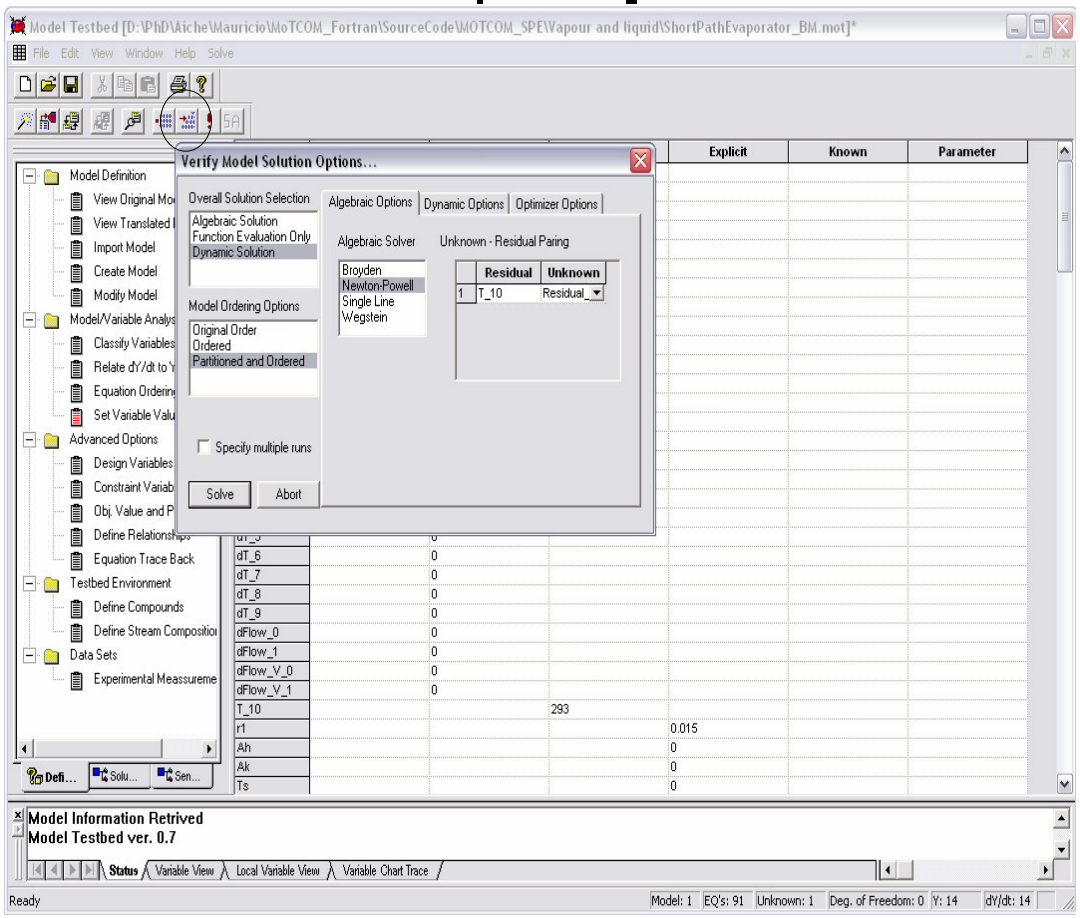
1. MoT


Model Testbed [D:\PhD\Aiche\Mauricio\MoTCOM_Fortran\SourceCode\MOTCOM_SPE\Vapour and liquid\ShortPathEvaporator_BM.mot]*
File Edit View Window Help Solve
Verify Model Solution Options...
Overall Solution Selection
Algebraic Solution
Function Evaluation Only
Dynamic Solution
Model Ordering Options
Original Order
Ordered
Partitioned and Ordered
Specify multiple runs
Solve
Abort
Algebraic Options
Dynamic Options
Optimizer Options
Algebraic Solver
Broyden
Newton-Powell
Single Line
Wegstein
Unknown - Residual Paring
Residual
Unknown
T_10
Residual_
Explicit
Known
Parameter
Model Definition
Model/Variable Analys
Advanced Options
Testbed Environment
Define Compounds
Data Sets
Equation Trace Back
dT_6
dT_7
dT_8
dT_9
dFlow_0
dFlow_1
dFlow_V_0
dFlow_V_1
T_10
r1
Ah
Ak
Ts
293
0.015
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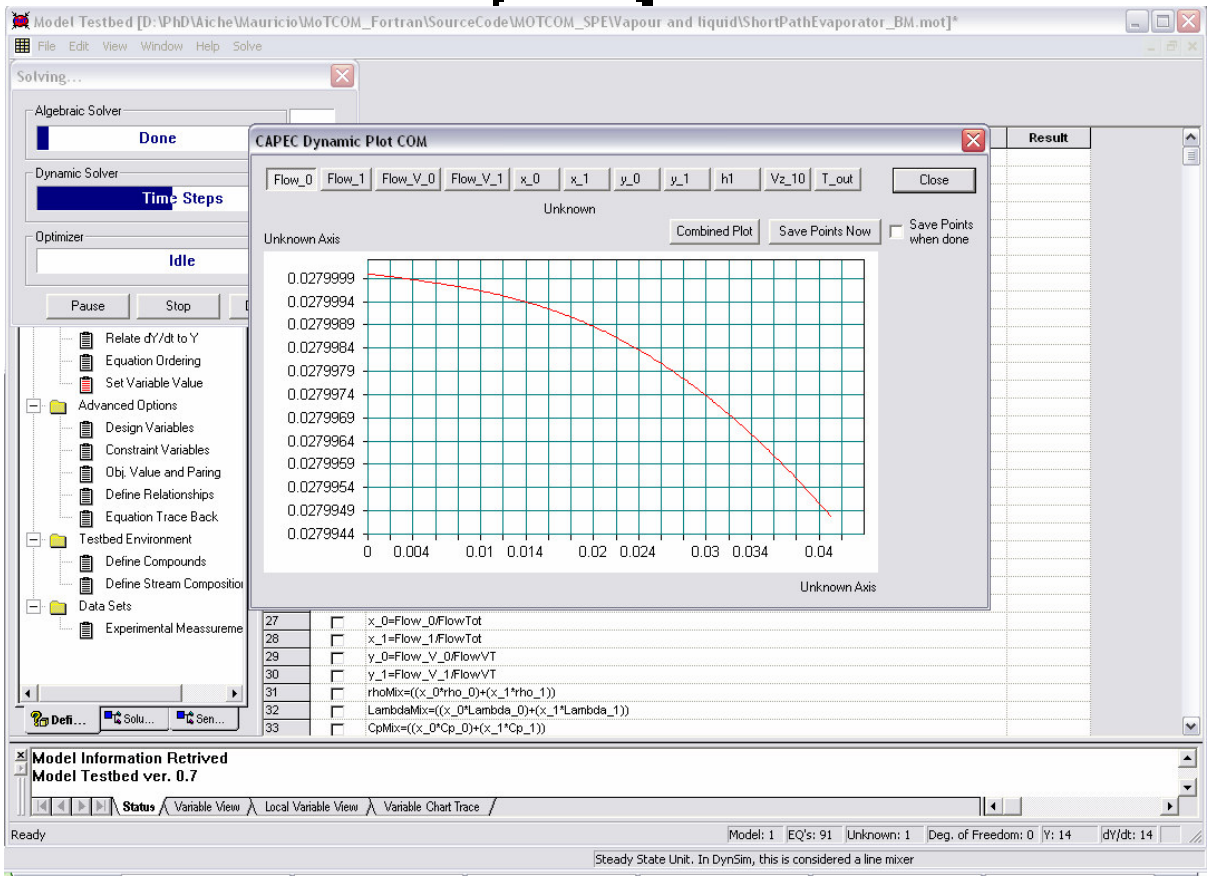
Model Testbed [D:\PhD\Aiche\Mauricio\MoTCOM_Fortran\SourceCode\MOTCOM_SPE\Vapour and liquid\ShortPathEvaporator_BM.mot]*
File Edit View Window Help Solve
Solving...
Algebraic Solver
Done
Dynamic Solver
Time Steps
Optimizer
Idle
Pause
Stop
Relate dY/dt to Y
Equation Ordering
Set Variable Value
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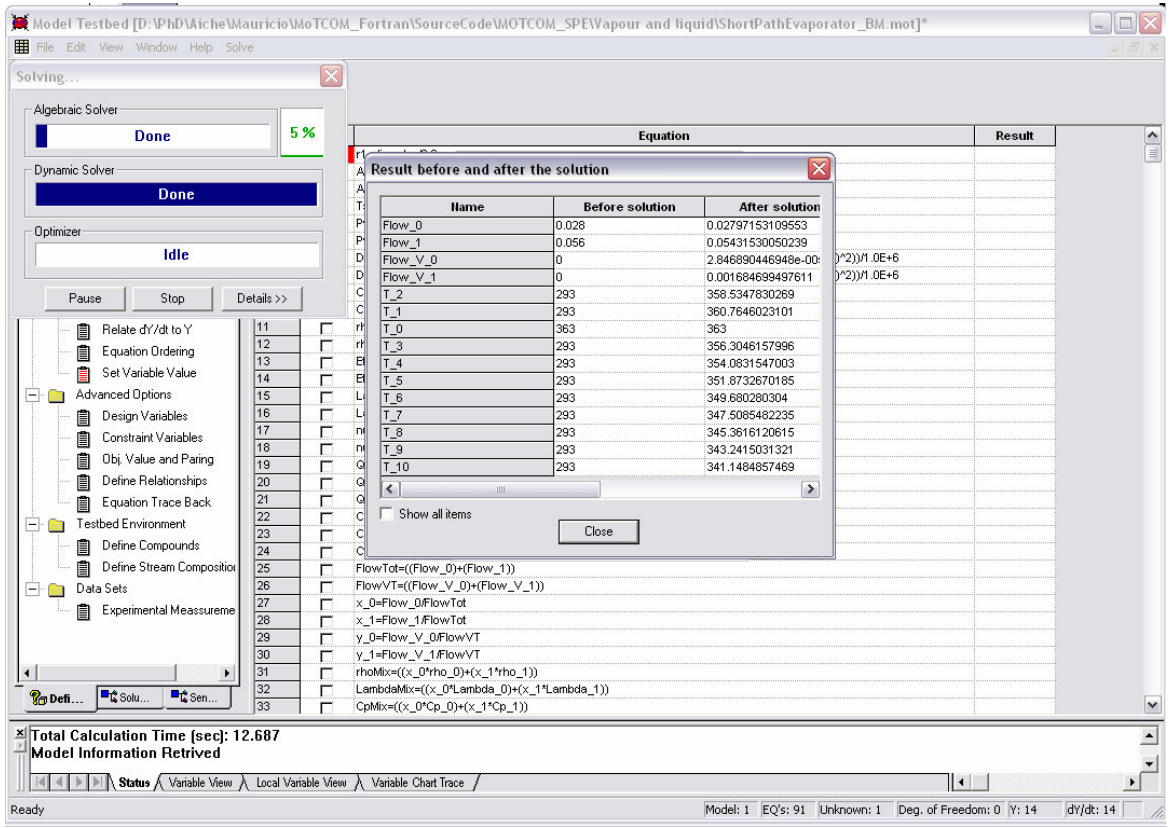
Data Sets
Experimental Meassureme
CAPEC Dynamic Plot COM
Flow_0 Flow_1 Flow_V_0 Flow_V_1 x_0 x_1 y_0 y_1 h1 Vz_10 T_out
Close
Unknown
Unknown Axis
Combined Plot
Save Points Now
Save Points when done
0.0279999
0.0279994
0.0279989
0.0279984
0.0279979
0.0279974
0.0279969
0.0279964
0.0279959
0.0279954
0.0279949
0.0279944
0 0.004 0.01 0.014 0.02 0.024 0.03 0.034 0.04
Unknown Axis
Result
27 x_0=Flow_0/FlowTot
28 x_1=Flow_1/FlowTot
29 y_0=Flow_V_0/FlowVT
30 y_1=Flow_V_1/FlowVT
31 rhoMix=((x_0*rho_0)+(x_1*rho_1))
32 LambdaMix=((x_0*Lambda_0)+(x_1*Lambda_1))
33 CpMix=((x_0*Cp_0)+(x_1*Cp_1))
Model Information Retrived
Model Testbed ver. 0.7
Status Variable View Local Variable View Variable Chart Trace
Ready
Model: 1 EQ's: 91 Unknown: 1 Deg. of Freedom: 0 Y: 14 dY/dt: 14
Steady State Unit. In DynSim, this is considered a line mixer

1. MoT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File Edit View Window Help Solve
Solving...
Algebraic Solver
Done
5 %
Dynamic Solver
Done
Optimizer
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Pause
Stop
Details >>
Relate dY/dt to Y
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Define Stream Compositio
Data Sets
Experimental Meassureme
Equation
Result
Result before and after the solution
Name
Before solution
After solution
Flow_0 0.028 0.02797153109553
Flow_1 0.056 0.05431530050239
Flow_V_0 0 2.846890446948e-00
Flow_V_1 0 0.001684699497611
T_2 293 358.5347830269
T_1 293 360.7646023101
T_0 363 363
T_3 293 356.3046157996
T_4 293 354.0831547003
T_5 293 351.8732670185
T_6 293 349.680280304
T_7 293 347.5085482235
T_8 293 345.3616120615
T_9 293 343.2415031321
T_10 293 341.1484857469
Show all items
Close
FlowTot=((Flow_0)+(Flow_1))
FlowVT=((Flow_V_0)+(Flow_V_1))
x_0=Flow_0/FlowTot
x_1=Flow_1/FlowTot
y_0=Flow_V_0/FlowVT
y_1=Flow_V_1/FlowVT
rhoMix=((x_0*rho_0)+(x_1*rho_1))
LambdaMix=((x_0*Lambda_0)+(x_1*Lambda_1))
CpMix=((x_0*Cp_0)+(x_1*Cp_1))
Total Calculation Time (sec): 12.687
Model Information Retrived
Status
Variable View
Local Variable View
Variable Chart Trace
Ready
Model: 1
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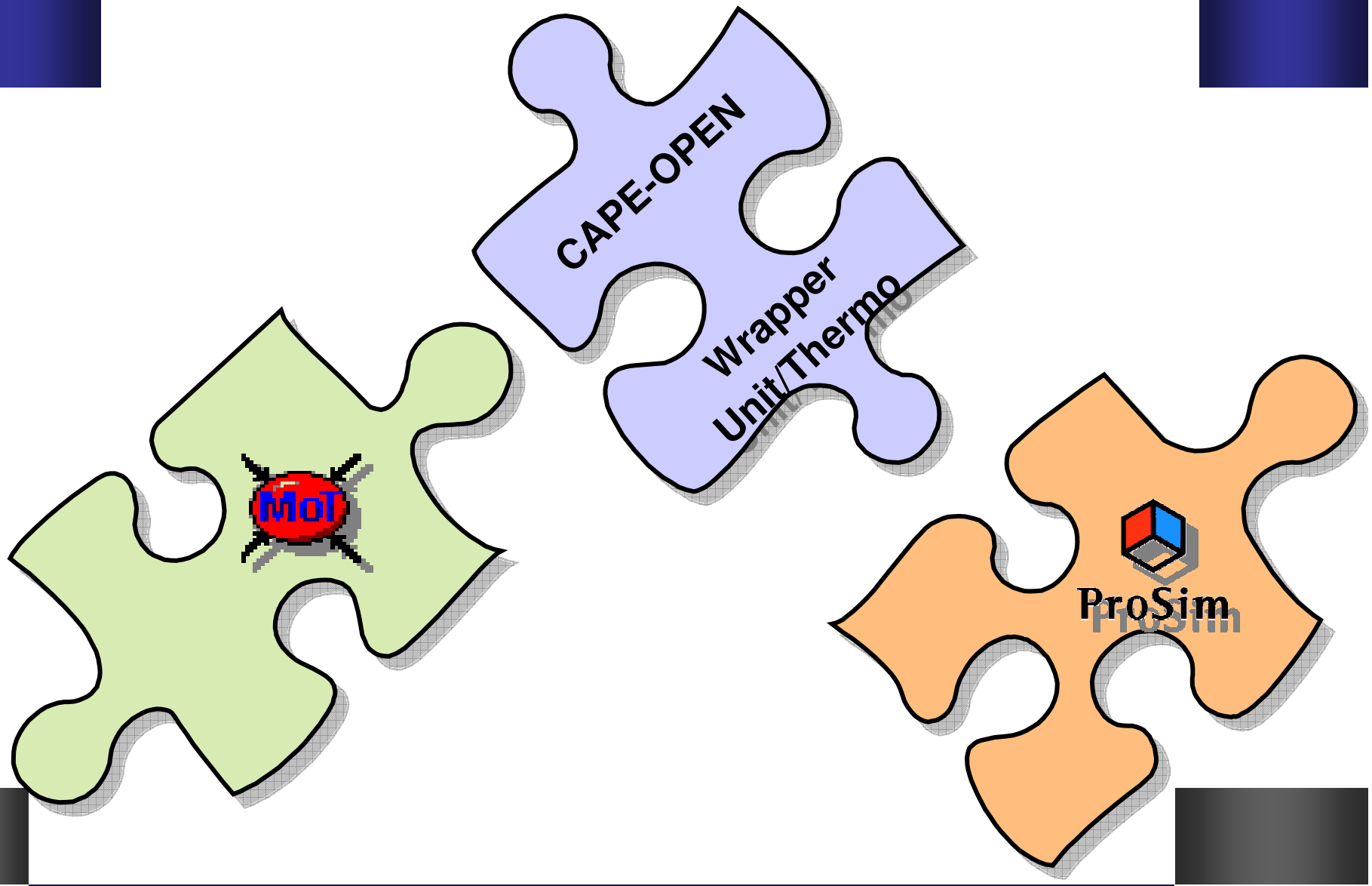
1. MoT

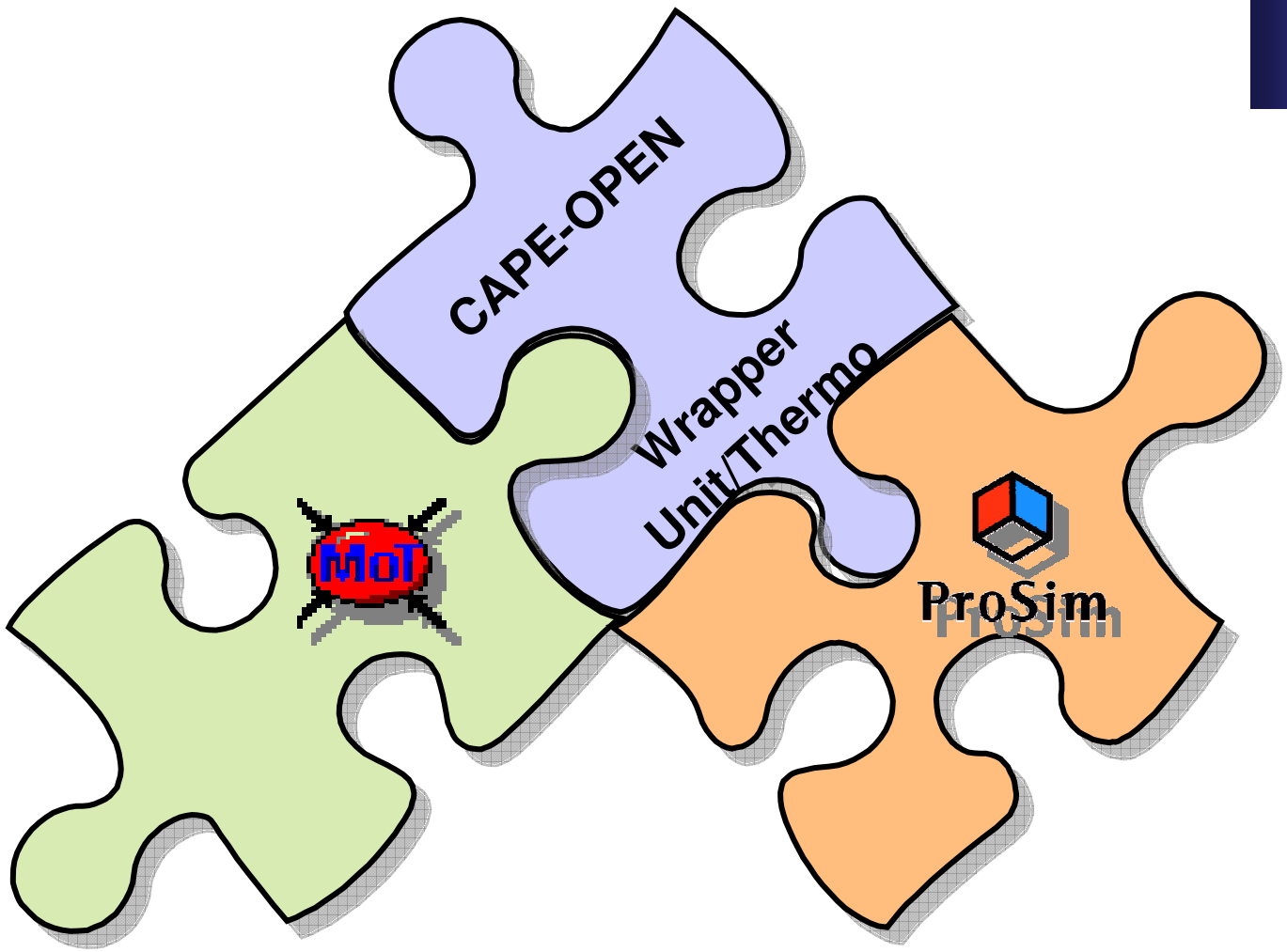
2. ProSim
   - Simulis thermodynamics
   - ProSimPlus
   - CO-wrapper

ProSim

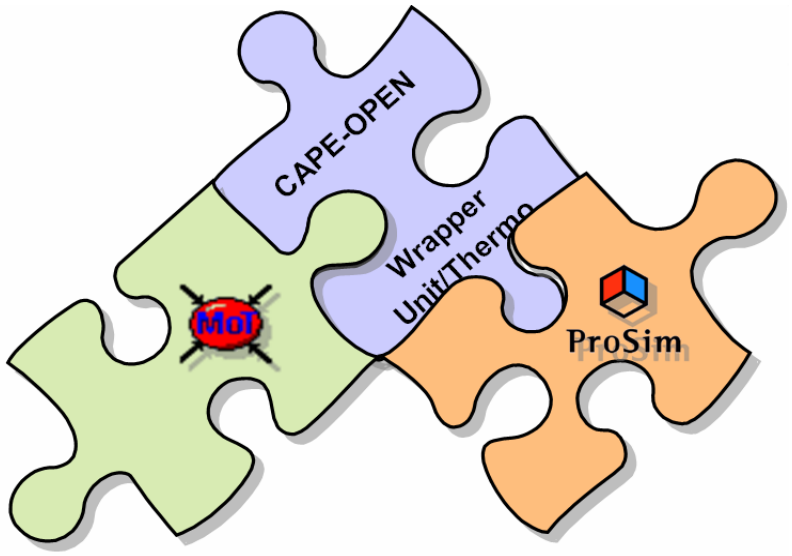
MoT-ProSim Integration

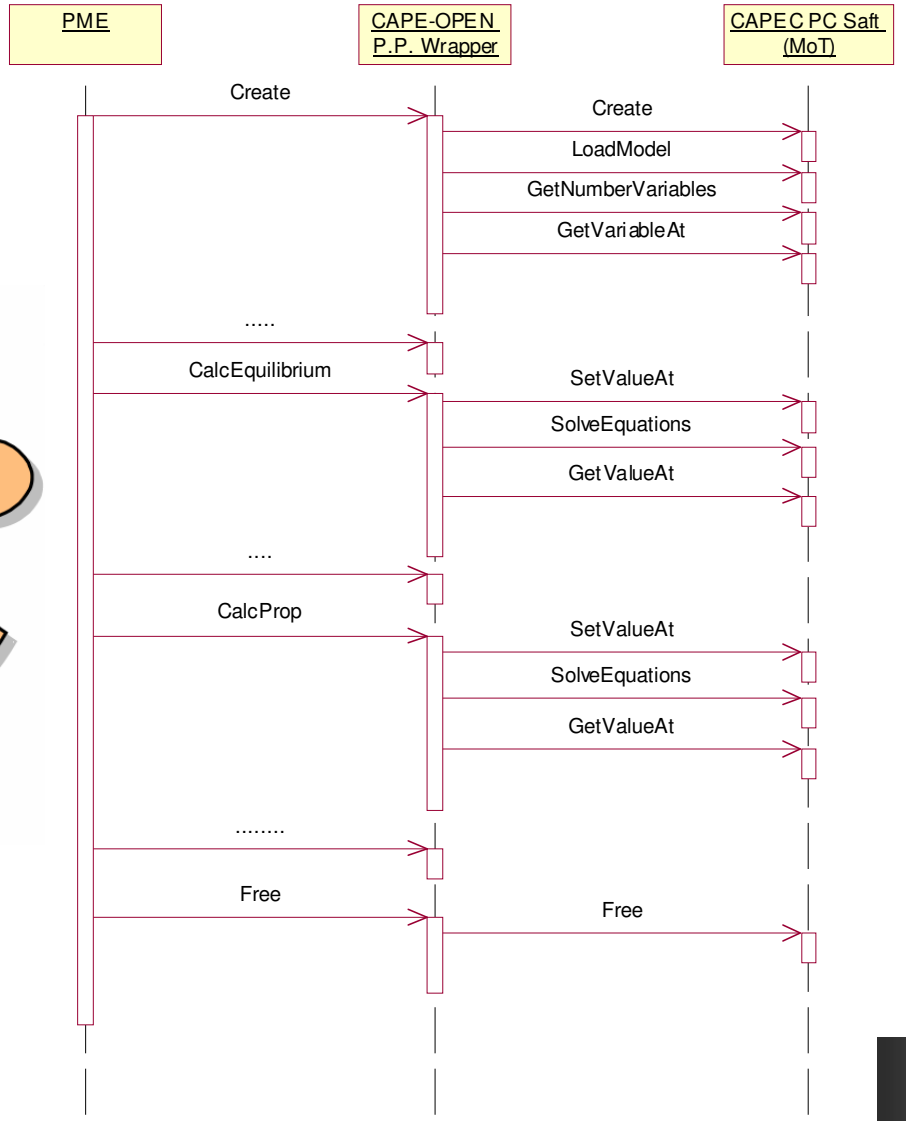


MoT-ProSim Integration

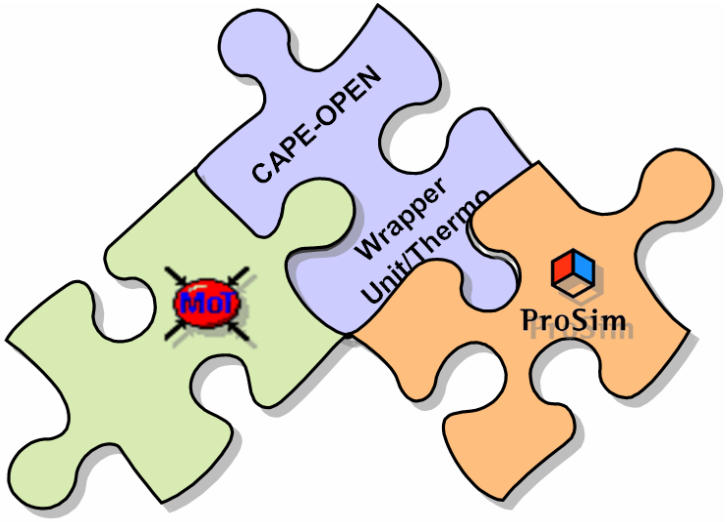


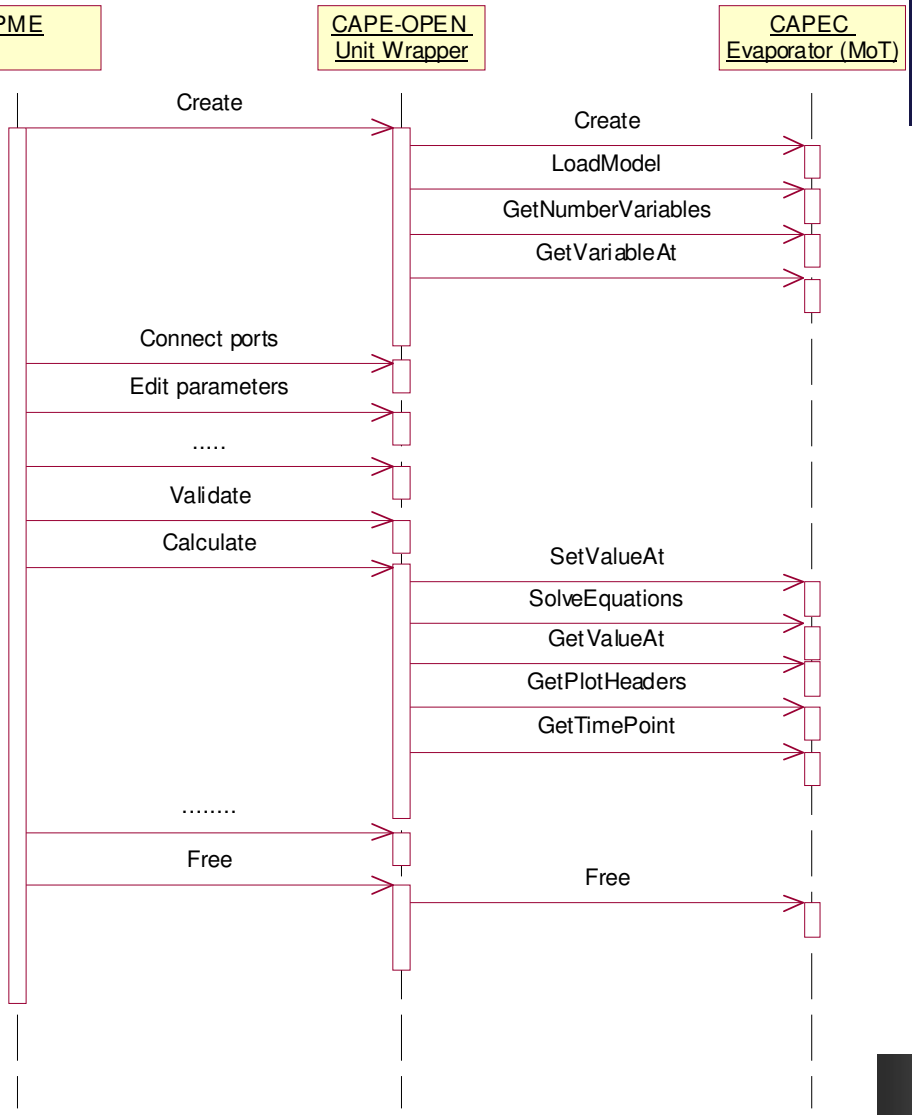
CO-thermo interface





CO-unit model interface

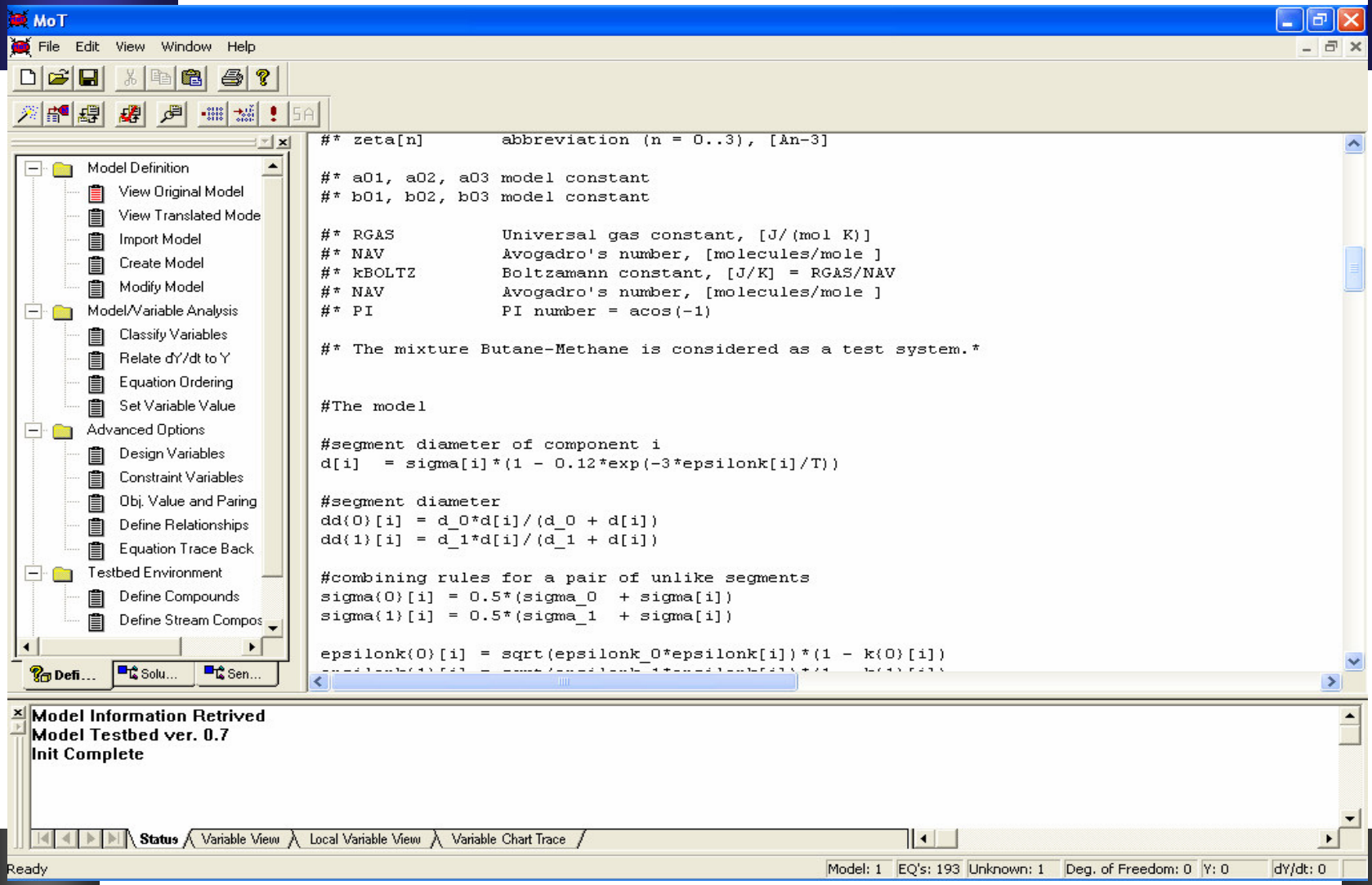




Case Studies

1. **Highlights interoperability through the use of an external model (PC-SAFT) through the CO-thermo interface in ProSim, which is run from EXCEL - for a binary mixture of methane/n-butane (saturation point & property calculations)**
2. **Highlights interoperability through the use of an external unit operation model (short-path evaporation) for the recovery of a chemical from a feed mixture using ProSim as the simulator and wrapping the MoT-model object for the CO-socket in ProSim**

Case Study: PC-SAFT EOS



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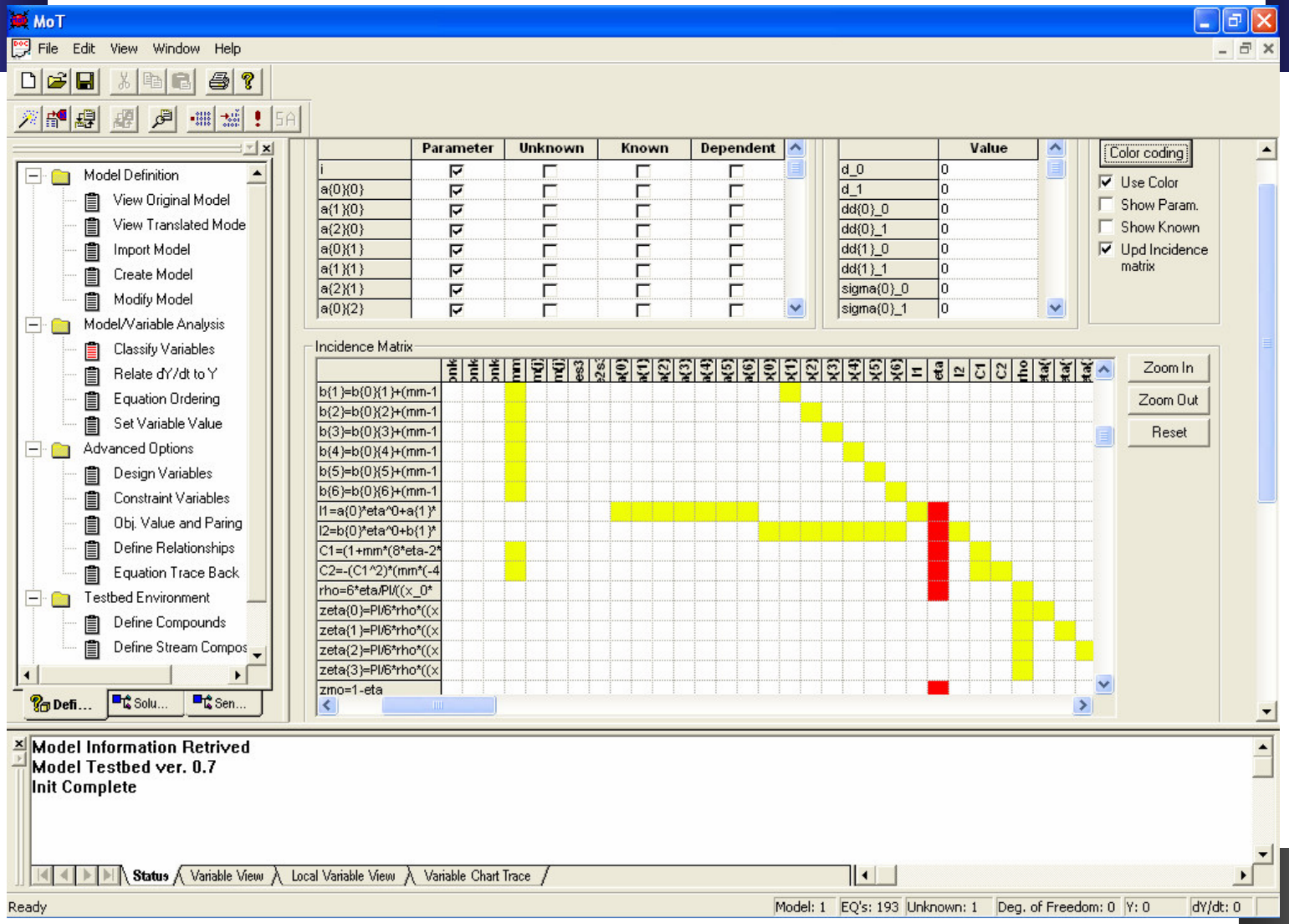

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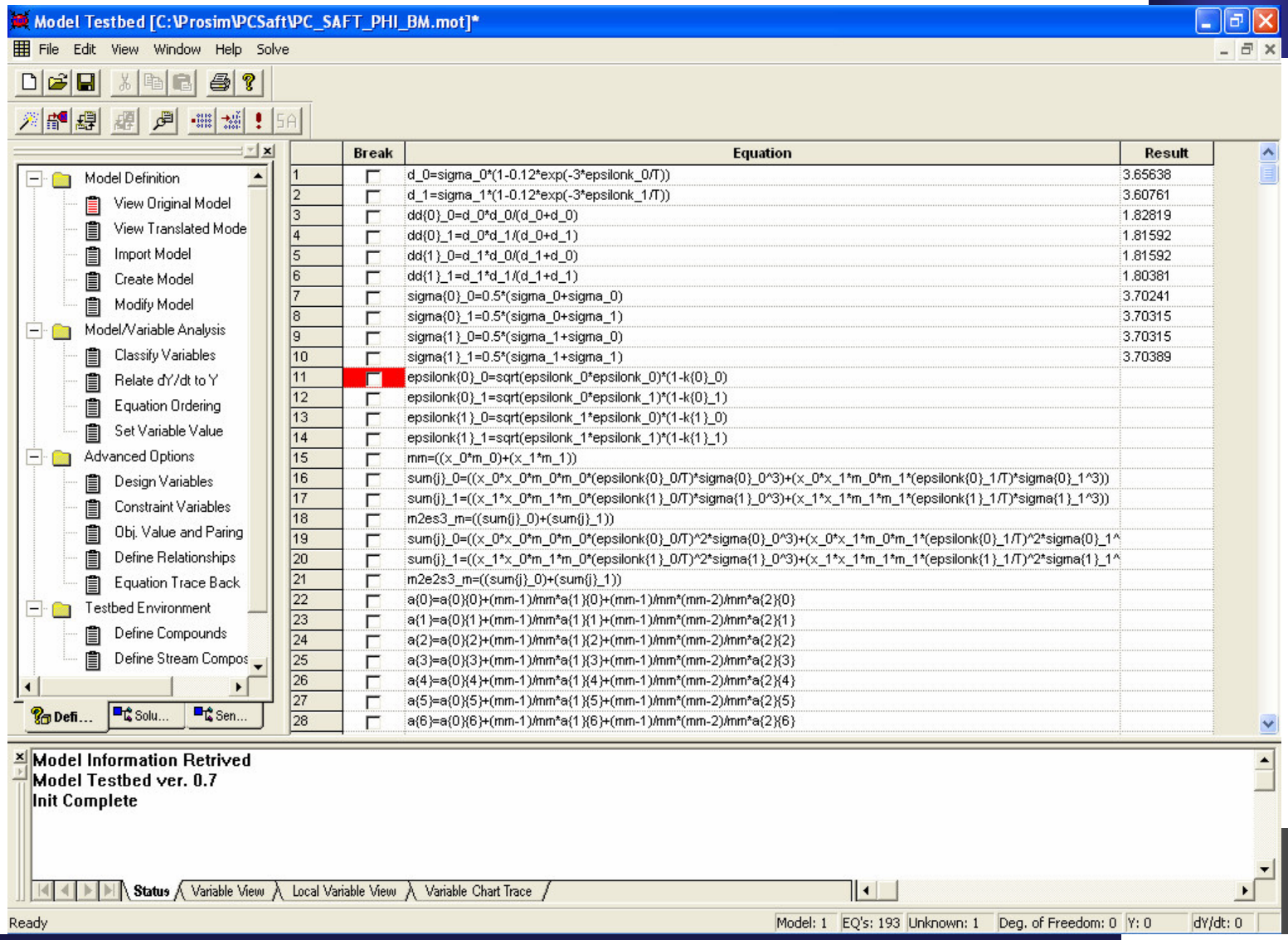
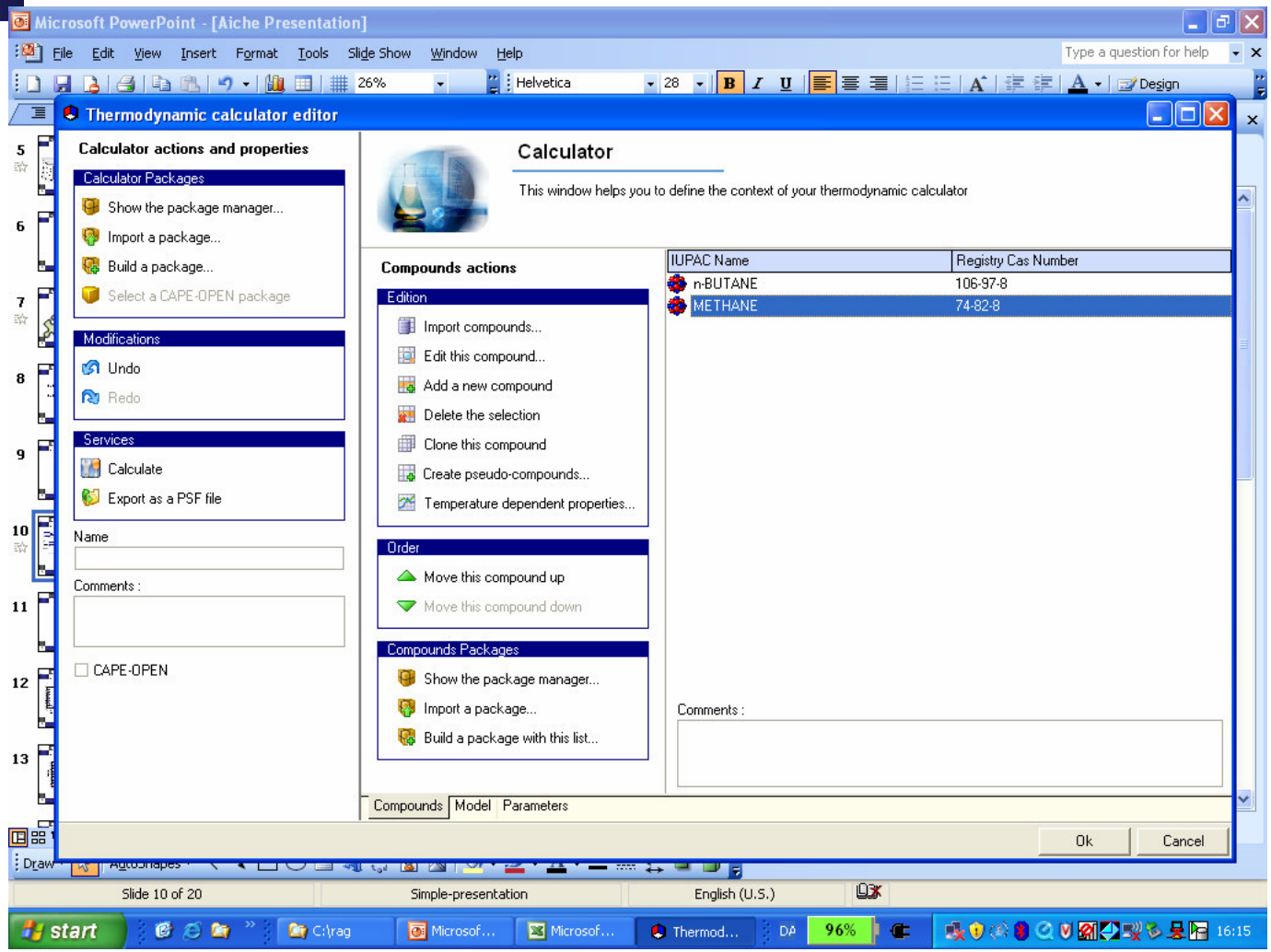


Case Study 1: Thermo Interface

1. External Thermo-model (PC-SAFT)



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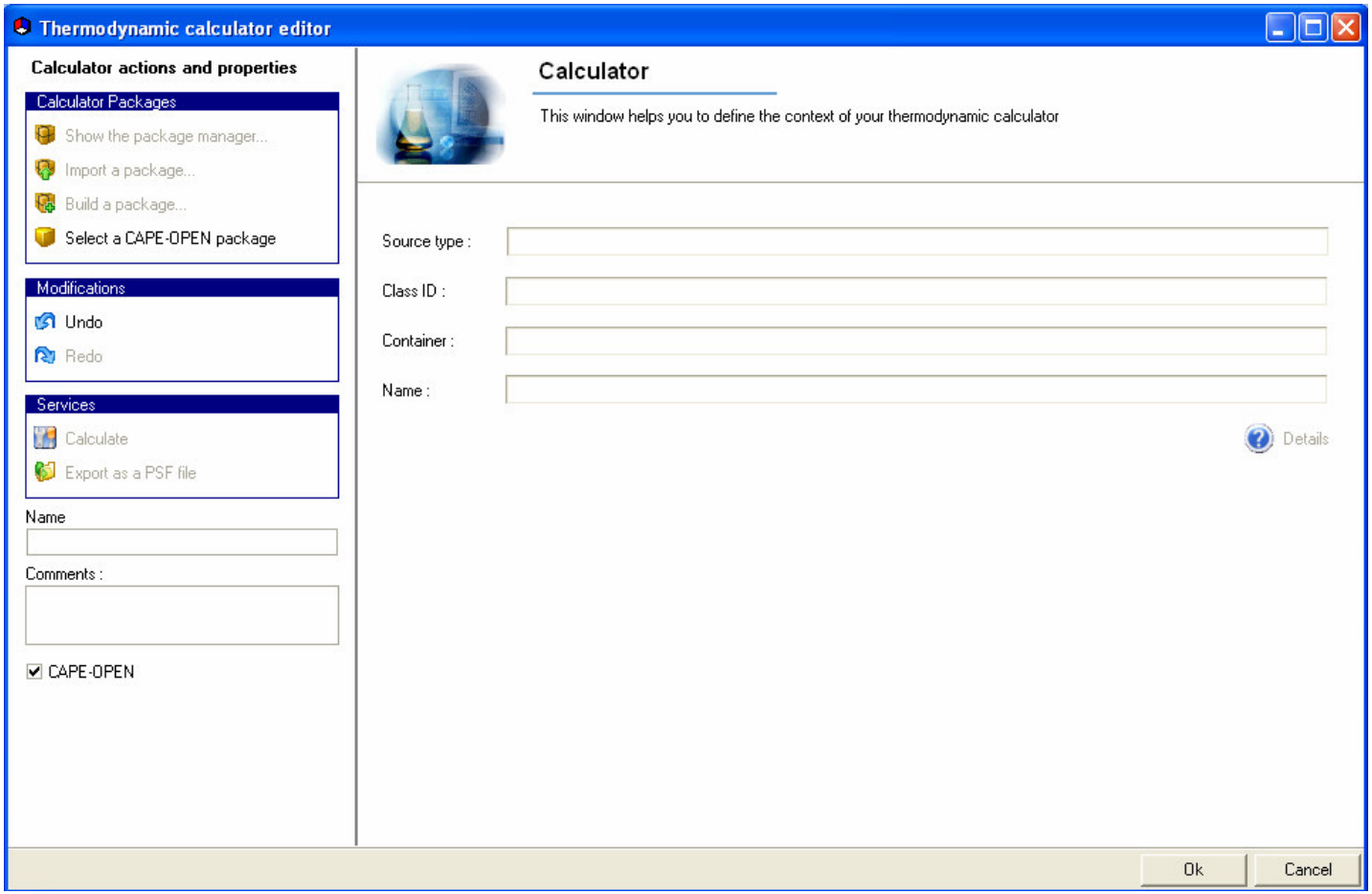

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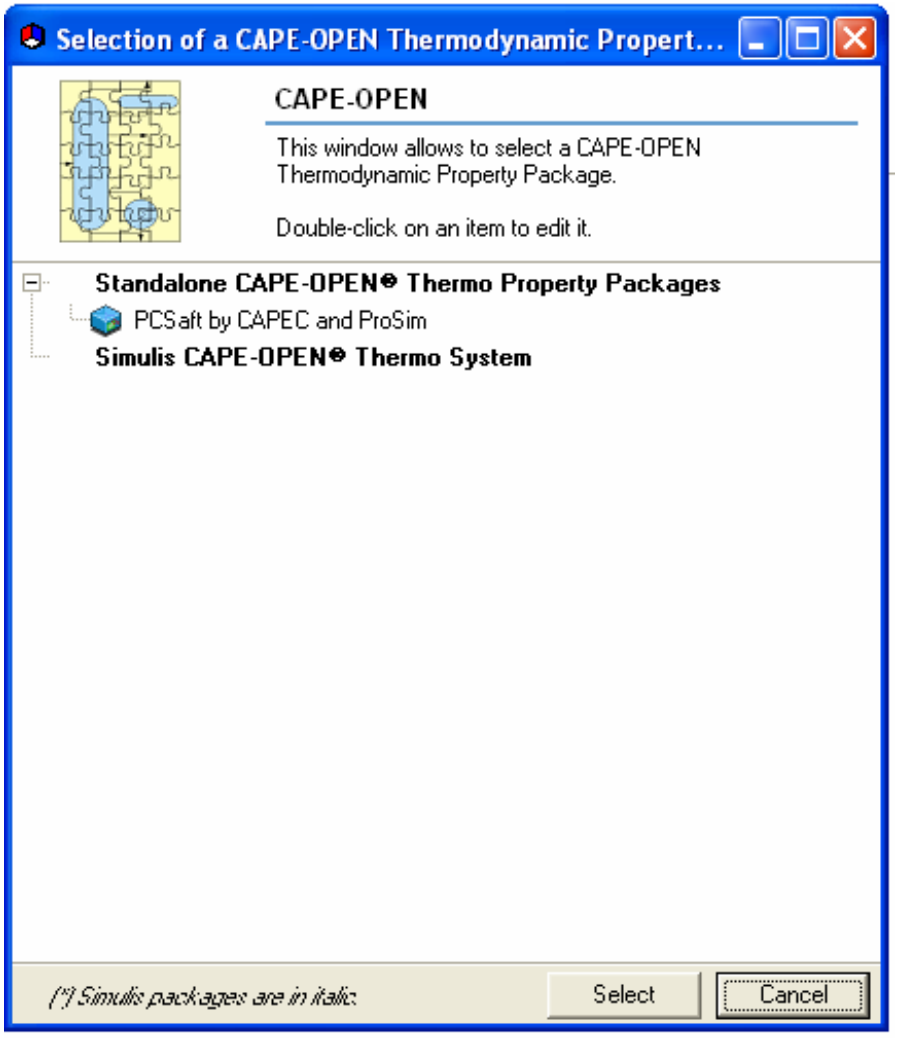

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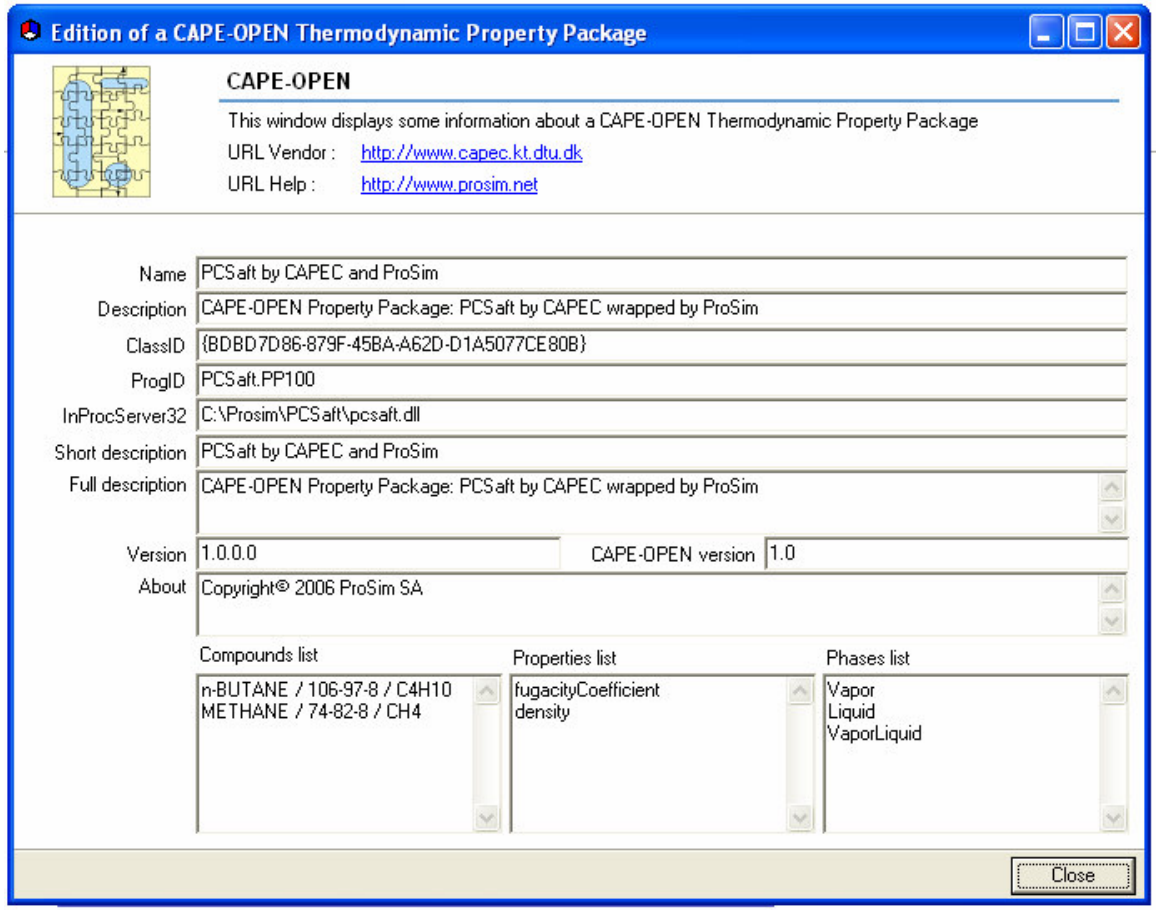

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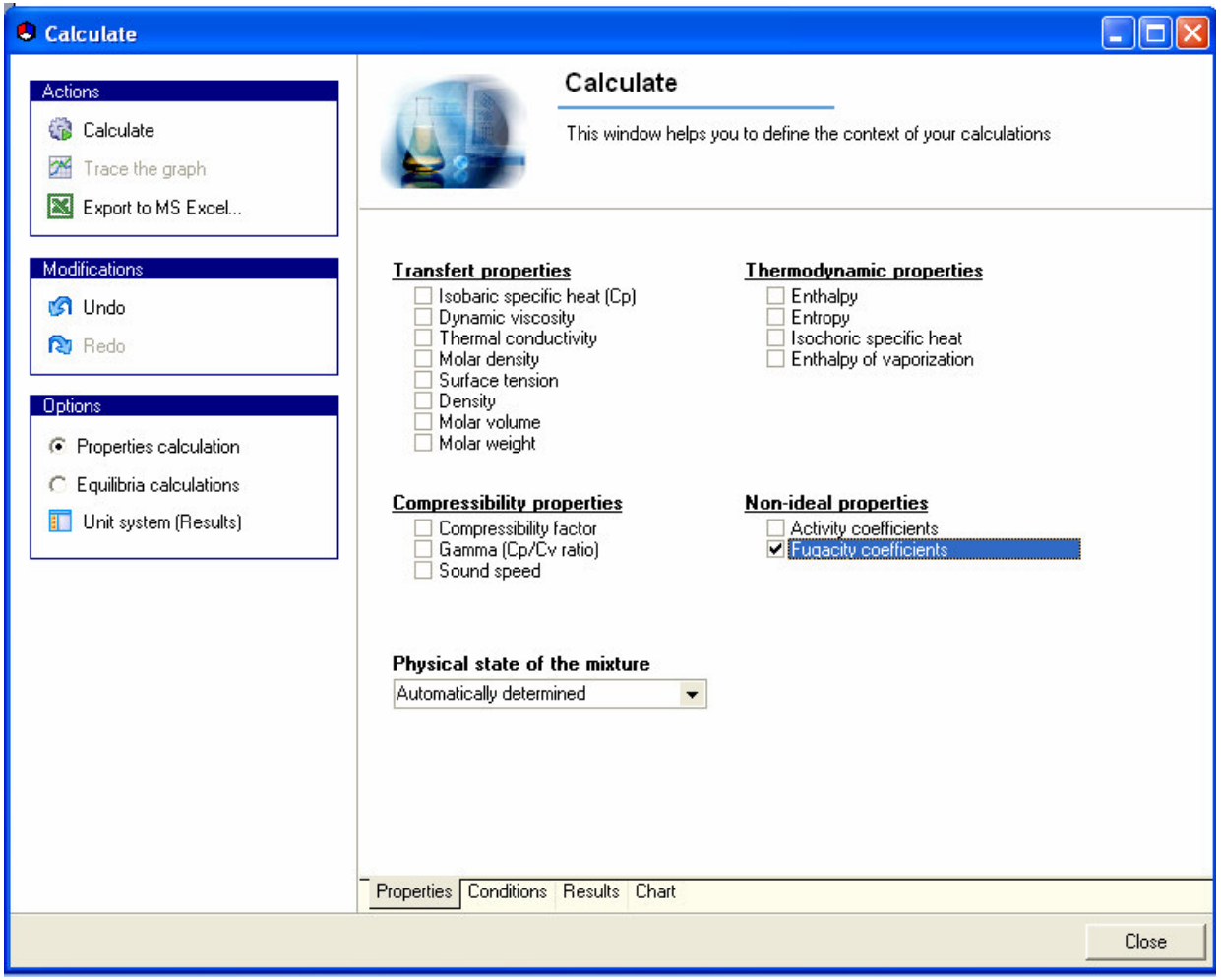

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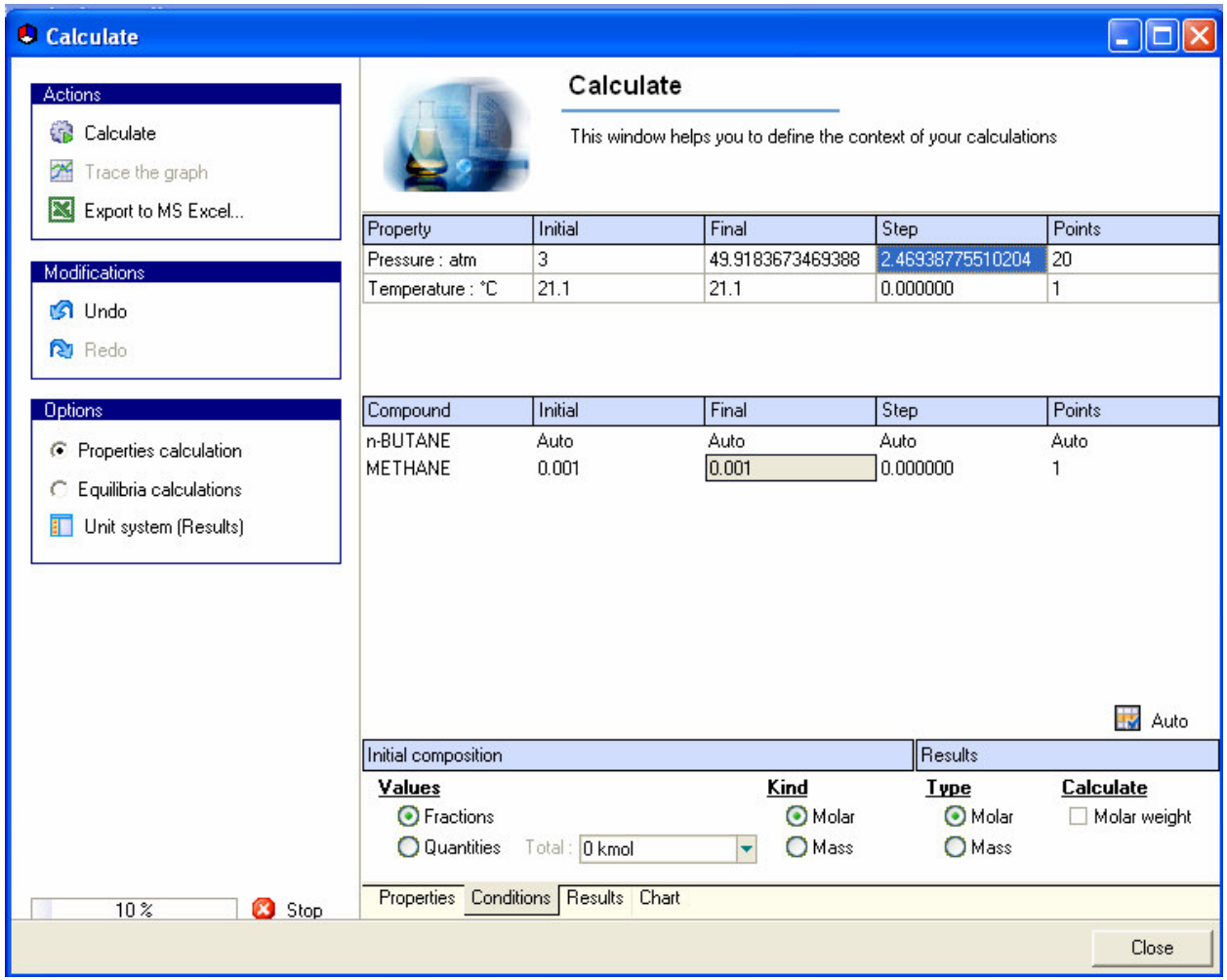

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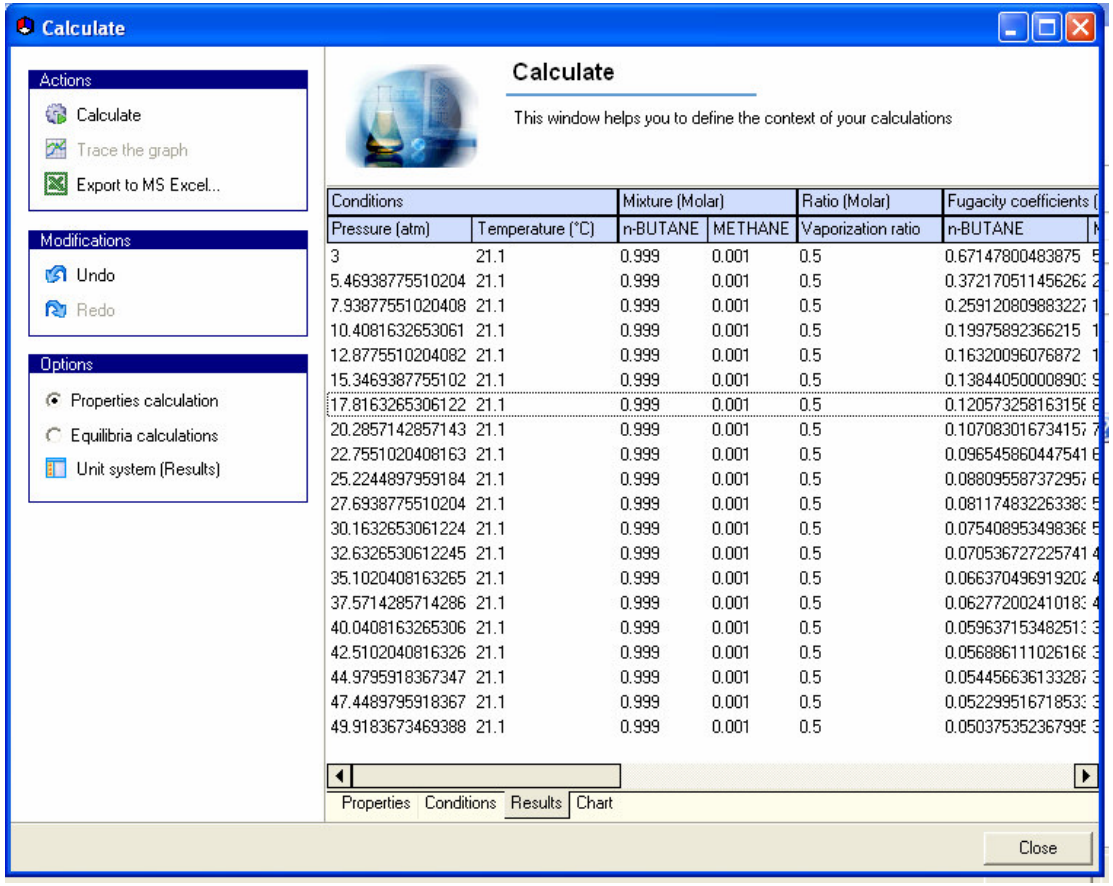
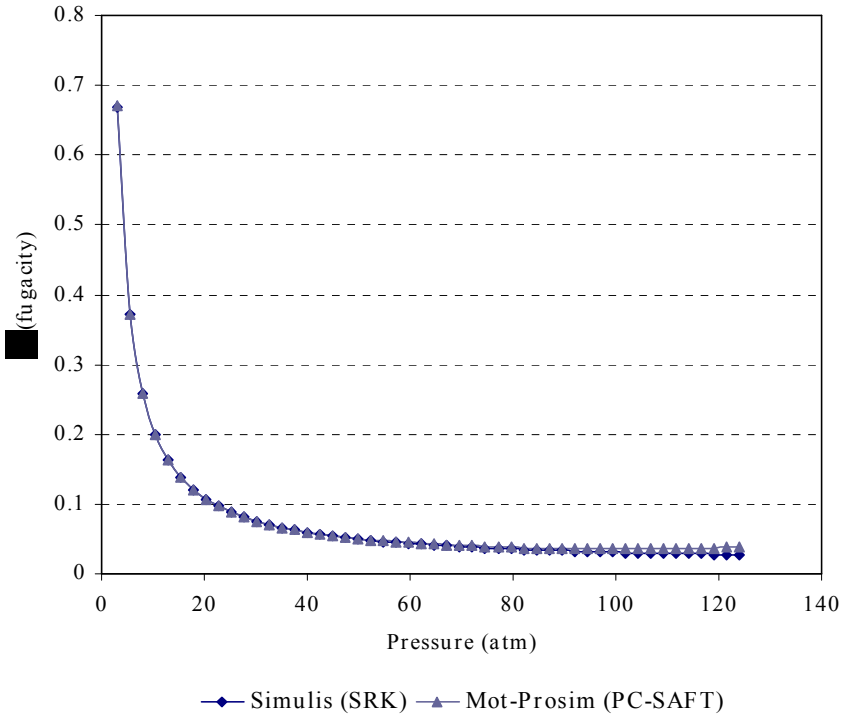


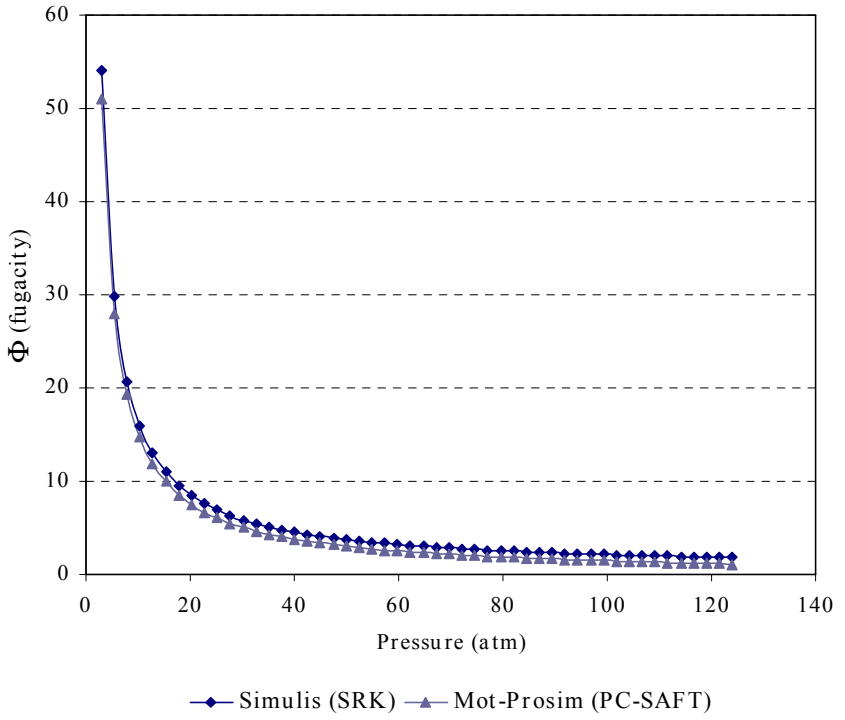
Case Study 1: Thermo Interface

1. Validation & comparison of results

Fugacity coefficient for n-butane (Liquid phase)

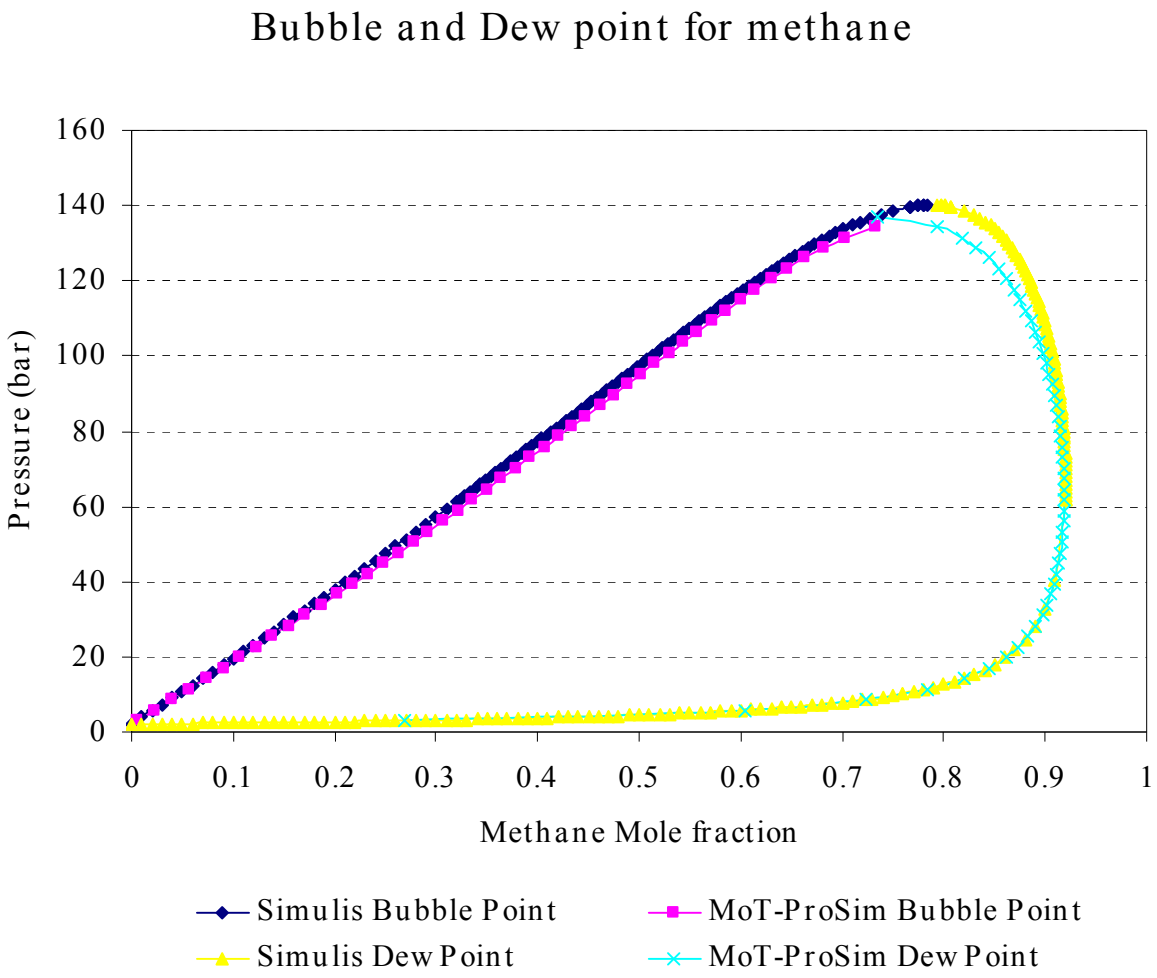


Fugacity coefficient for methane (Liquid phase)



Case Study 1: Thermo Interface

1. Validation & comparison of results



T = 21.1 °C

$x_{n\text{-}but} = 0.999$

$x_{CH4} = 0.001$

Short-Path Evaporator Model

Momentum balance

$$\nu \frac{\partial^2 v(y,z)}{\partial y^2} = -g$$

Rate of Evaporization

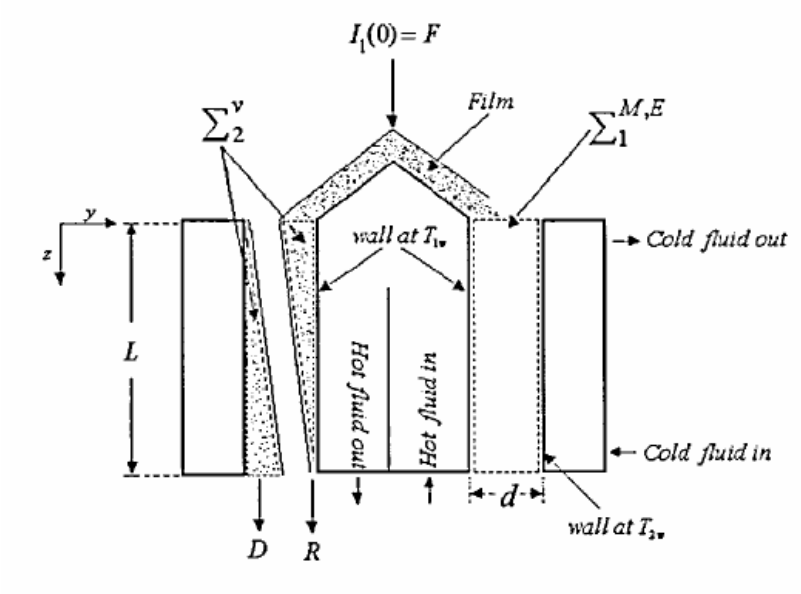
$$\frac{\partial I_i(z)}{\partial z} = -2\pi \cdot R \cdot k_i; \quad k_i = \frac{\gamma_i P_i^{vap}}{\sqrt{2\pi R_g M_i T_s(z)}} \left(\frac{P}{P_{ref}}\right) \left\{1-(1-F)\left[1-e^{d/(\kappa\beta)}\right]^n\right\}$$

Energy balance

$$v(y,z)\frac{\partial T(y,z)}{\partial z} = \frac{\lambda}{\rho Cp}\left[\frac{\partial^2 T(y,z)}{\partial y^2} + \frac{\partial^2 T(y,z)}{\partial z^2}\right]$$

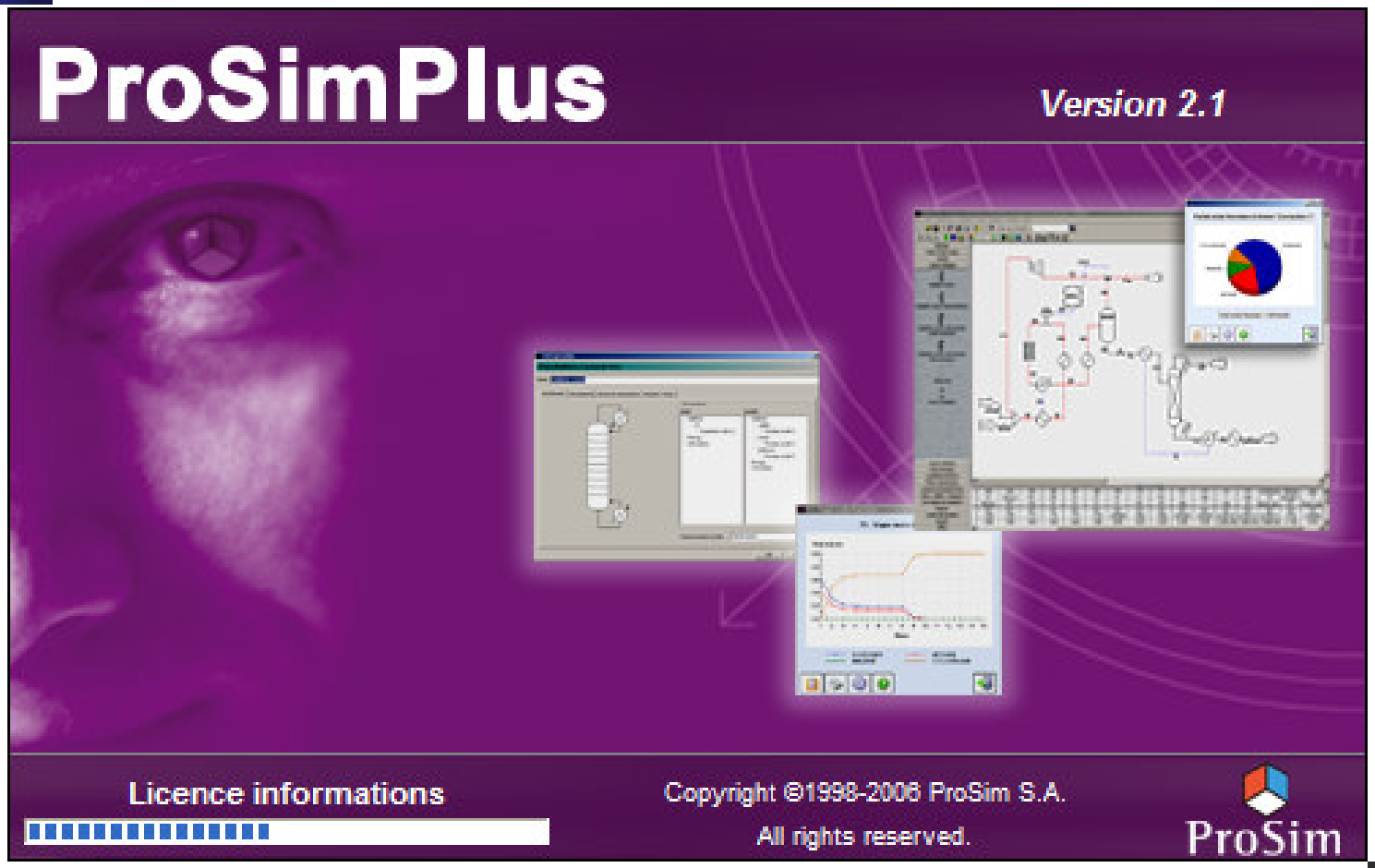
Mass Balance

$$v(y,z)\frac{\partial C_i(y,z)}{\partial z} = D_i\left[\frac{\partial^2 C_i(y,z)}{\partial y^2} + \frac{\partial^2 C_i(y,z)}{\partial z^2}\right]$$

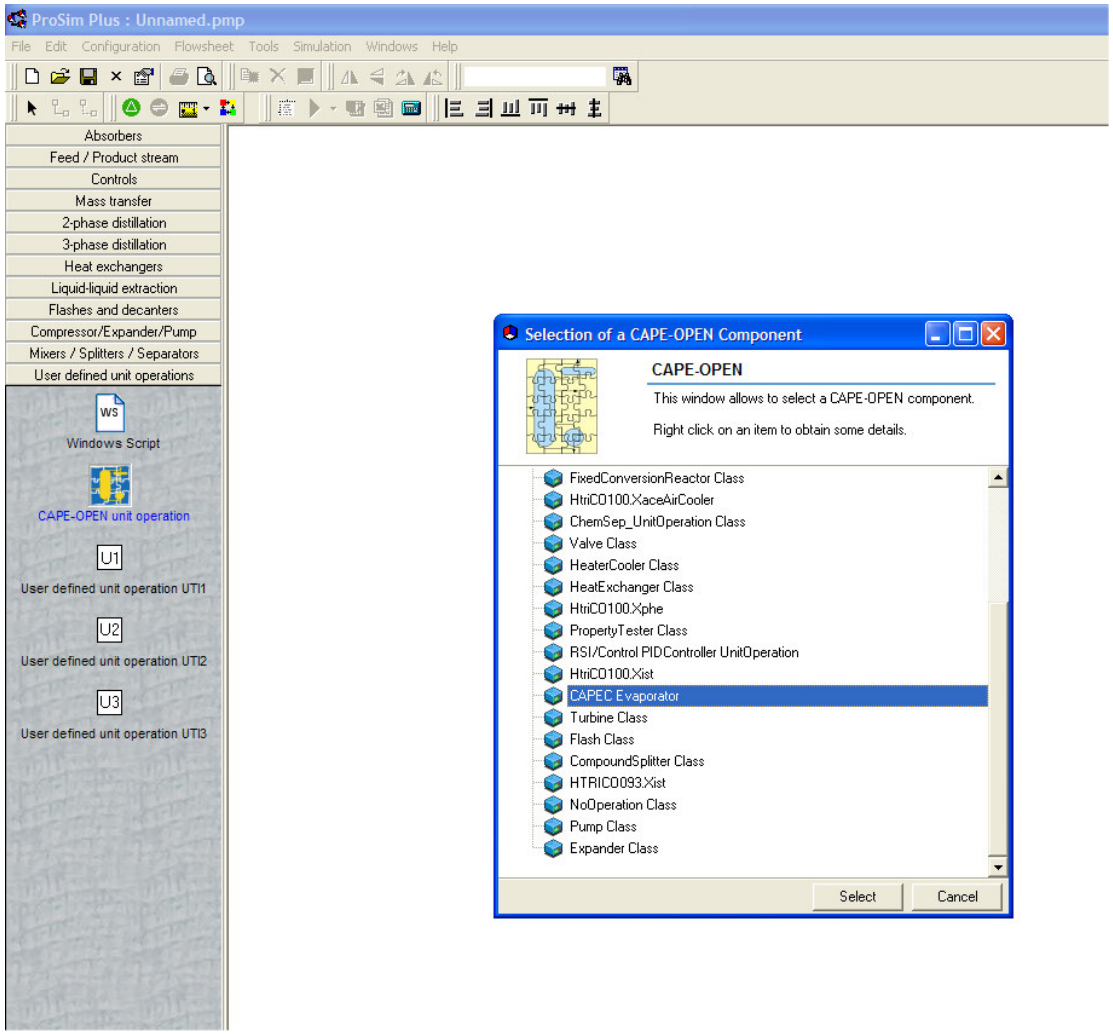


*Sales-Cruz, M. And Gani, R., 2006; "Computer-Aided modelling of short path evaporation for chemical product purifications, analysis and design", *Chem. Eng. Res. and Des*. 84, 7, 583-594

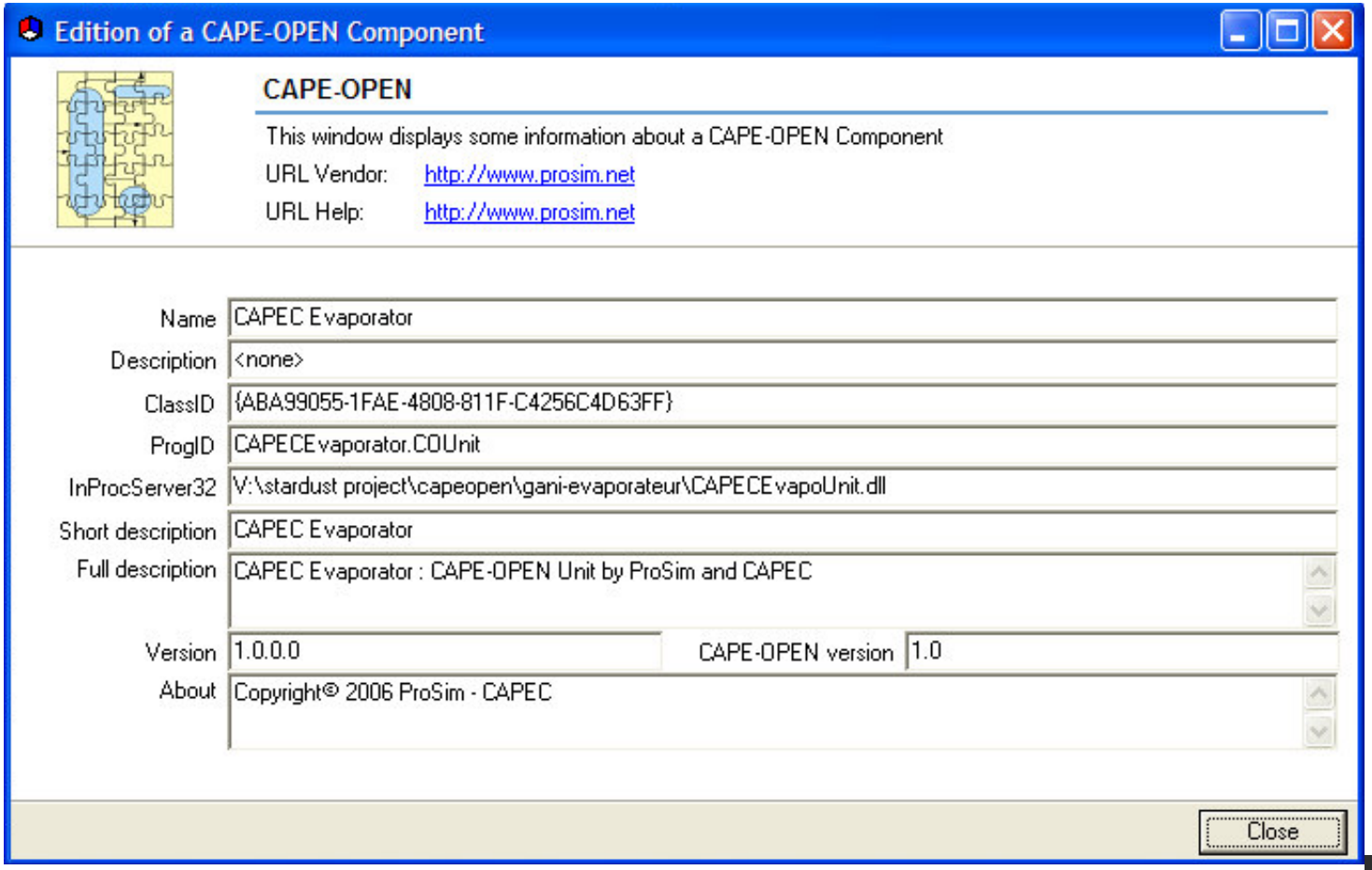
Case Study 2: Unit Interface



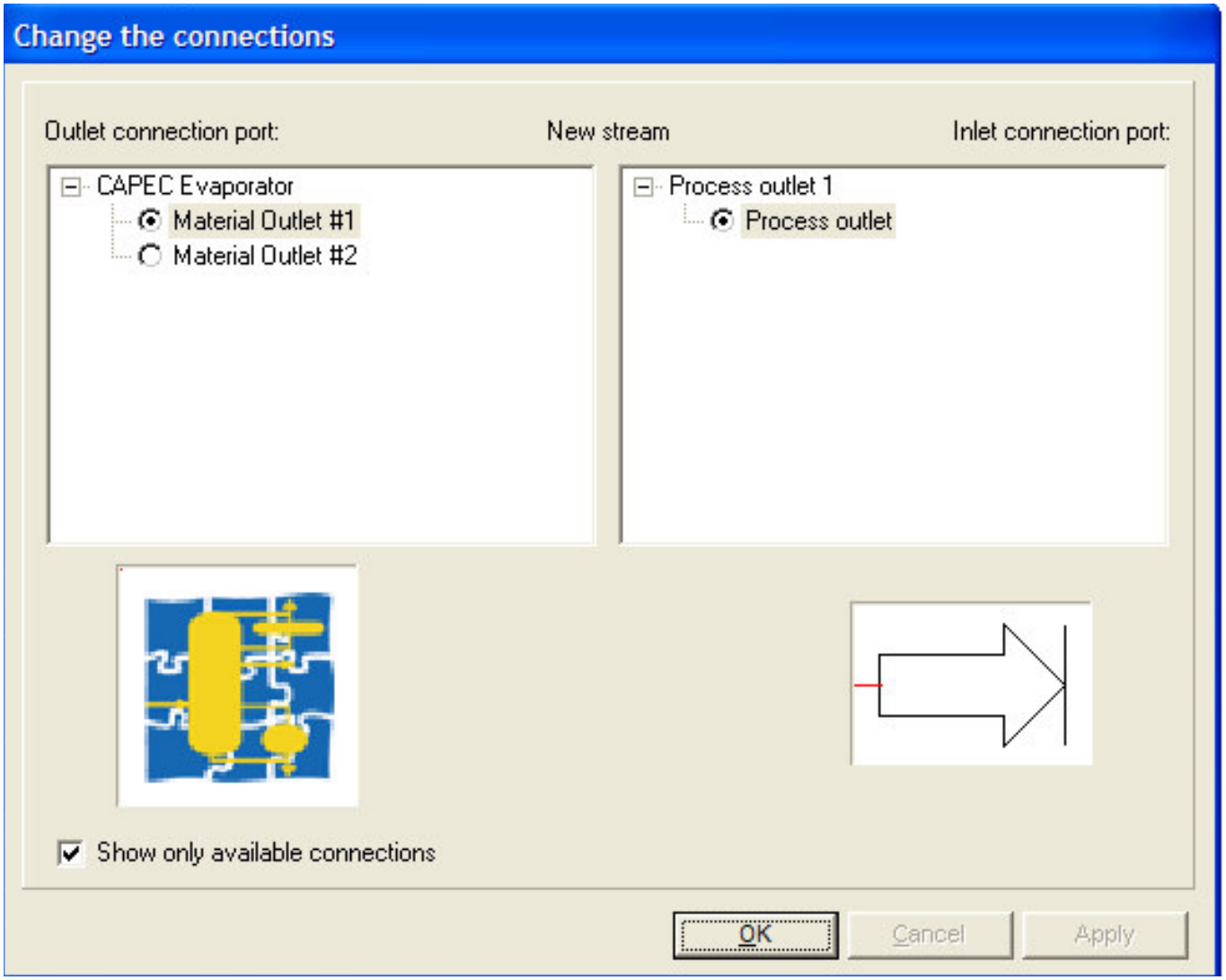
Case Study 2: Unit Interface



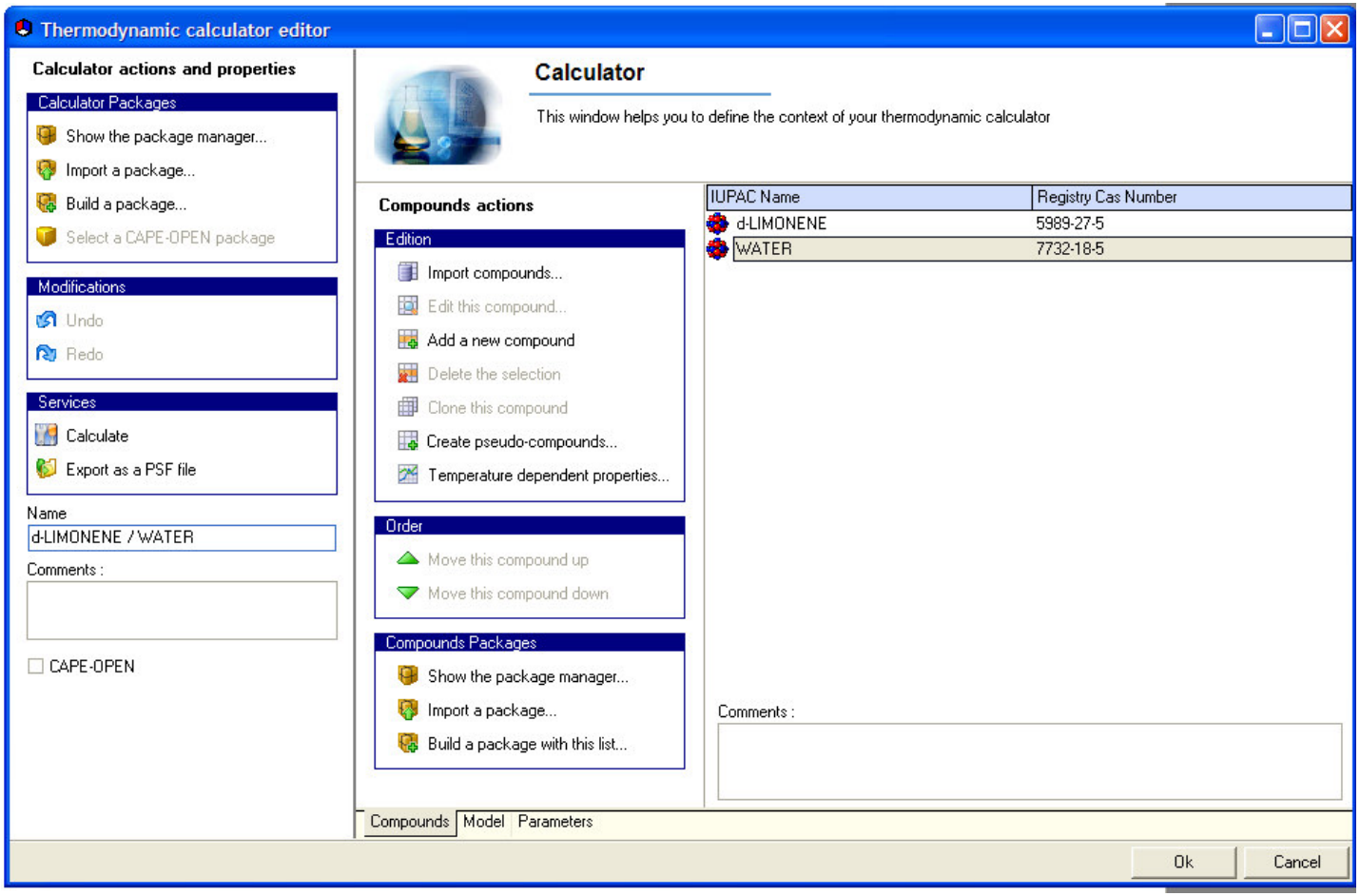
Case Study 2: Unit Interface



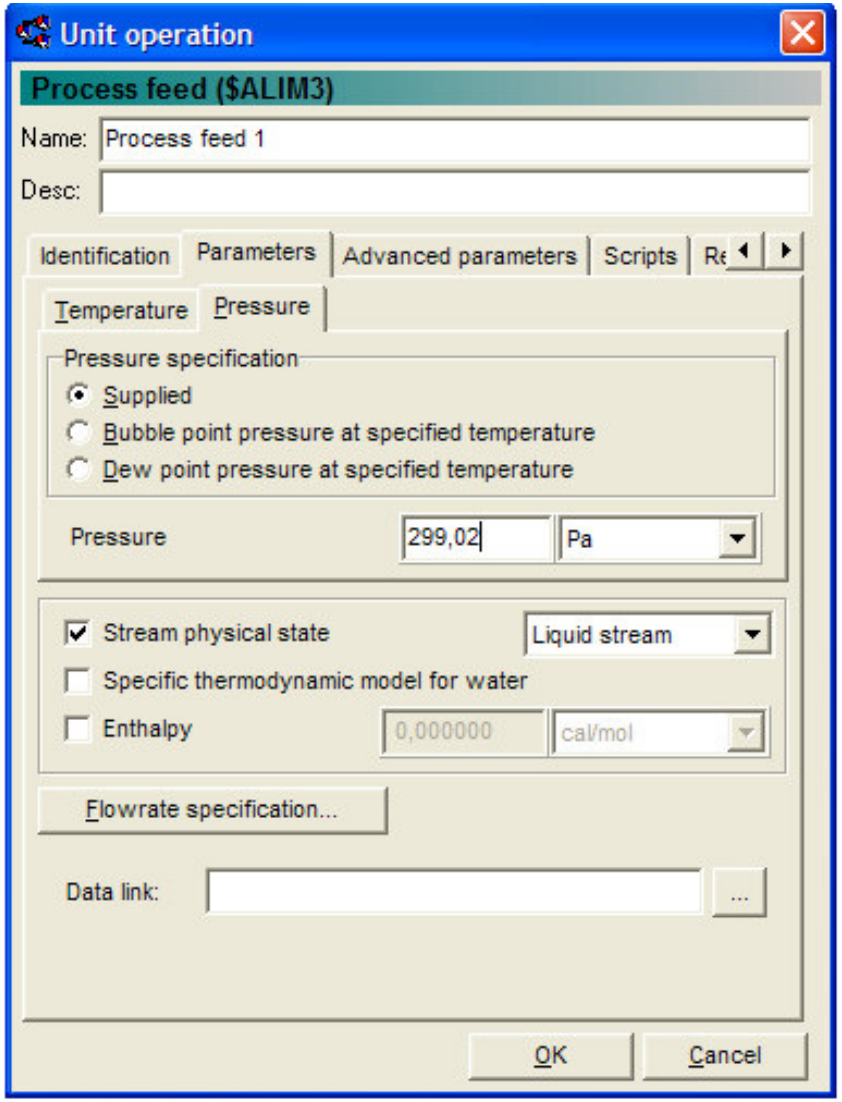
Case Study 2: Unit Interface



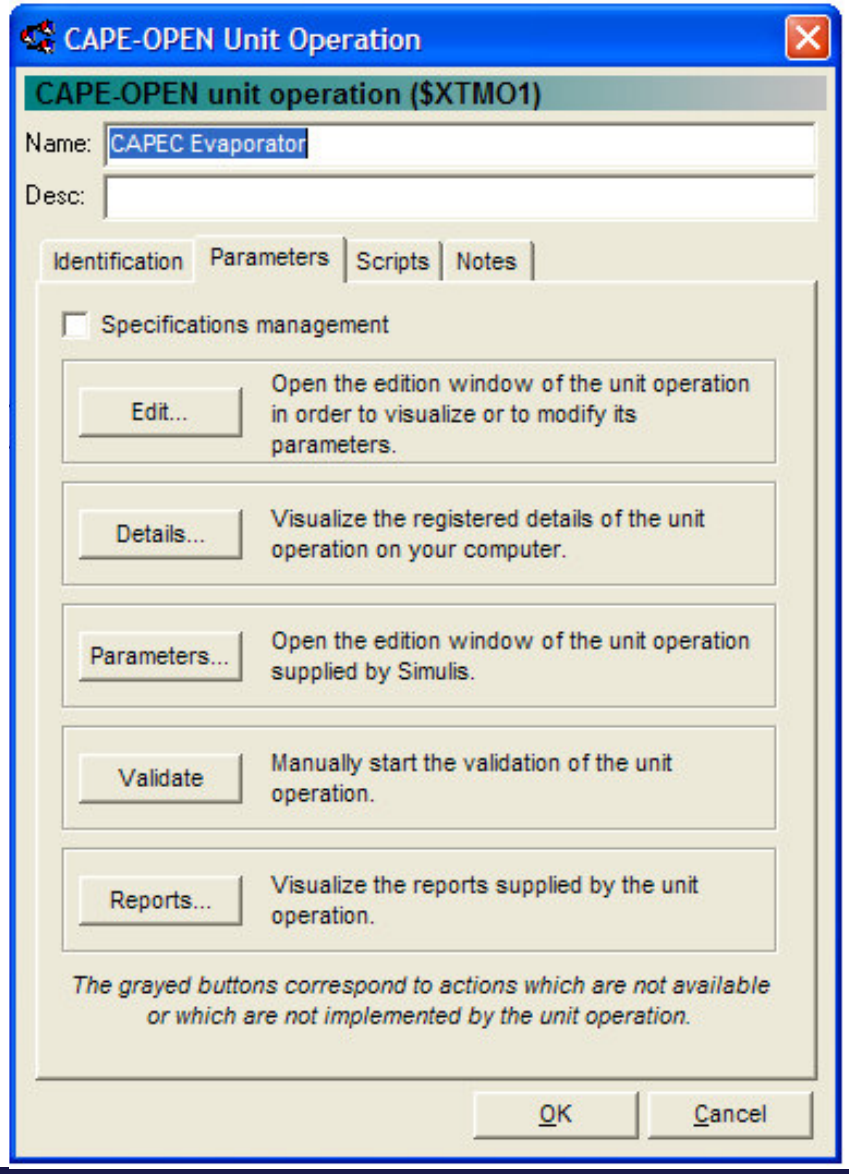
Case Study 2: Unit Interface



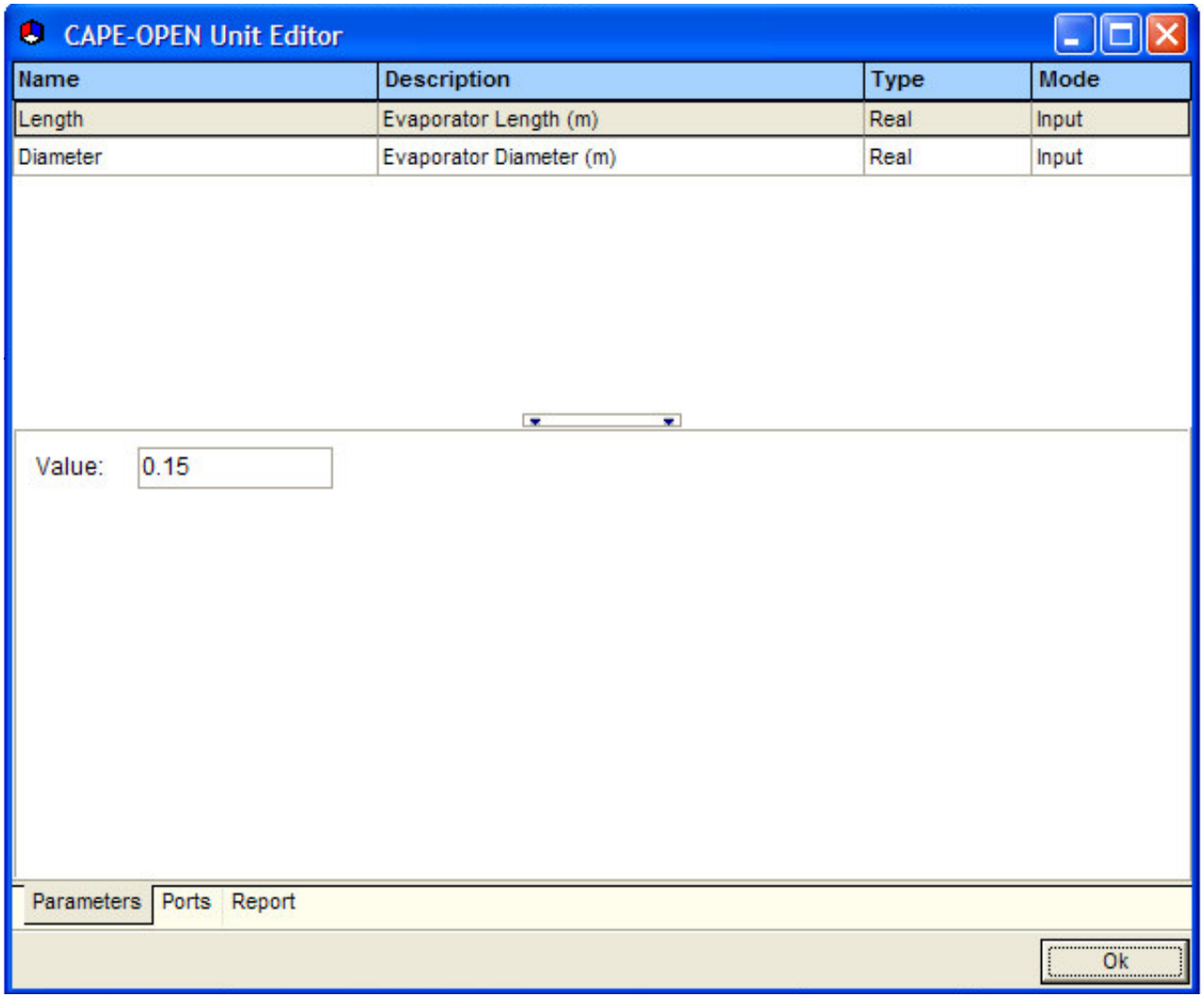
Case Study 2: Unit Interface



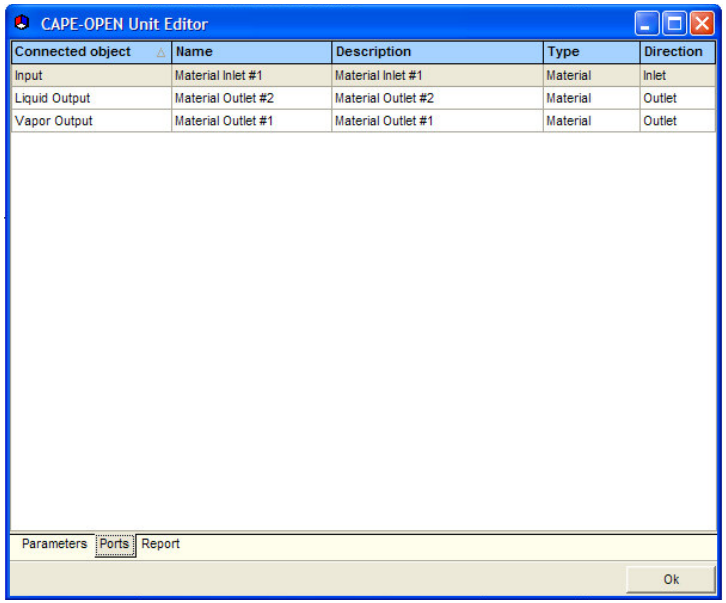
Case Study 2: Unit Interface

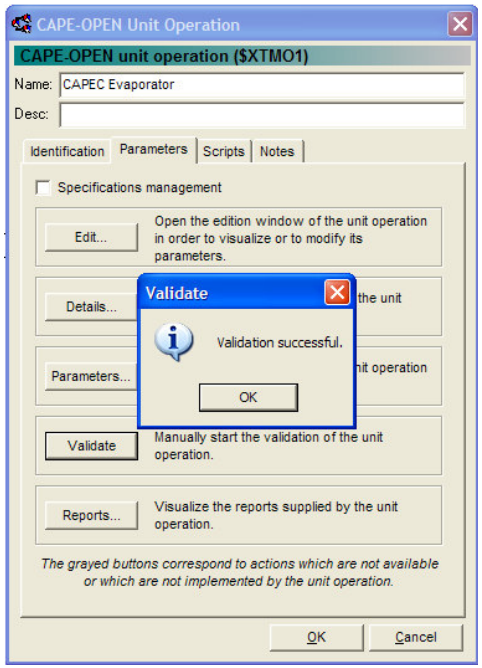


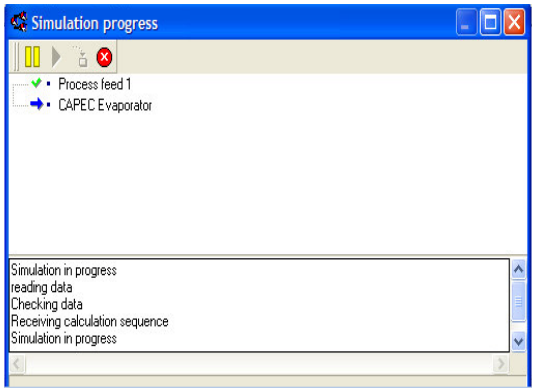
Case Study 2: Unit Interface



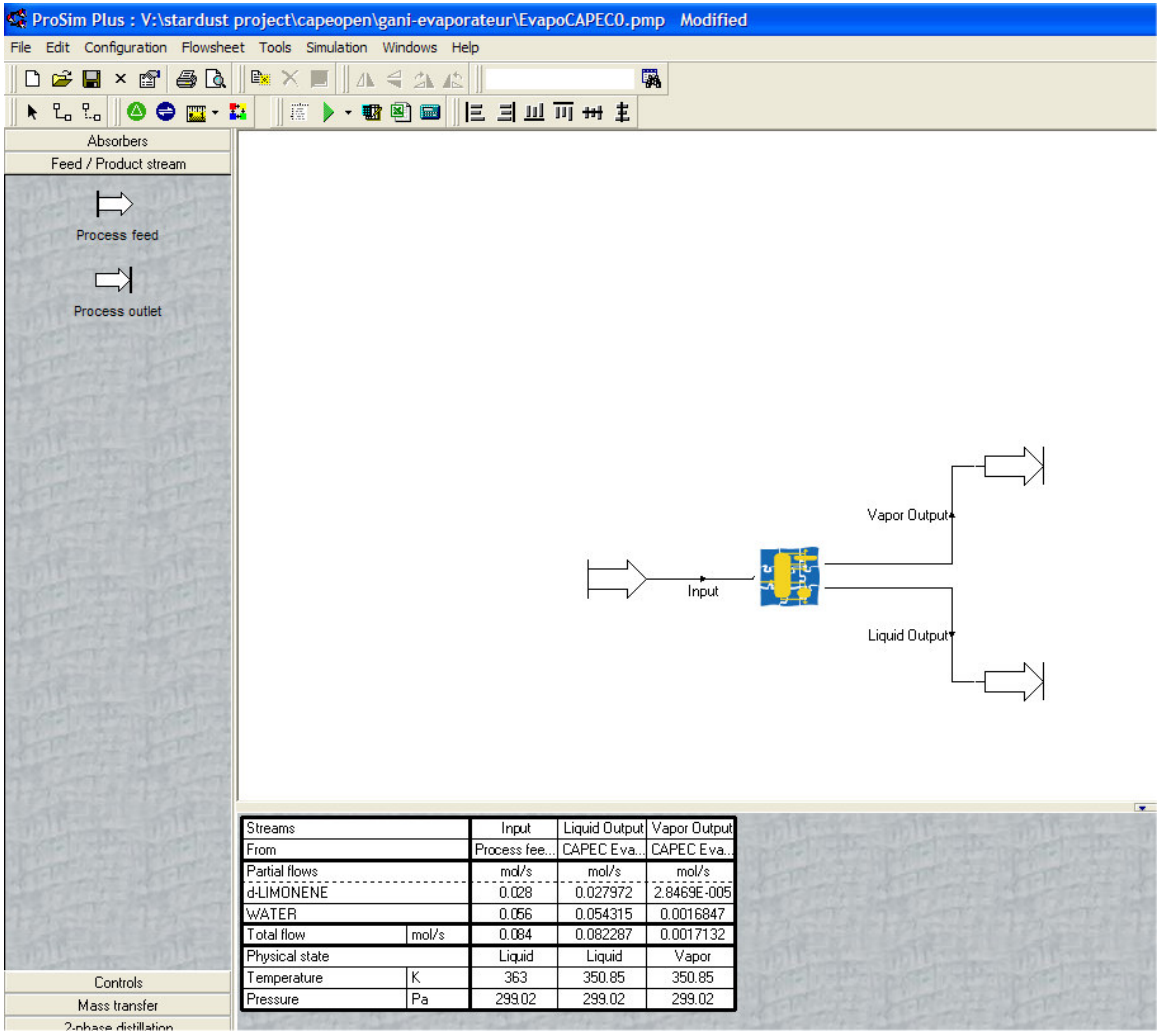
Case Study 2: Unit Interface







Case Study 2: Unit Interface

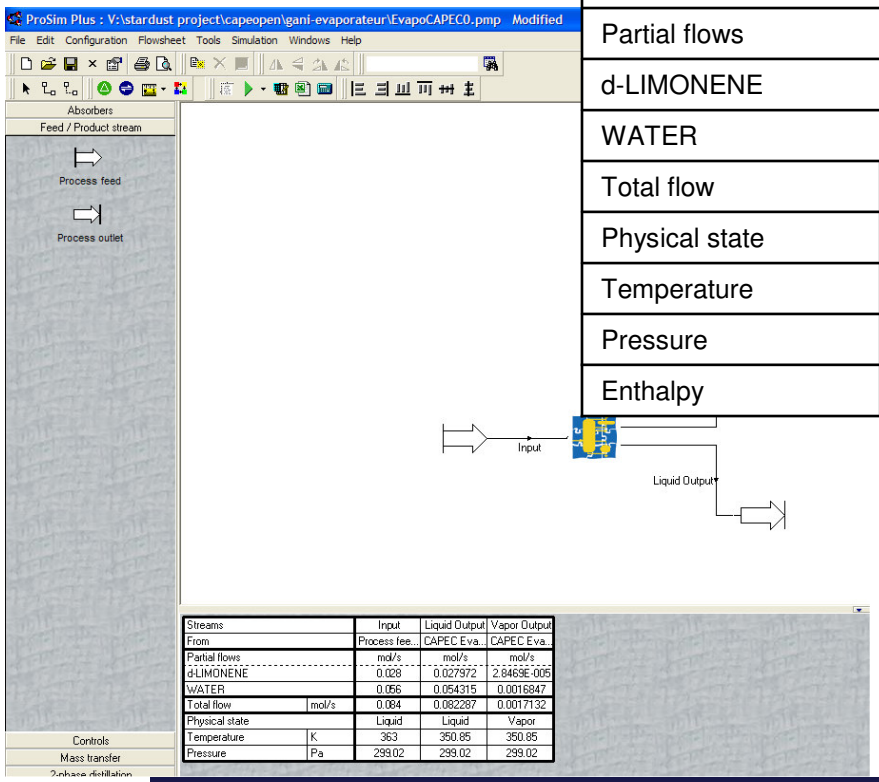


Streams		Input	Liquid Output	Vapor Output
From		Process fee...	CAPEC Eva...	CAPEC Eva...
Partial flows		mol/s	mol/s	mol/s
d-LIMONENE		0.028	0.027972	2.8469E-005
WATER		0.056	0.054315	0.0016847
Total flow	mol/s	0.084	0.082287	0.0017132
Physical state		Liquid	Liquid	Vapor
Temperature	K	363	350.85	350.85
Pressure	Pa	299.02	299.02	299.02

Case Study 2: Unit Interface

2. Short-Path Evaporator Model

Streams		Liaison 1	Liaison 2	Liaison 3
From		Entrée du procédé 1	CAPEC Evaporator	CAPEC Evaporator
Partial flows		kg/h	kg/h	kg/h
d-LIMONENE		13.7323872	0.013962354	13.71842485
WATER		3.63188448	0.109261291	3.522623189
Partial flows		mol/s	mol/s	mol/s
d-LIMONENE		0.028	2.84689E-05	0.027971531
WATER		0.056	0.001684699	0.054315301
Total flow	kg/h	17.36427168	0.123223645	17.24104803
Physical state		Vapor	Vapor	Vapor
Temperature	K	363	350.8500852	350.8500852
Pressure	Pa	299.0199192	299.0199192	299.0199192
Enthalpy	kcal/h	431.2384293	5.53628E-05	13.35118618



Conclusions

- **Through two (MoT & ProSimPlus) modelling/simulation tools, it has been shown how to apply the CO-interfaces with few additional programming effort**
- **Using the highlighted approach, any new thermo-model or unit operation model can be converted into a model object, which is then connected to a simulation environment supporting CO-interfaces, thereby achieving plug & play (interoperability) of software tools and models**
- **Current and future work is extending this approach to other modelling problems, such as, parameter estimation, customized simulators, and modelling for product behaviour analysis**