

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

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- 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

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

1. MoT

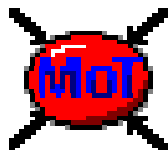
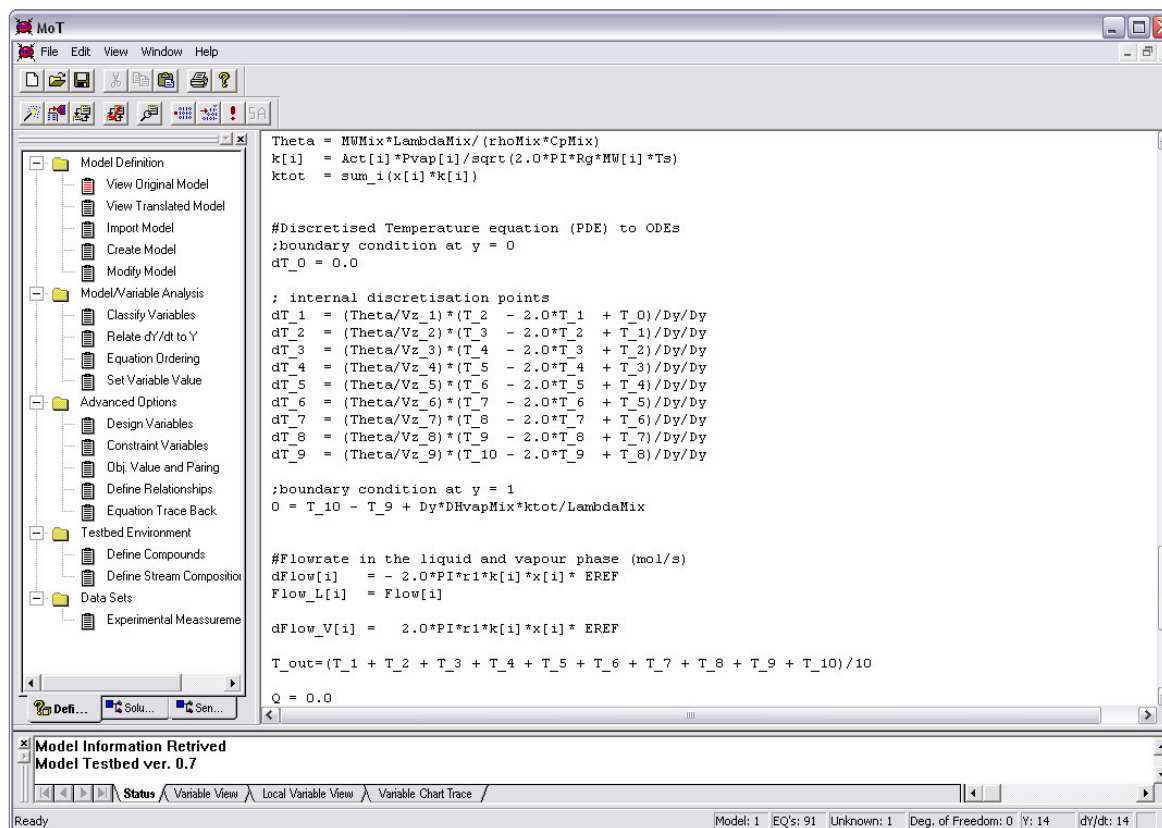


2. ProSim

- 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 Pairing
  Define Relationships
  Equation Trace Back
Testbed Environment
  Define Compounds
  Define Stream Composition
Data Sets
  Experimental Measureme

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

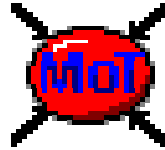
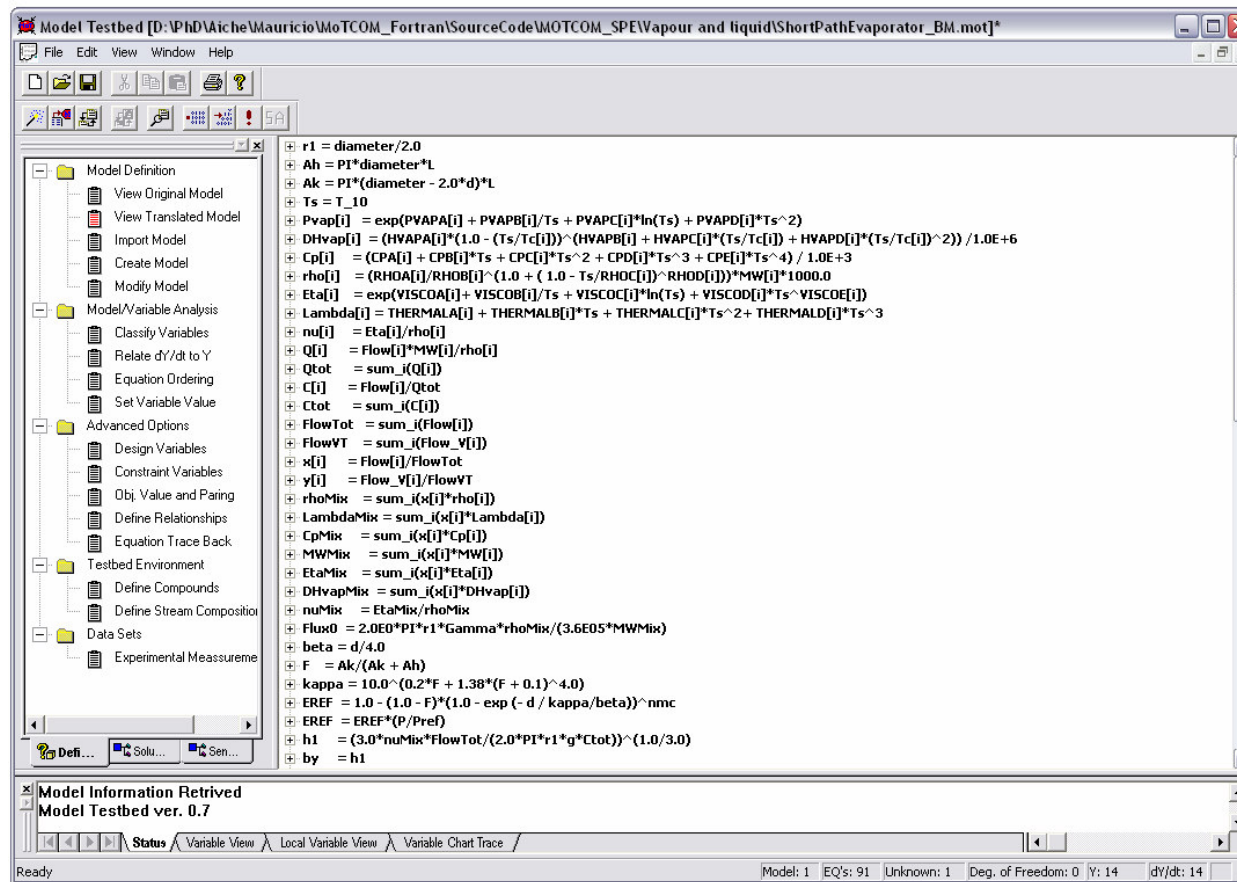
Q = 0.0
    
```

Model Information Retrieved
Model Testbed ver. 0.7

Ready Model: 1 EQ's: 91 Unknown: 1 Deg. of Freedom: 0 Y: 14 dy/dt: 14



1. MoT

```

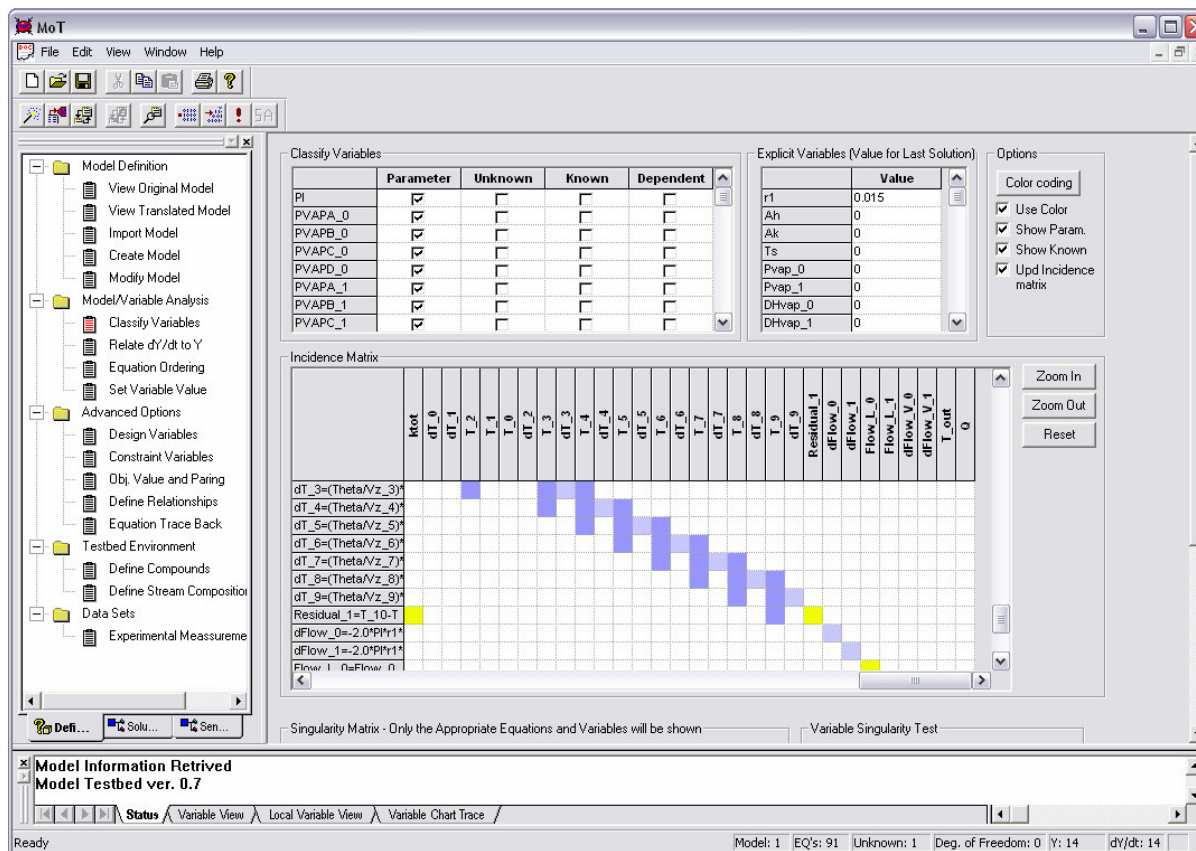
Model Testbed [D:\PhD\Aiche\Mauricio\MoT\COM_Fortran\SourceCode\MOTCOM_SPE\vapour and liquid\ShortPathEvaporator_BM.mot]*
File Edit View Window Help
Model Definition
  View Original Model
  View Translated Model
  Import Model
  Create Model
  Modify Model
Model/Variable Analysis
  Classify Variables
  Relate dy/dt to Y
  Equation Ordering
  Set Variable Value
Advanced Options
  Design Variables
  Constraint Variables
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Testbed Environment
  Define Compounds
  Define Stream Composition
  Data Sets
  Experimental Measureme

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^2 + 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

Model Information Retrieved
Model Testbed ver. 0.7
Ready
Model: 1 EQ's: 91 Unknown: 1 Deg. of Freedom: 0 Y: 14 dy/dt: 14
  
```



1. MoT

Classify Variables

	Parameter	Unknown	Known	Dependent
PI	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PVAPA_0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PVAPB_0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PVAPC_0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PVAPD_0	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PVAPA_1	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PVAPB_1	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
PVAPC_1	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Explicit Variables (Value for Last Solution)

	Value
r1	0.015
Ah	0
Ak	0
Ts	0
Pvvp_0	0
Pvvp_1	0
DHvp_0	0
DHvp_1	0

Incidence Matrix

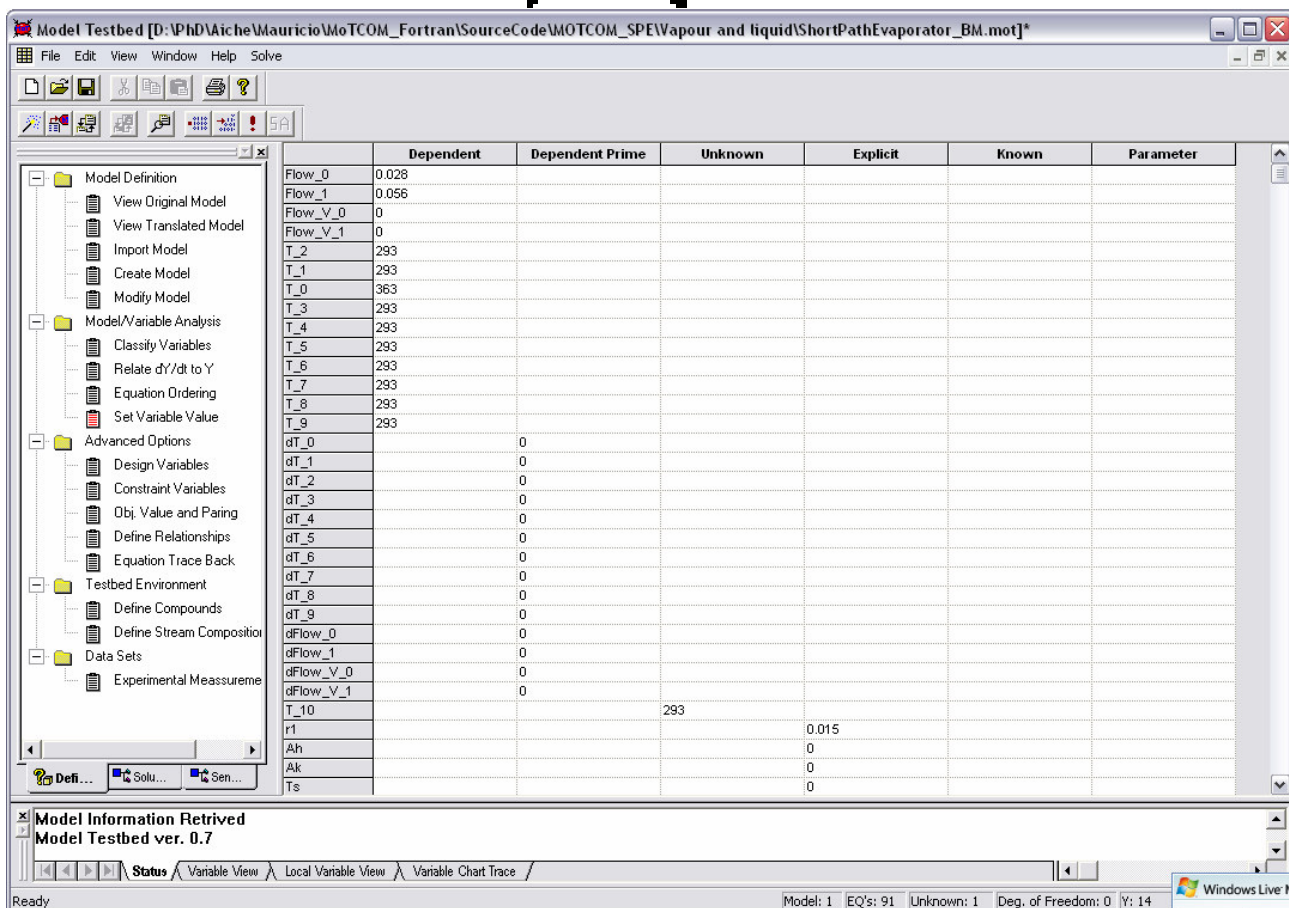
	root	dT_0	dT_1	T_2	T_1	T_0	dT_2	T_3	dT_3	T_4	dT_4	T_5	dT_5	T_6	dT_6	T_7	dT_7	T_8	dT_8	T_9	Residual_1	dFlow_0	Flow_L_0	Flow_L_1	dFlow_V_0	dFlow_V_1	T_out	0		
dT_3=(Theta/Vz_3)*																														
dT_4=(Theta/Vz_4)*																														
dT_5=(Theta/Vz_5)*																														
dT_6=(Theta/Vz_6)*																														
dT_7=(Theta/Vz_7)*																														
dT_8=(Theta/Vz_8)*																														
dT_9=(Theta/Vz_9)*																														
Residual_1=T_10-T																														
dFlow_0=-2.0*Pr1*																														
dFlow_1=-2.0*Pr1*																														
Flow_1 = 0																														

Model Information Retrieved
Model Testbed ver. 0.7

Ready Model: 1 EQ's: 91 Unknown: 1 Deg. of Freedom: 0 Y: 14 dY/dt: 14



1. MoT

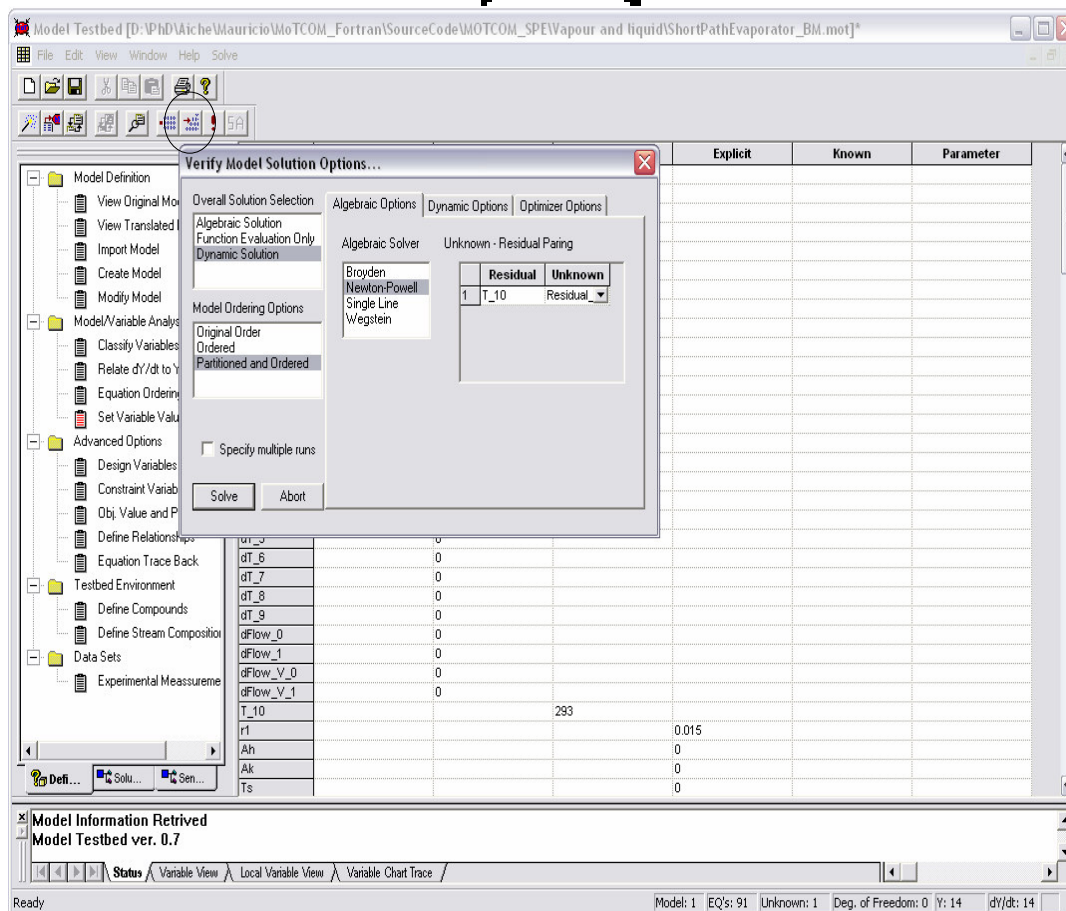



The screenshot shows the Model Testbed software interface. The main window displays a table of variables and their properties. The table has the following columns: Variable Name, Dependent, Dependent Prime, Unknown, Explicit, Known, and Parameter.

Variable Name	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		

The interface also includes a left-hand navigation pane with categories like 'Model Definition', 'Model/Variable Analysis', 'Advanced Options', 'Testbed Environment', and 'Data Sets'. At the bottom, a status bar shows 'Model: 1 | EQ's: 91 | Unknown: 1 | Deg. of Freedom: 0 | Y: 14'.

1. MoT

The screenshot shows the ProSim software interface. A dialog box titled "Verify Model Solution Options..." is open, displaying various solver options. The "Algebraic Solver" section is active, showing "Newton-Powell" selected. The "Unknown - Residual Pairing" table is visible:

Residual	Unknown
1	T_10
	Residual_

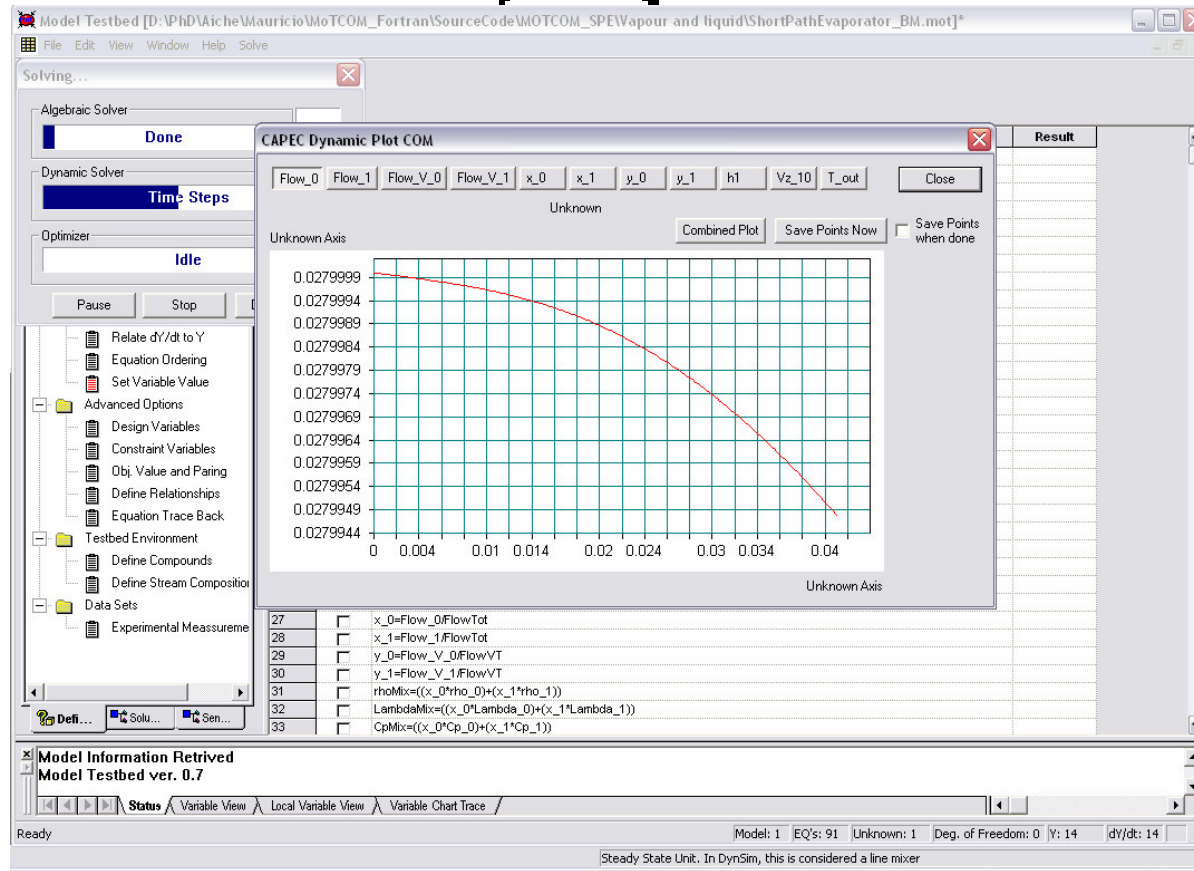
The background window shows a model testbed with a table of variables and their values:

Variable	Value	Explicit	Known	Parameter
ur_0	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			

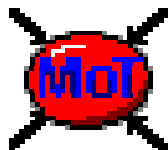
At the bottom of the interface, a status bar indicates: "Model: 1 EQ's: 91 Unknown: 1 Deg. of Freedom: 0 Y: 14 dy/dt: 14".



1. MoT



1. MoT



Model Testbed [D:\PhD\Aiche\Mauricio\MoT\COM_Fortran\SourceCode\MOTCOM_SPE\Vapour and liquid\ShortPathEvaporator_BM.mot]*

Solving...

Algebraic Solver: Done 5%

Dynamic Solver: Done

Optimizer: Idle

Equation

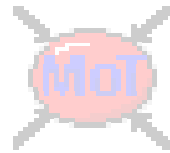
Name	Before solution	After solution
Flow_0	0.028	0.02797153109553
Flow_1	0.056	0.05431530050239
Flow_V_0	0	2.846890446949e-003
Flow_V_1	0	0.001684699497611
T_2	293	358.5347830269
T_1	293	360.7646023101
T_0	363	363
T_3	293	356.3046157996
T_4	293	354.0831547003
T_5	293	351.8732670185
T_6	293	349.680280304
T_7	293	347.5085482235
T_8	293	345.3616120615
T_9	293	343.2415031321
T_10	293	341.1484857469
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 Retrieved

Ready | Model: 1 | EQ's: 91 | Unknown: 1 | Deg. of Freedom: 0 | V: 14 | dj/dt: 14



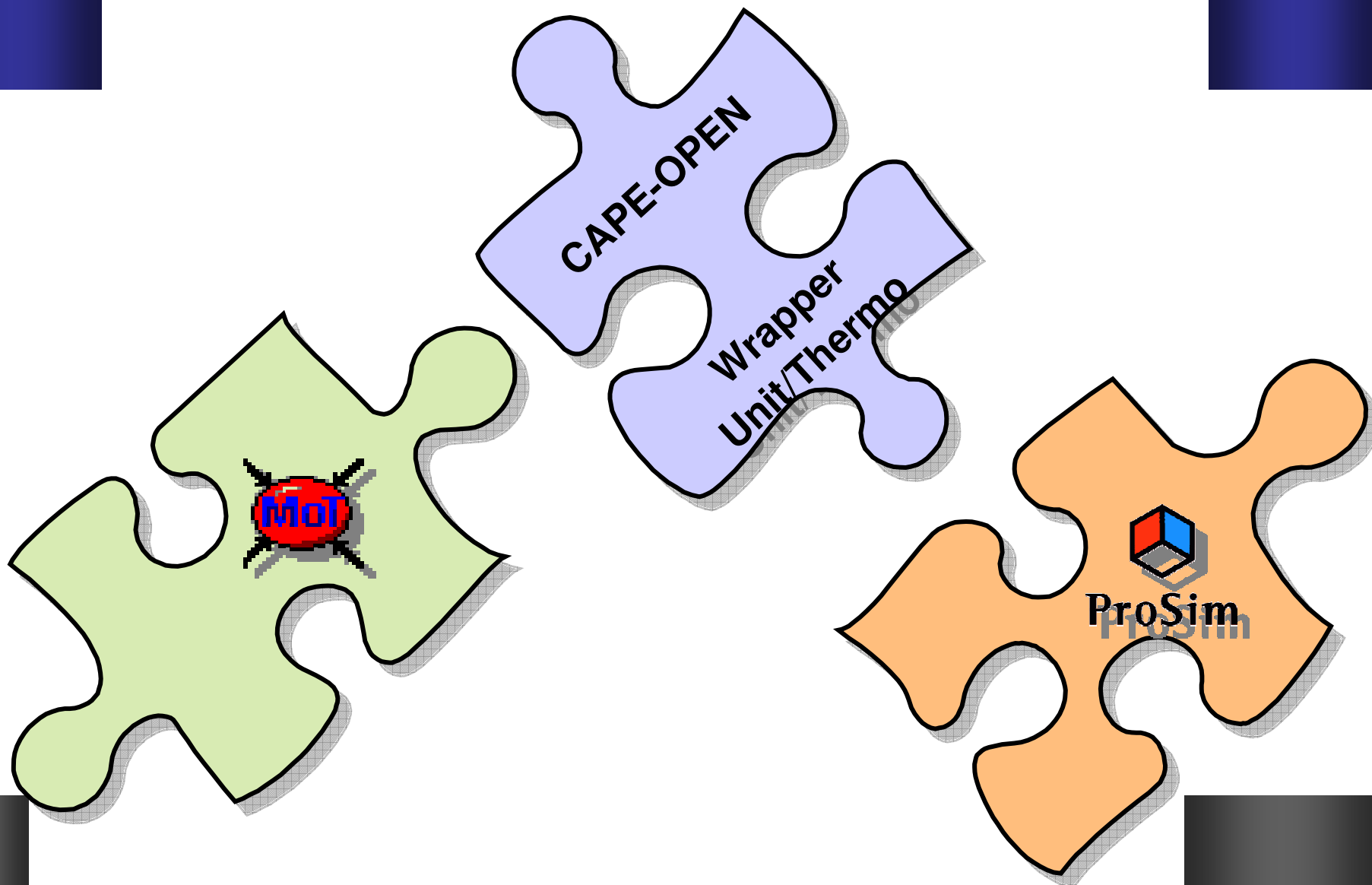
1. MoT

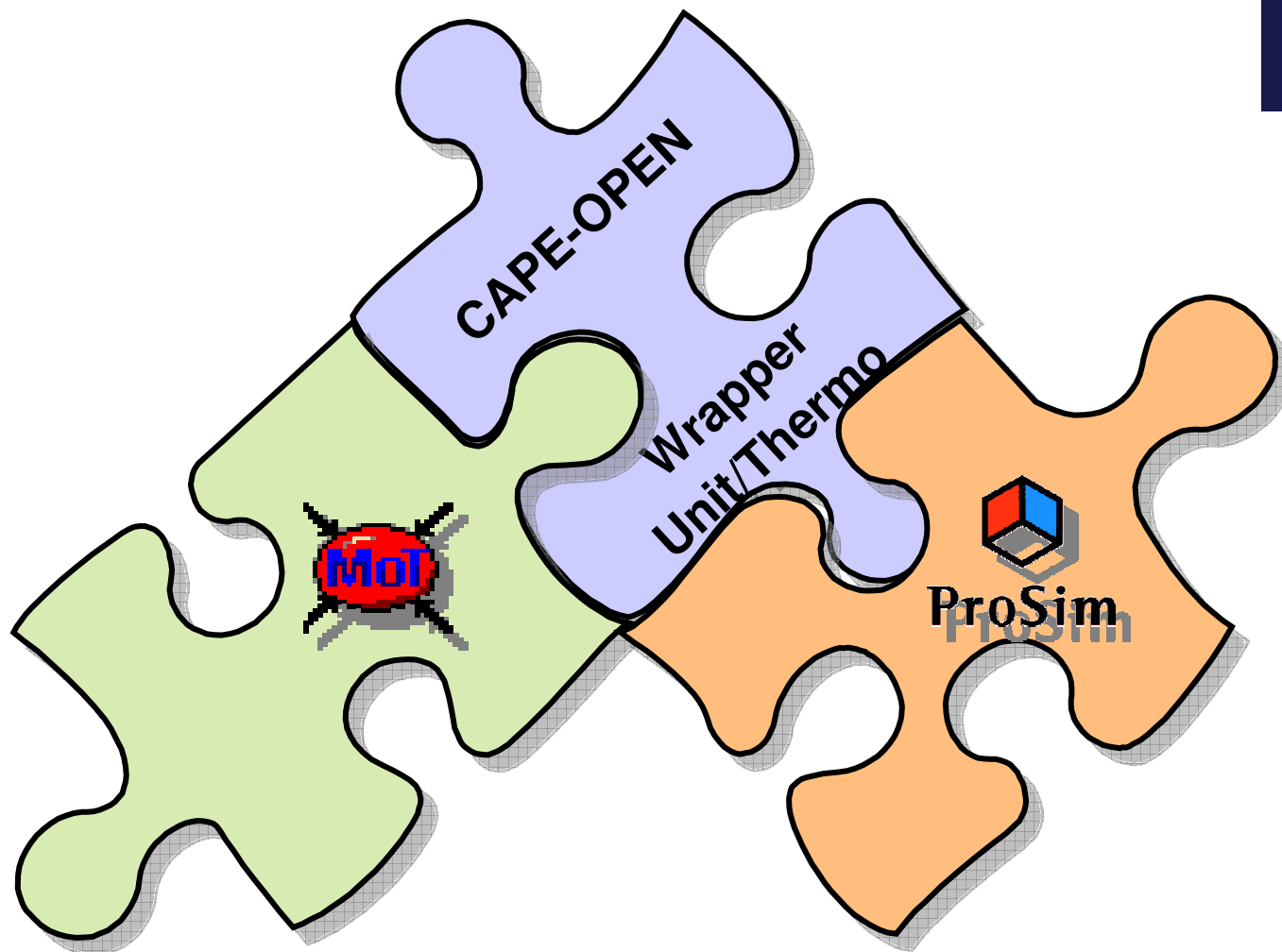


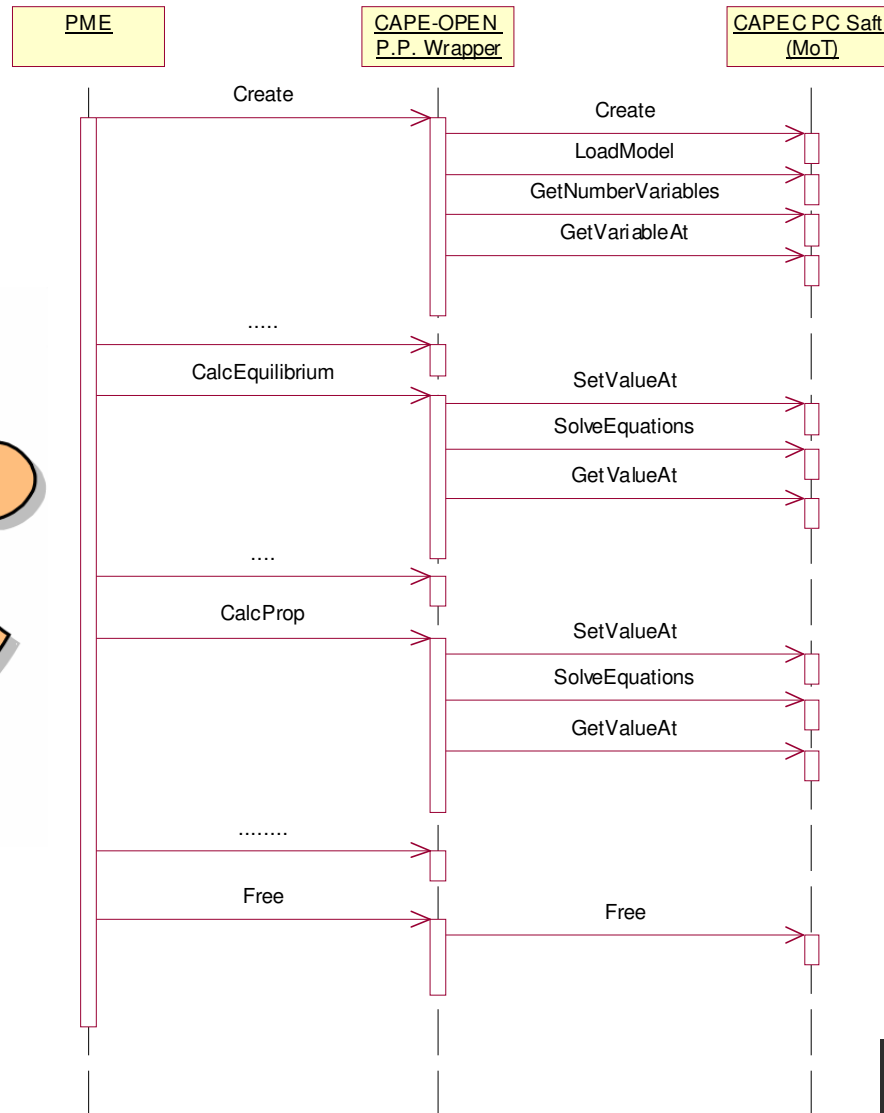
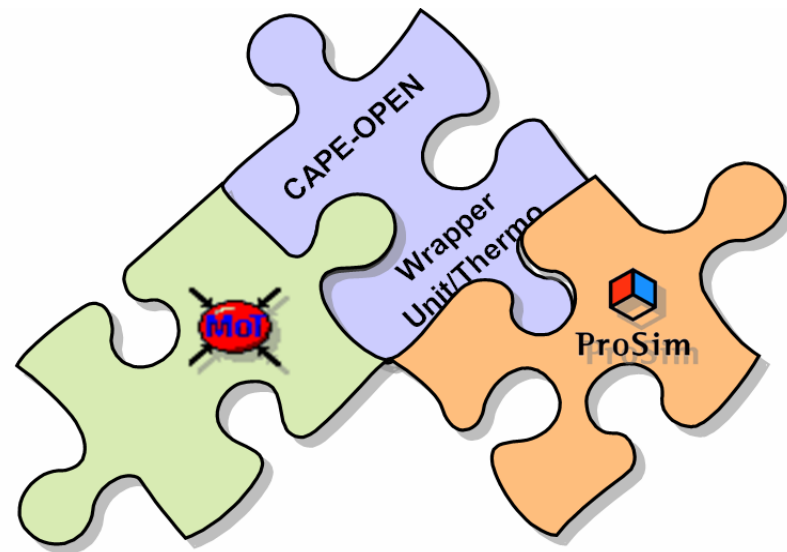
2. ProSim

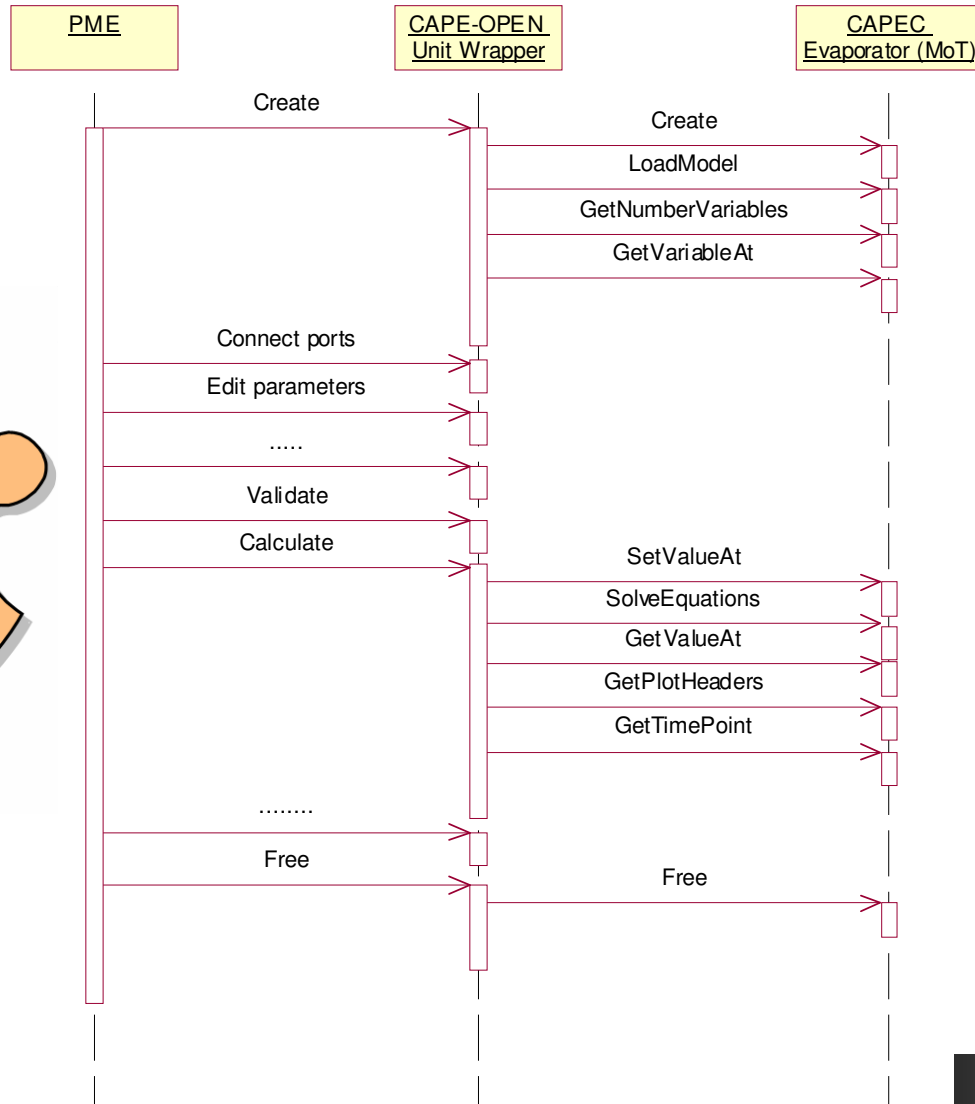
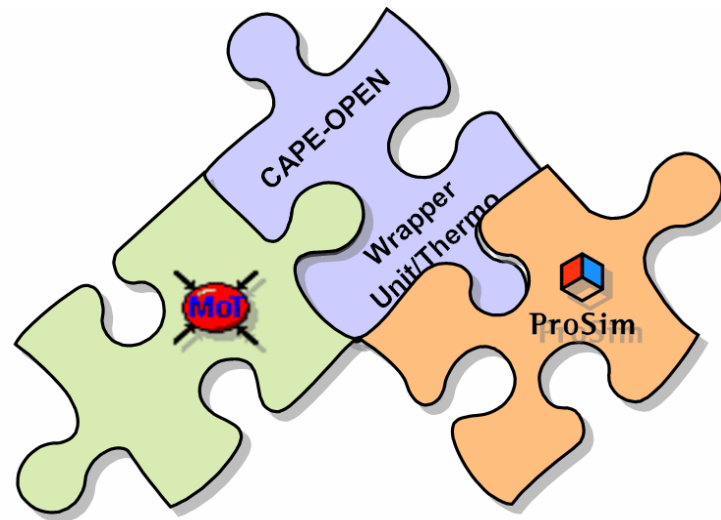
- Simulis thermodynamics
- ProSimPlus
- CO-wrapper



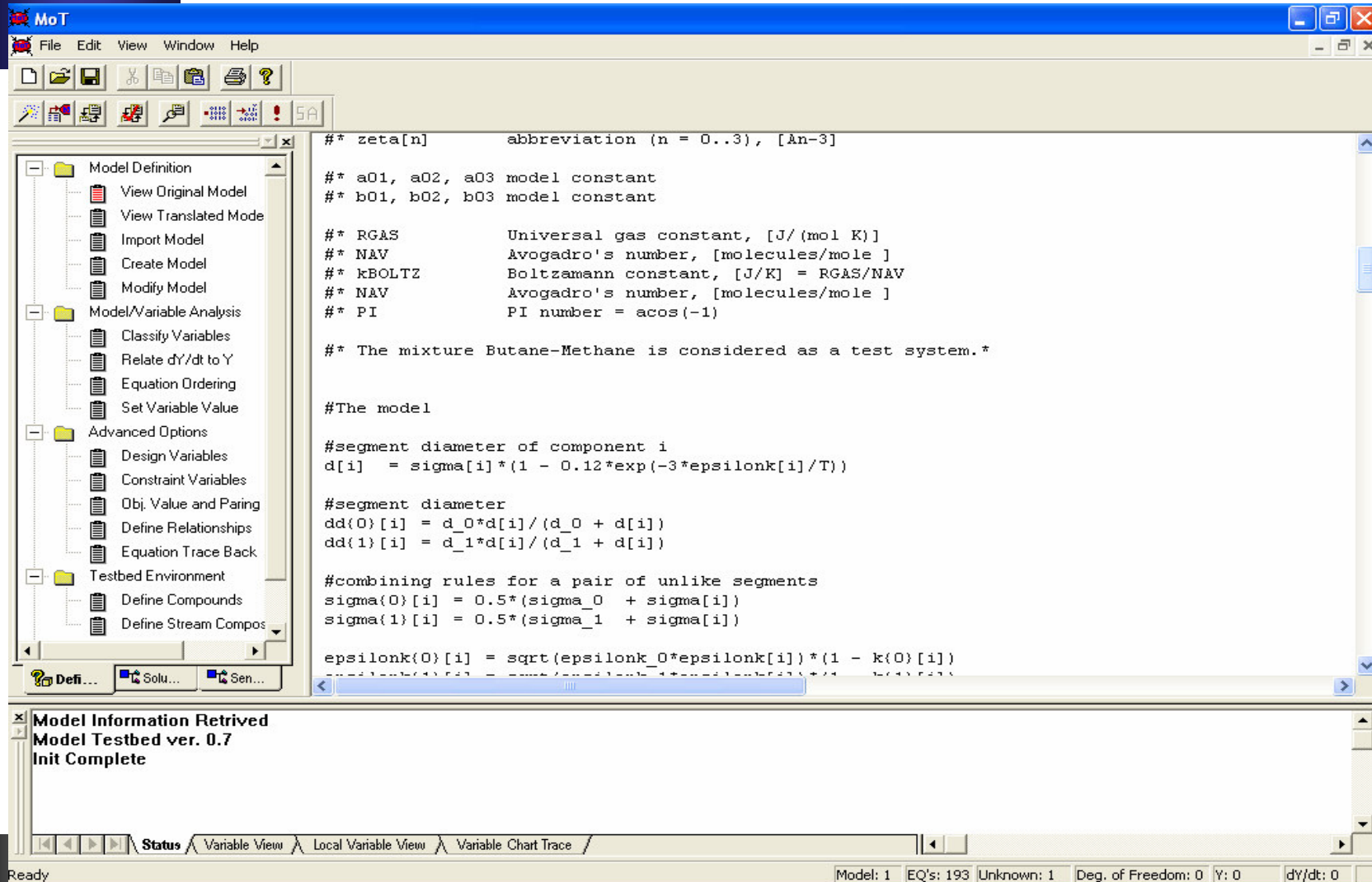








- 1. Highlights interoperability through the use of an external model (PC-SAFT) through the CO-thermo interface in ProSim, which is run from EXCEL - for a binary mixture of methane/n-butane (saturation point & property calculations)**
- 2. Highlights interoperability through the use of an external unit 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**



The screenshot shows the MoT software interface. The main window displays the following code:

```

** zeta[n]      abbreviation (n = 0..3), [Ån-3]

** a01, a02, a03 model constant
** b01, b02, b03 model constant

** RGAS        Universal gas constant, [J/(mol K)]
** NAV         Avogadro's number, [molecules/mole]
** kBOLTZ      Boltzmann constant, [J/K] = RGAS/NAV
** NAV         Avogadro's number, [molecules/mole]
** PI          PI number = acos(-1)

** The mixture Butane-Methane is considered as a test system.*

#The model

#segment diameter of component i
d[i] = sigma[i]*(1 - 0.12*exp(-3*epsilonk[i]/T))

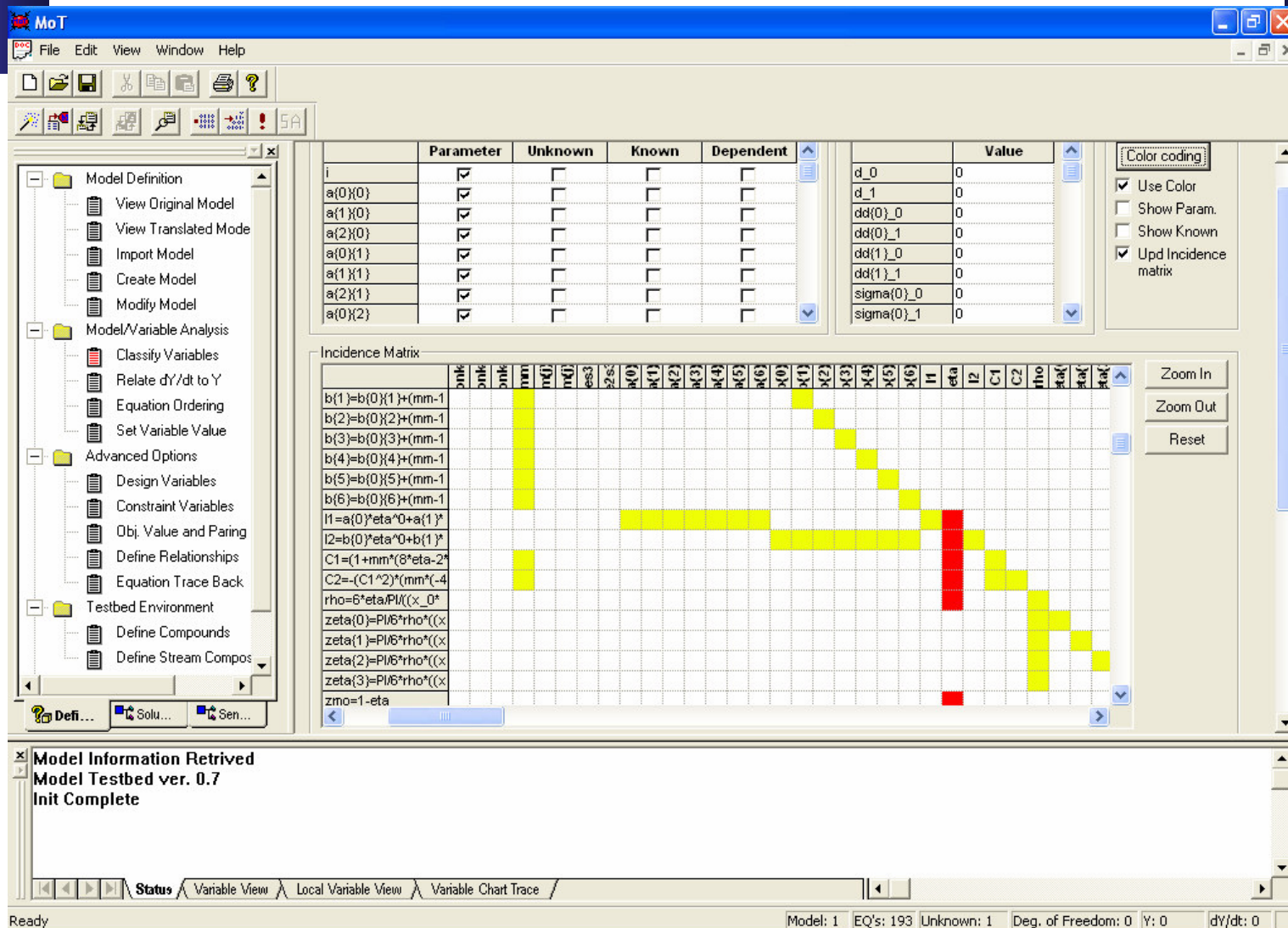
#segment diameter
dd(0)[i] = d_0*d[i]/(d_0 + d[i])
dd(1)[i] = d_1*d[i]/(d_1 + d[i])

#combining rules for a pair of unlike segments
sigma(0)[i] = 0.5*(sigma_0 + sigma[i])
sigma(1)[i] = 0.5*(sigma_1 + sigma[i])

epsilonk(0)[i] = sqrt(epsilonk_0*epsilonk[i]*(1 - k(0)[i]))
epsilonk(1)[i] = sqrt(epsilonk_1*epsilonk[i]*(1 - k(1)[i]))

```

The left sidebar shows a tree view with categories: Model Definition, Model/Variable Analysis, Advanced Options, and Testbed Environment. The bottom status bar indicates: Ready, Model: 1, EQ's: 193, Unknown: 1, Deg. of Freedom: 0, Y: 0, dY/dt: 0.



MoT

File Edit View Window Help

Model Definition

- View Original Model
- View Translated Mode
- 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

- Define Compounds
- Define Stream Compos

Parameter	Unknown	Known	Dependent
i	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
a(0){0}	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
a(1){0}	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
a(2){0}	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
a(0){1}	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
a(1){1}	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
a(2){1}	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>
a(0){2}	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="checkbox"/>

Value	
d_0	0
d_1	0
dd(0)_0	0
dd(0)_1	0
dd(1)_0	0
dd(1)_1	0
sigma(0)_0	0
sigma(0)_1	0

Incidence Matrix

	bnk	bnk	bnk	mm	ndf	ndf	ess3	2ss	a(0)	a(1)	a(2)	a(3)	a(4)	a(5)	a(6)	a(0)	a(1)	a(2)	a(3)	a(4)	a(5)	a(6)	l1	eta	l2	C1	C2	rho	zeta	zeta	zeta	zeta	zmo		
b(1)=b(0){1}+(mm-1																																			
b(2)=b(0){2}+(mm-1																																			
b(3)=b(0){3}+(mm-1																																			
b(4)=b(0){4}+(mm-1																																			
b(5)=b(0){5}+(mm-1																																			
b(6)=b(0){6}+(mm-1																																			
l1=a(0)*eta^0+a(1)^2																																			
l2=b(0)*eta^0+b(1)^2																																			
C1=(1+mm*(8*eta-2*																																			
C2=-(C1^2)*(mm*-4																																			
rho=6*eta/PI/(x_0*																																			
zeta(0)=PI/6*rho*(x																																			
zeta(1)=PI/6*rho*(x																																			
zeta(2)=PI/6*rho*(x																																			
zeta(3)=PI/6*rho*(x																																			
zmo=1-eta																																			

Model Information Retrieved
Model Testbed ver. 0.7
Init Complete

Status Variable View Local Variable View Variable Chart Trace

Ready Model: 1 EQ's: 193 Unknown: 1 Deg. of Freedom: 0 Y: 0 dy/dt: 0

Model Testbed [C:\Prosim\PCSAft\PC_SAFT_PHI_BM.mot]*

File Edit View Window Help Solve

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

- Define Compounds
- Define Stream Compos

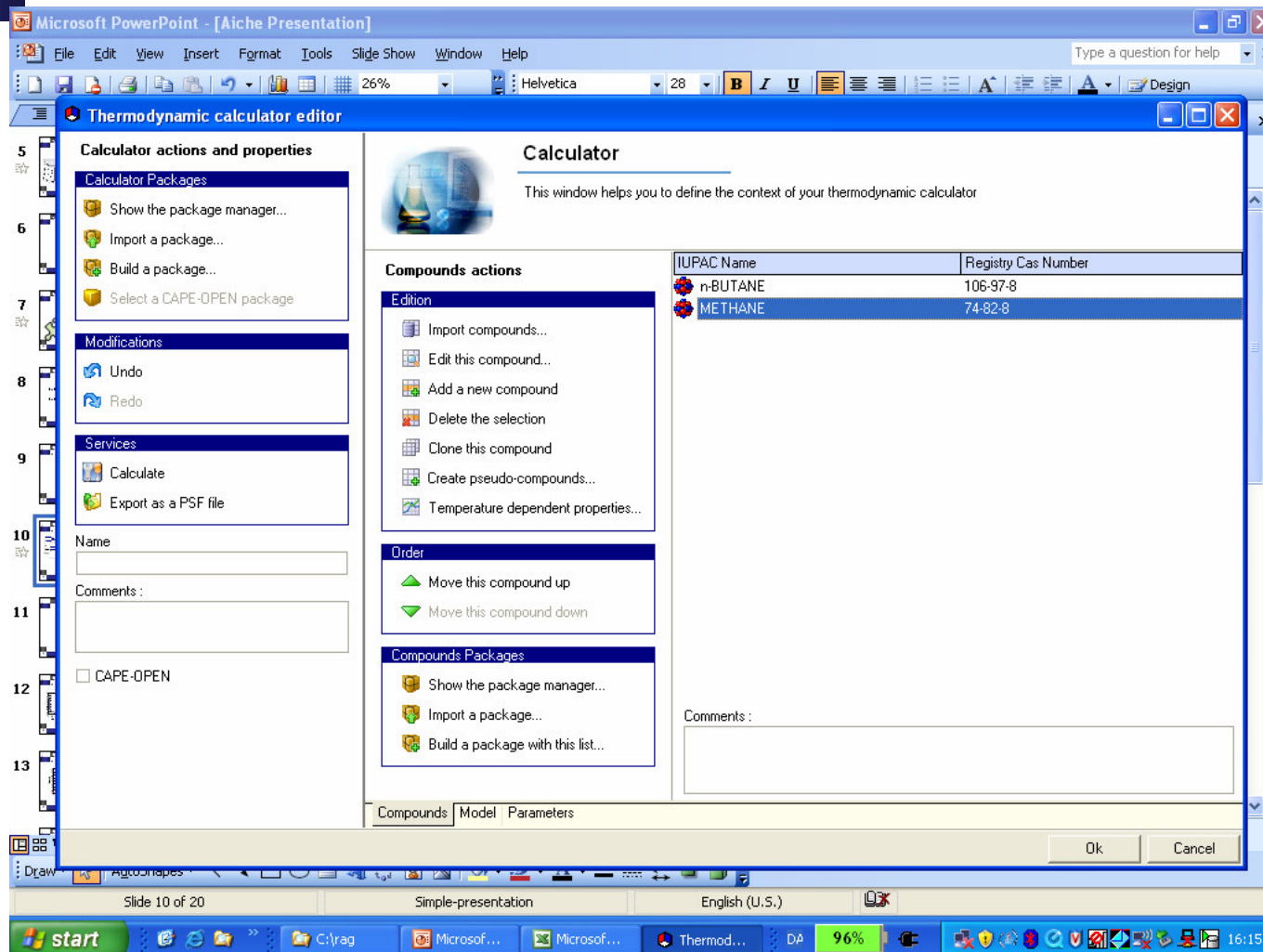
Break	Equation	Result
<input type="checkbox"/>	d_0=sigma_0*(1-0.12*exp(-3*epsilon_k_0/T))	3.65638
<input type="checkbox"/>	d_1=sigma_1*(1-0.12*exp(-3*epsilon_k_1/T))	3.60761
<input type="checkbox"/>	dd(0)_0=d_0*d_0/(d_0+d_0)	1.82819
<input type="checkbox"/>	dd(0)_1=d_0*d_1/(d_0+d_1)	1.81592
<input type="checkbox"/>	dd(1)_0=d_1*d_0/(d_1+d_0)	1.81592
<input type="checkbox"/>	dd(1)_1=d_1*d_1/(d_1+d_1)	1.80381
<input type="checkbox"/>	sigma(0)_0=0.5*(sigma_0+sigma_0)	3.70241
<input type="checkbox"/>	sigma(0)_1=0.5*(sigma_0+sigma_1)	3.70315
<input type="checkbox"/>	sigma(1)_0=0.5*(sigma_1+sigma_0)	3.70315
<input type="checkbox"/>	sigma(1)_1=0.5*(sigma_1+sigma_1)	3.70389
<input checked="" type="checkbox"/>	epsilon_k(0)_0=sqrt(epsilon_k_0*epsilon_k_0)*(1-k(0)_0)	
<input type="checkbox"/>	epsilon_k(0)_1=sqrt(epsilon_k_0*epsilon_k_1)*(1-k(0)_1)	
<input type="checkbox"/>	epsilon_k(1)_0=sqrt(epsilon_k_1*epsilon_k_0)*(1-k(1)_0)	
<input type="checkbox"/>	epsilon_k(1)_1=sqrt(epsilon_k_1*epsilon_k_1)*(1-k(1)_1)	
<input type="checkbox"/>	mm=((x_0*m_0)+(x_1*m_1))	
<input type="checkbox"/>	sum(j)_0=((x_0*x_0*m_0*m_0*(epsilon_k(0)_0/T)*sigma(0)_0^3)+(x_0*x_1*m_0*m_1*(epsilon_k(0)_1/T)*sigma(0)_1^3))	
<input type="checkbox"/>	sum(j)_1=((x_1*x_0*m_1*m_0*(epsilon_k(1)_0/T)*sigma(1)_0^3)+(x_1*x_1*m_1*m_1*(epsilon_k(1)_1/T)*sigma(1)_1^3))	
<input type="checkbox"/>	m2es3_m=((sum(j)_0)+(sum(j)_1))	
<input type="checkbox"/>	sum(j)_0=((x_0*x_0*m_0*m_0*(epsilon_k(0)_0/T)^2*sigma(0)_0^3)+(x_0*x_1*m_0*m_1*(epsilon_k(0)_1/T)^2*sigma(0)_1^3)	
<input type="checkbox"/>	sum(j)_1=((x_1*x_0*m_1*m_0*(epsilon_k(1)_0/T)^2*sigma(1)_0^3)+(x_1*x_1*m_1*m_1*(epsilon_k(1)_1/T)^2*sigma(1)_1^3)	
<input type="checkbox"/>	m2e2s3_m=((sum(j)_0)+(sum(j)_1))	
<input type="checkbox"/>	a(0)=a(0){0}+(mm-1)/mm*a(1){0}+(mm-1)/mm*(mm-2)/mm*a(2){0}	
<input type="checkbox"/>	a(1)=a(0){1}+(mm-1)/mm*a(1){1}+(mm-1)/mm*(mm-2)/mm*a(2){1}	
<input type="checkbox"/>	a(2)=a(0){2}+(mm-1)/mm*a(1){2}+(mm-1)/mm*(mm-2)/mm*a(2){2}	
<input type="checkbox"/>	a(3)=a(0){3}+(mm-1)/mm*a(1){3}+(mm-1)/mm*(mm-2)/mm*a(2){3}	
<input type="checkbox"/>	a(4)=a(0){4}+(mm-1)/mm*a(1){4}+(mm-1)/mm*(mm-2)/mm*a(2){4}	
<input type="checkbox"/>	a(5)=a(0){5}+(mm-1)/mm*a(1){5}+(mm-1)/mm*(mm-2)/mm*a(2){5}	
<input type="checkbox"/>	a(6)=a(0){6}+(mm-1)/mm*a(1){6}+(mm-1)/mm*(mm-2)/mm*a(2){6}	

Model Information Retrieved
Model Testbed ver. 0.7
Init Complete

Status Variable View Local Variable View Variable Chart Trace

Ready Model: 1 EQ's: 193 Unknown: 1 Deg. of Freedom: 0 Y: 0 dY/dt: 0

1. External Thermo-model (PC-SAFT)



Thermodynamic calculator editor

Calculator actions and properties

- Calculator Packages
 - Show the package manager...
 - Import a package...
 - Build a package...
 - Select a CAPE-OPEN package
- Modifications
 - Undo
 - Redo
- Services
 - Calculate
 - Export as a PSF file

Name:

Comments:

CAPE-OPEN

Calculator

This window helps you to define the context of your thermodynamic calculator

Compounds actions

- Edition
 - Import compounds...
 - Edit this compound...
 - Add a new compound
 - Delete the selection
 - Clone this compound
 - Create pseudo-compounds...
 - Temperature dependent properties...
- Order
 - Move this compound up
 - Move this compound down
- Compounds Packages
 - Show the package manager...
 - Import a package...
 - Build a package with this list...

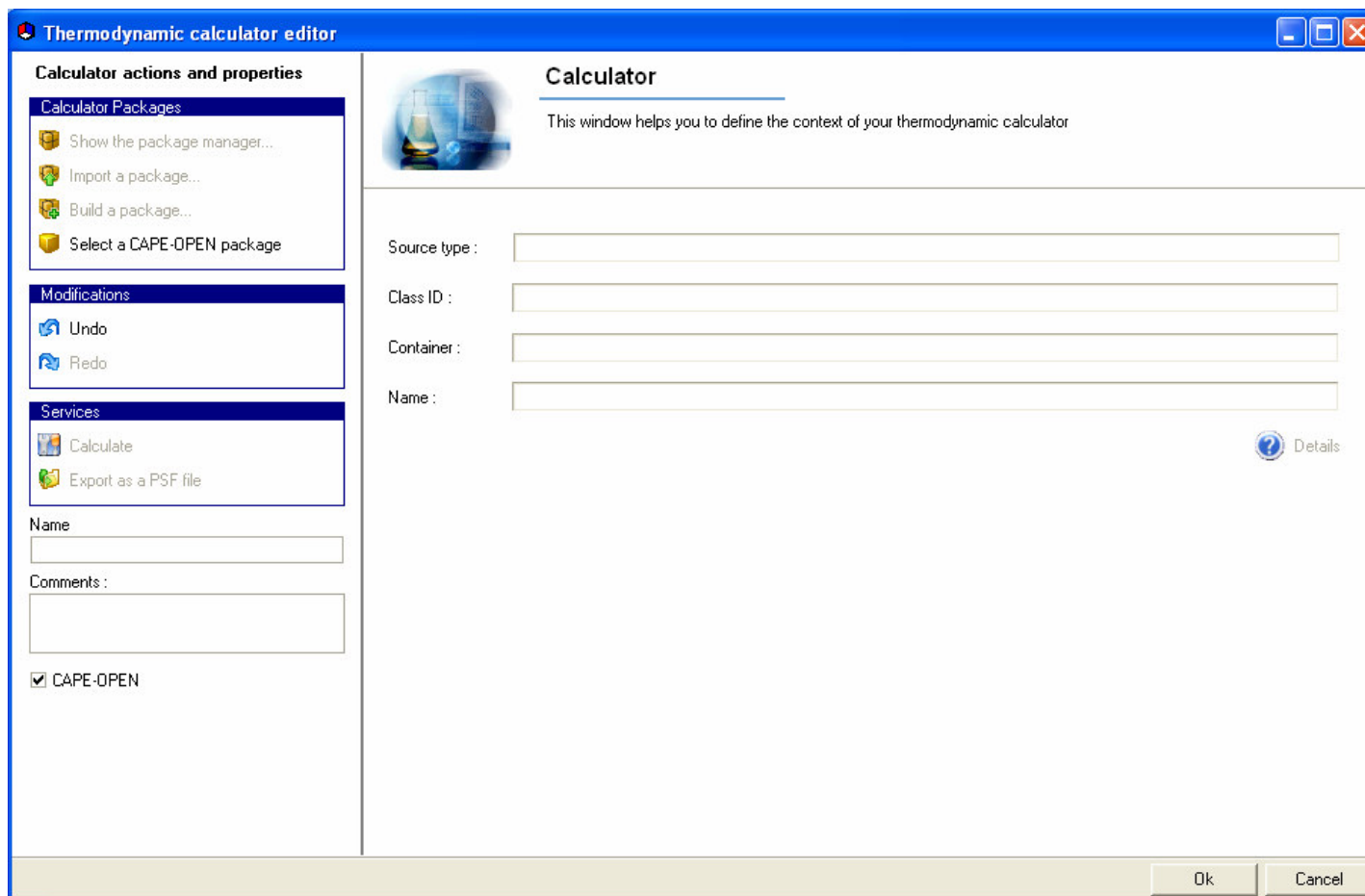
IUPAC Name	Registry Cas Number
n-BUTANE	106-97-8
METHANE	74-82-8

Comments:

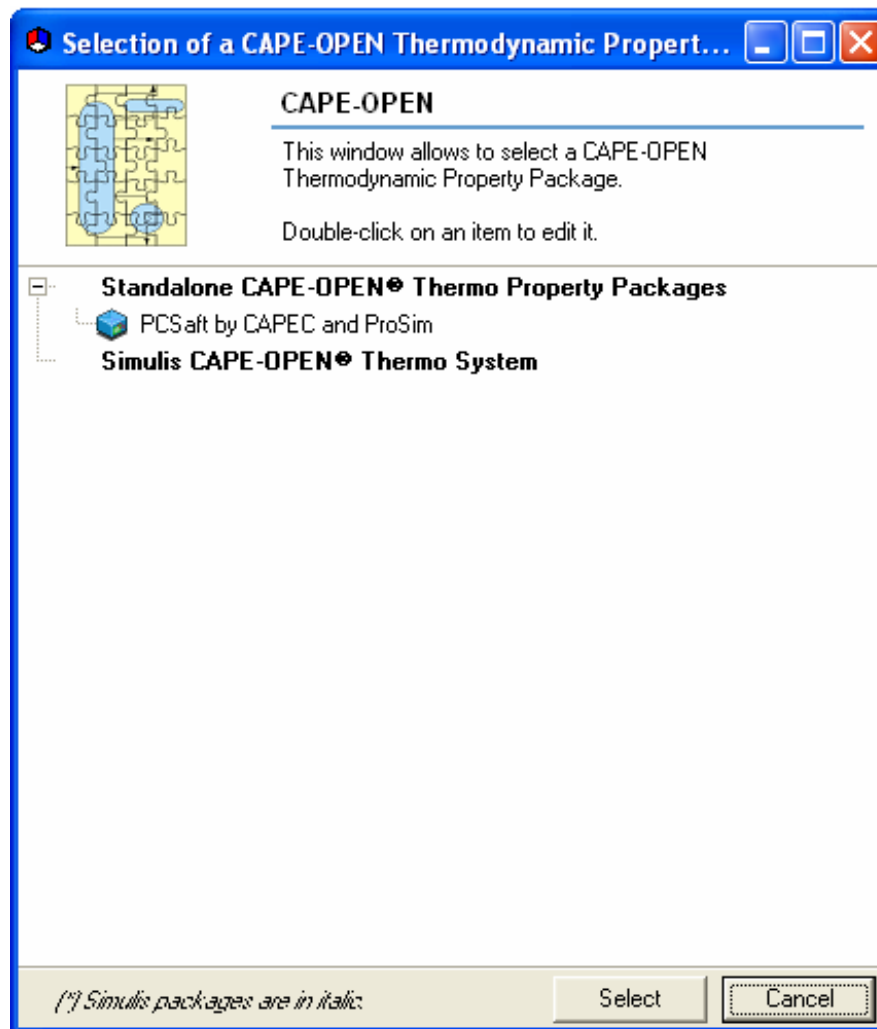
Compounds | Model | Parameters

Ok Cancel

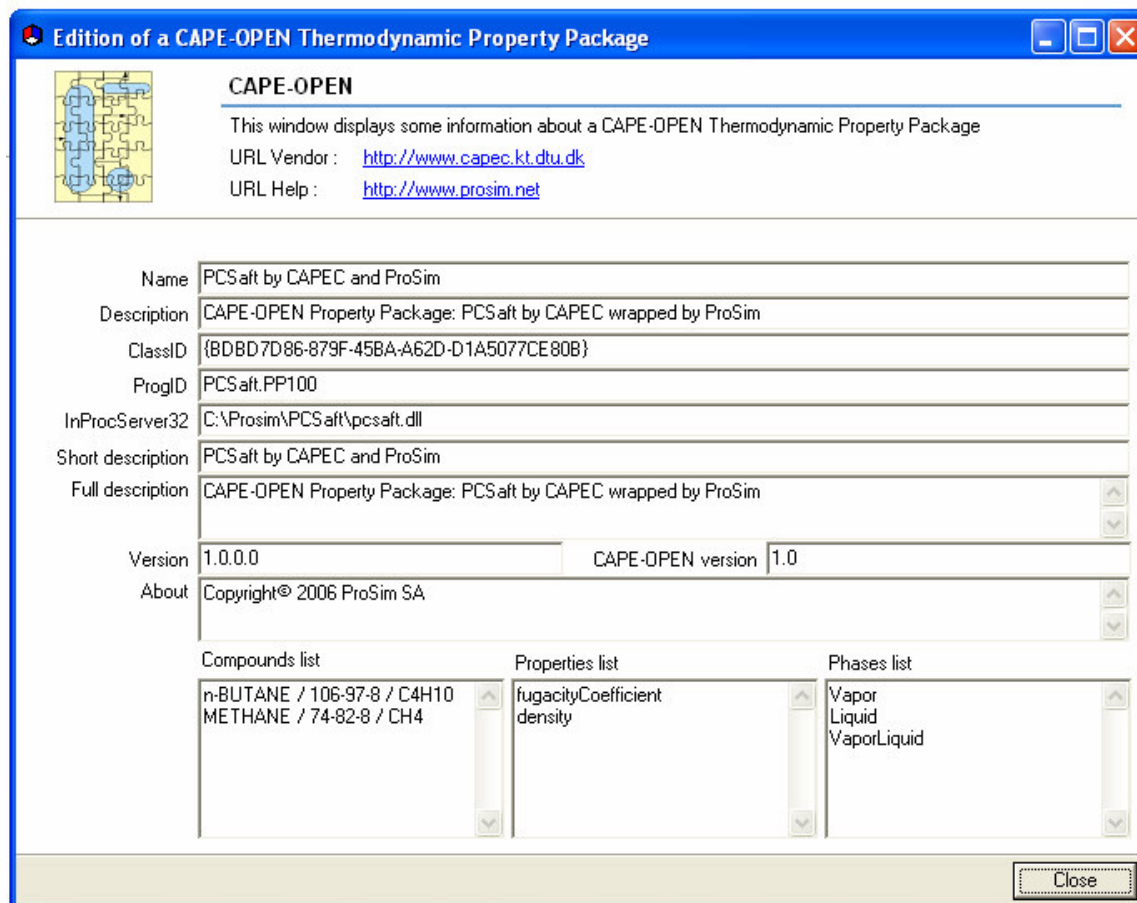
1. External Thermo-model (PC-SAFT)



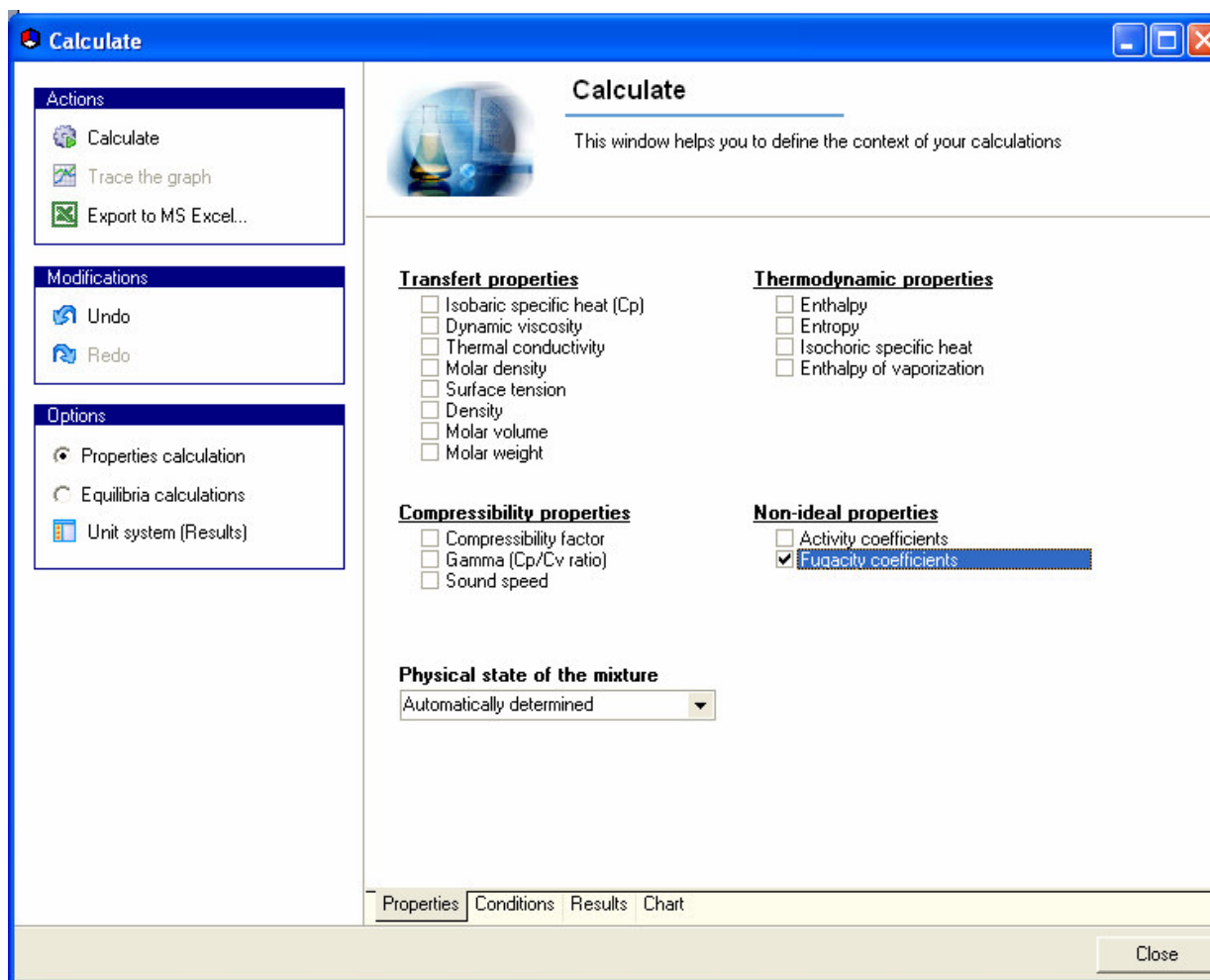
1. External Thermo-model (PC-SAFT)



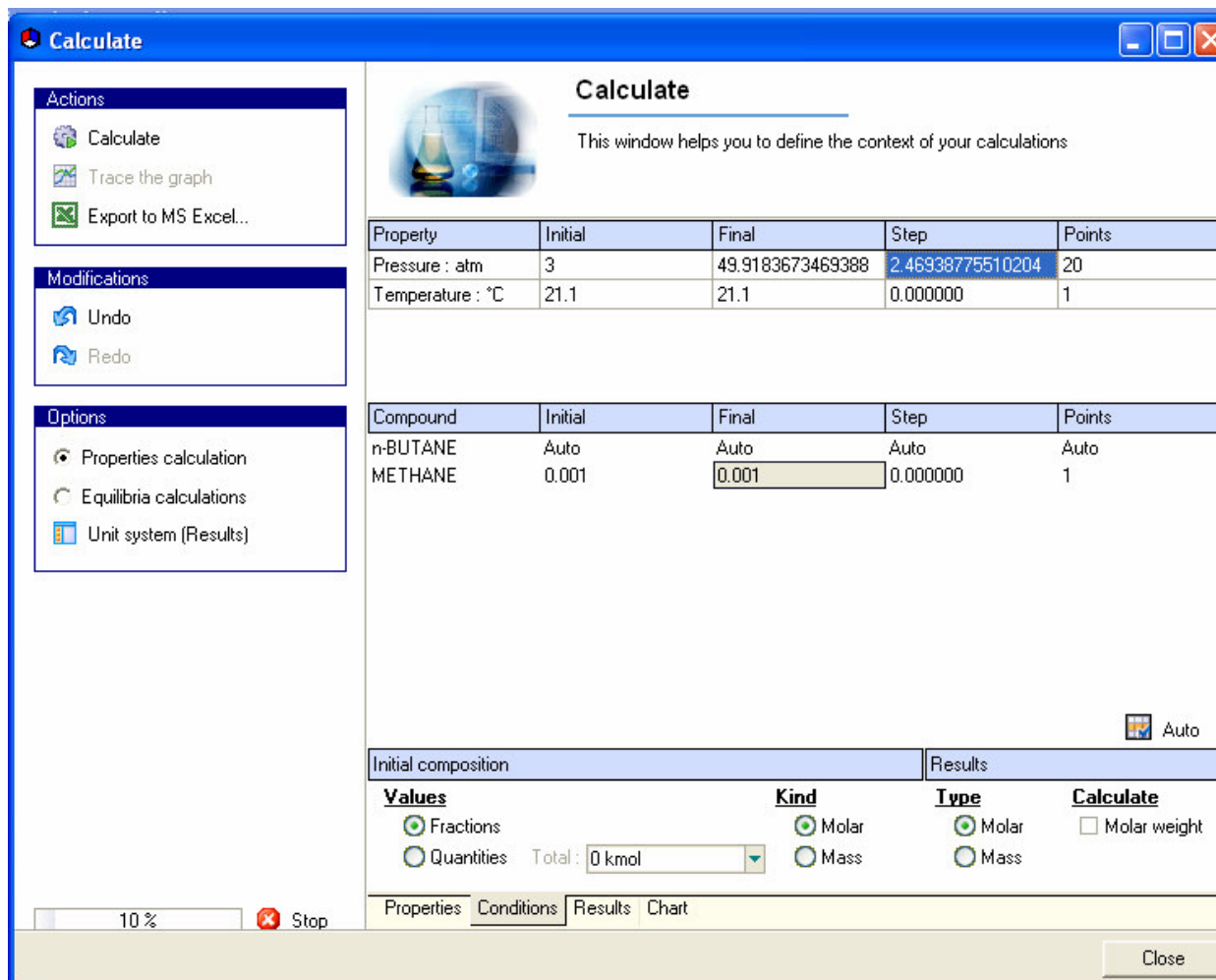
1. External Thermo-model (PC-SAFT)



1. External Thermo-model (PC-SAFT)



1. External Thermo-model (PC-SAFT)



Calculate

This window helps you to define the context of your calculations

Property	Initial	Final	Step	Points
Pressure : atm	3	49.9183673469388	2.46938775510204	20
Temperature : °C	21.1	21.1	0.000000	1

Compound	Initial	Final	Step	Points
n-BUTANE	Auto	Auto	Auto	Auto
METHANE	0.001	0.001	0.000000	1

Auto

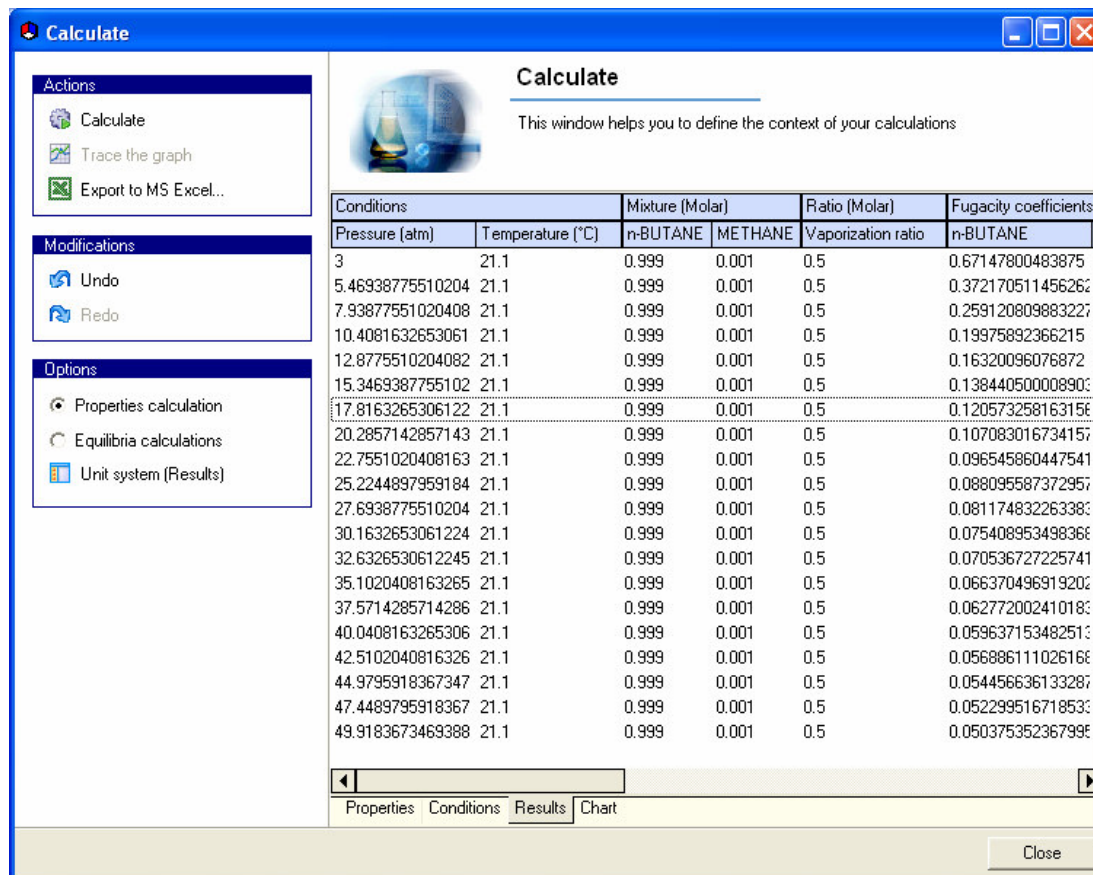
Initial composition		Results	
Values	Kind	Type	Calculate
<input checked="" type="radio"/> Fractions	<input checked="" type="radio"/> Molar	<input checked="" type="radio"/> Molar	<input type="checkbox"/> Molar weight
<input type="radio"/> Quantities Total: 0 kmol	<input type="radio"/> Mass	<input type="radio"/> Mass	

10% Stop

Properties Conditions Results Chart

Close

1. External Thermo-model (PC-SAFT)



Calculate

This window helps you to define the context of your calculations

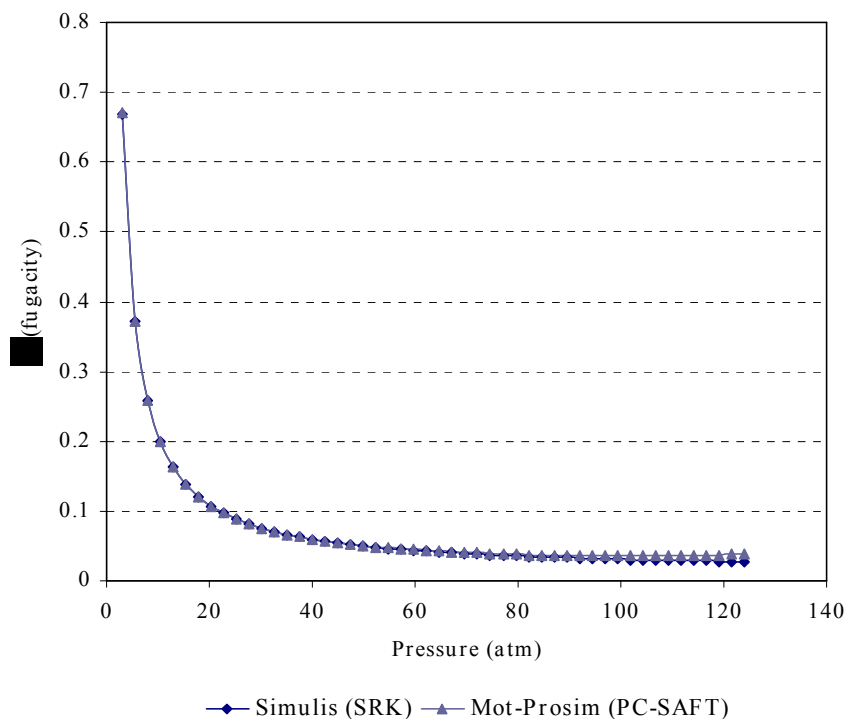
Conditions		Mixture (Molar)		Ratio (Molar)	Fugacity coefficients (
Pressure (atm)	Temperature (°C)	n-BUTANE	METHANE	Vaporization ratio	n-BUTANE
3	21.1	0.999	0.001	0.5	0.67147800483875
5.46938775510204	21.1	0.999	0.001	0.5	0.37217051145626
7.93877551020408	21.1	0.999	0.001	0.5	0.25912080988322
10.4081632653061	21.1	0.999	0.001	0.5	0.19975892366215
12.8775510204082	21.1	0.999	0.001	0.5	0.16320096076872
15.3469387755102	21.1	0.999	0.001	0.5	0.13844050000890
17.8163265306122	21.1	0.999	0.001	0.5	0.12057325816315
20.2857142857143	21.1	0.999	0.001	0.5	0.10708301673415
22.7551020408163	21.1	0.999	0.001	0.5	0.09654586044754
25.2244897959184	21.1	0.999	0.001	0.5	0.08809558737295
27.6938775510204	21.1	0.999	0.001	0.5	0.08117483226338
30.1632653061224	21.1	0.999	0.001	0.5	0.07540895349836
32.6326530612245	21.1	0.999	0.001	0.5	0.07053672722574
35.1020408163265	21.1	0.999	0.001	0.5	0.06637049691920
37.5714285714286	21.1	0.999	0.001	0.5	0.06277200241018
40.0408163265306	21.1	0.999	0.001	0.5	0.05963715348251
42.5102040816326	21.1	0.999	0.001	0.5	0.05688611102616
44.9795918367347	21.1	0.999	0.001	0.5	0.05445663613328
47.4489795918367	21.1	0.999	0.001	0.5	0.05229951671853
49.9183673469388	21.1	0.999	0.001	0.5	0.05037535236799

Properties | Conditions | Results | Chart

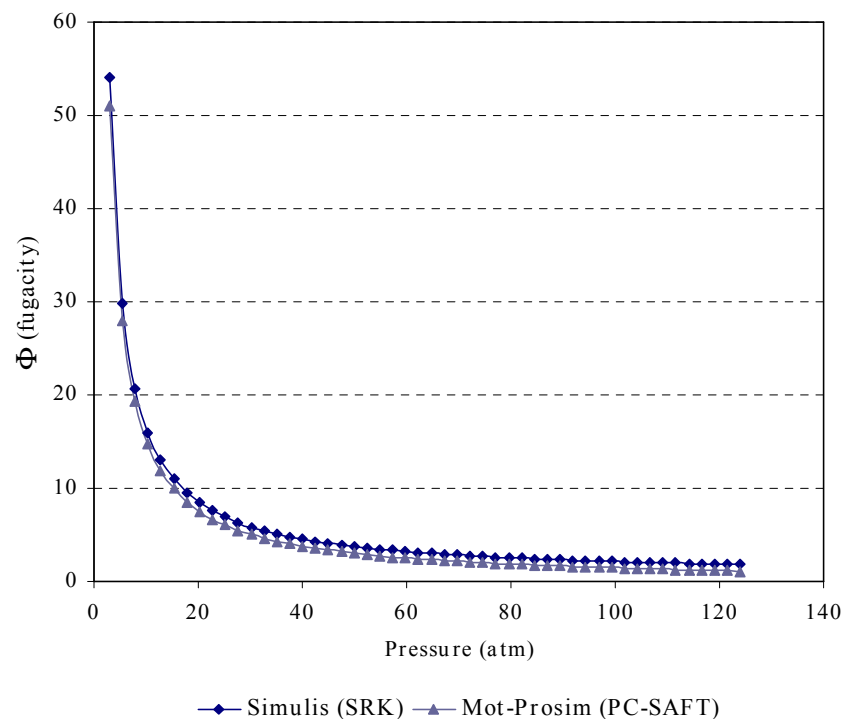
Close

1. Validation & comparison of results

Fugacity coefficient for n-butane (Liquid phase)

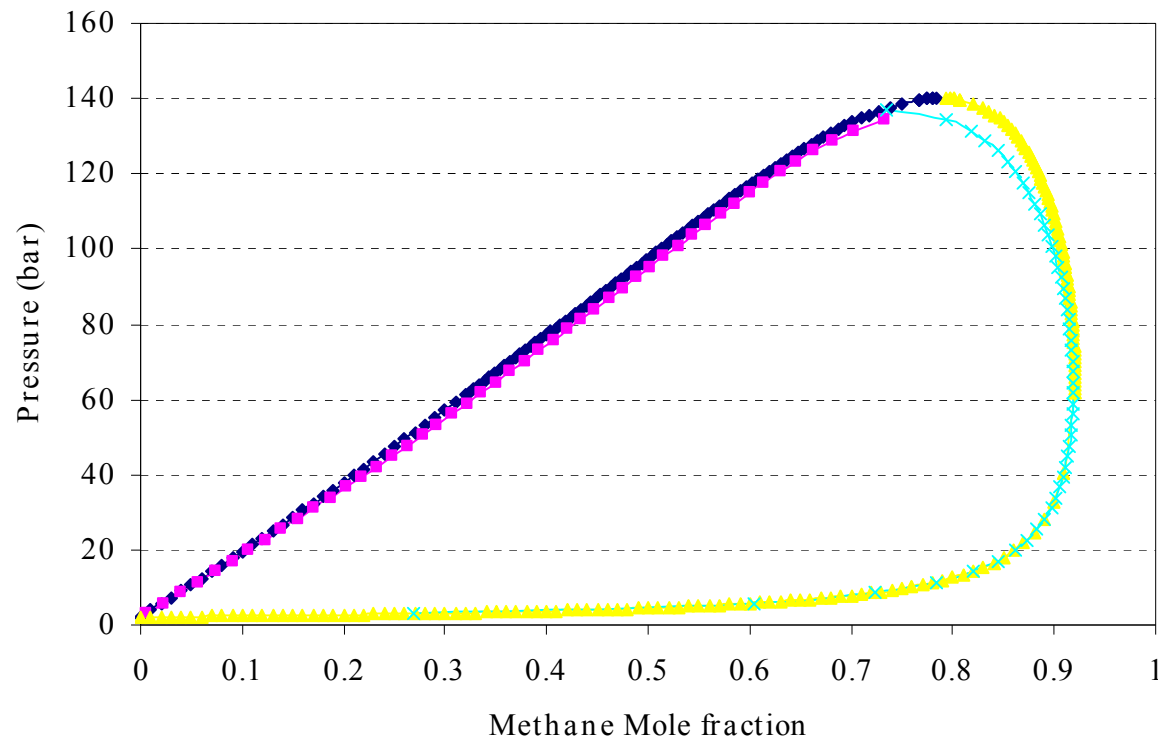


Fugacity coefficient for methane (Liquid phase)



1. Validation & comparison of results

Bubble and Dew point for methane



$T = 21.1 \text{ }^\circ\text{C}$

$x_{n-but} = 0.999$

$x_{CH_4} = 0.001$

◆ Simulis Bubble Point ■ MoT-ProSim Bubble Point
▲ Simulis Dew Point × MoT-ProSim Dew Point

Momentum balance

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

Rate of Evaporation

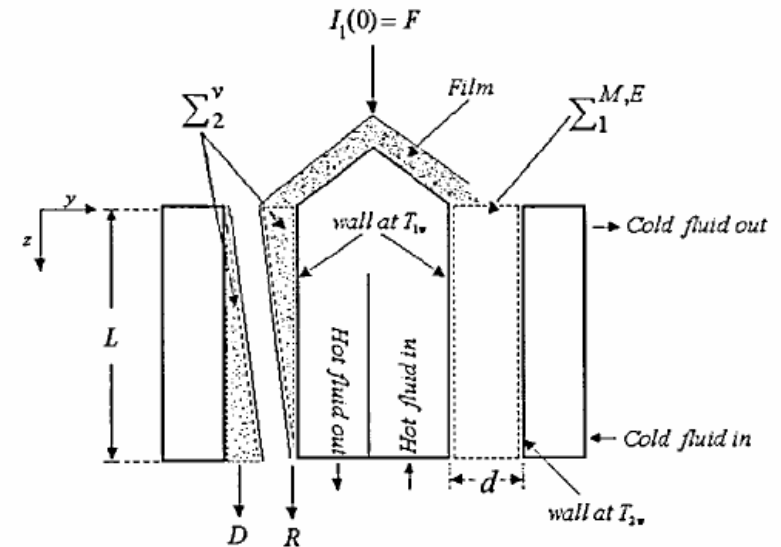
$$\frac{\partial I_i(z)}{\partial z} = -2\pi \cdot R \cdot k_i; \quad k_i = \frac{\gamma_i P_i^{\text{vap}}}{\sqrt{2\pi R_g M_i T_s(z)}} \left(\frac{P}{P_{\text{ref}}} \right) \left\{ 1 - (1-F) \left[1 - e^{d/(x\beta)} \right]^n \right\}$$

Energy balance

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

Mass Balance

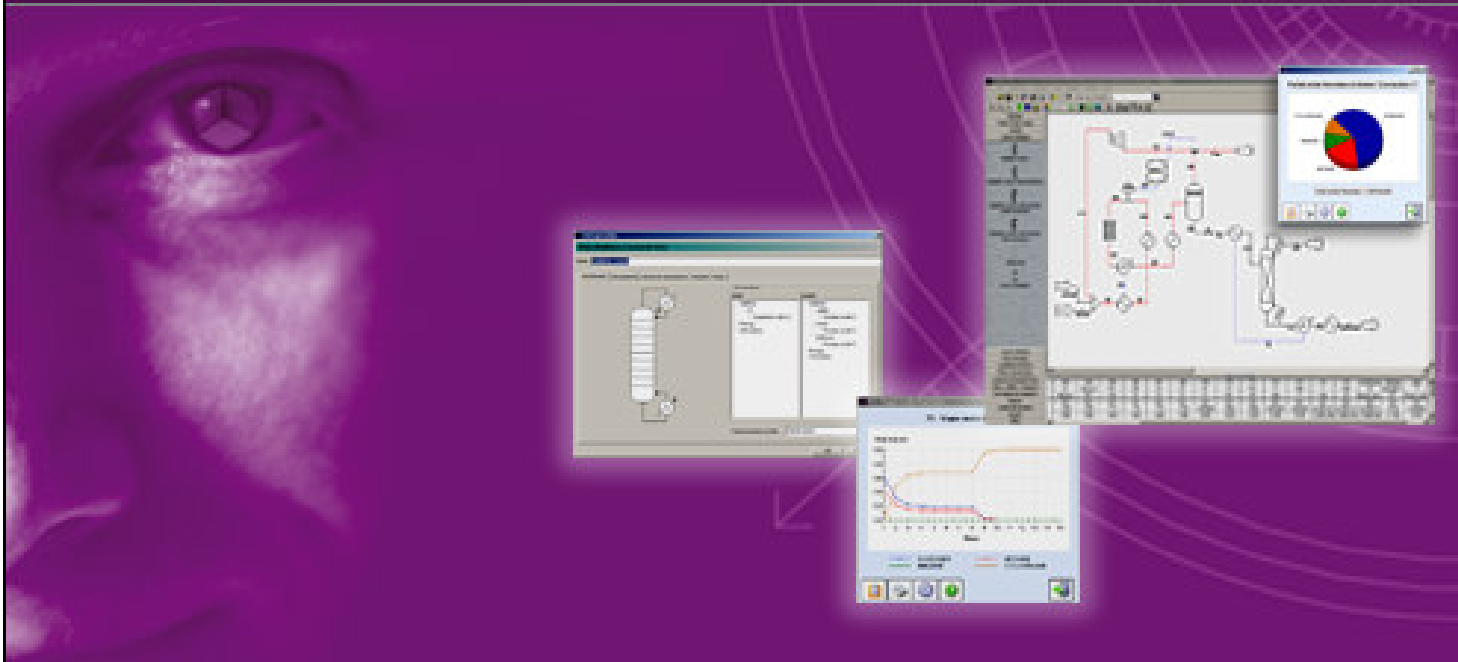
$$v(y, z) \frac{\partial C_i(y, z)}{\partial z} = D_i \left[\frac{\partial^2 C_i(y, z)}{\partial y^2} + \frac{\partial^2 C_i(y, z)}{\partial z^2} \right]$$



*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

ProSimPlus

Version 2.1



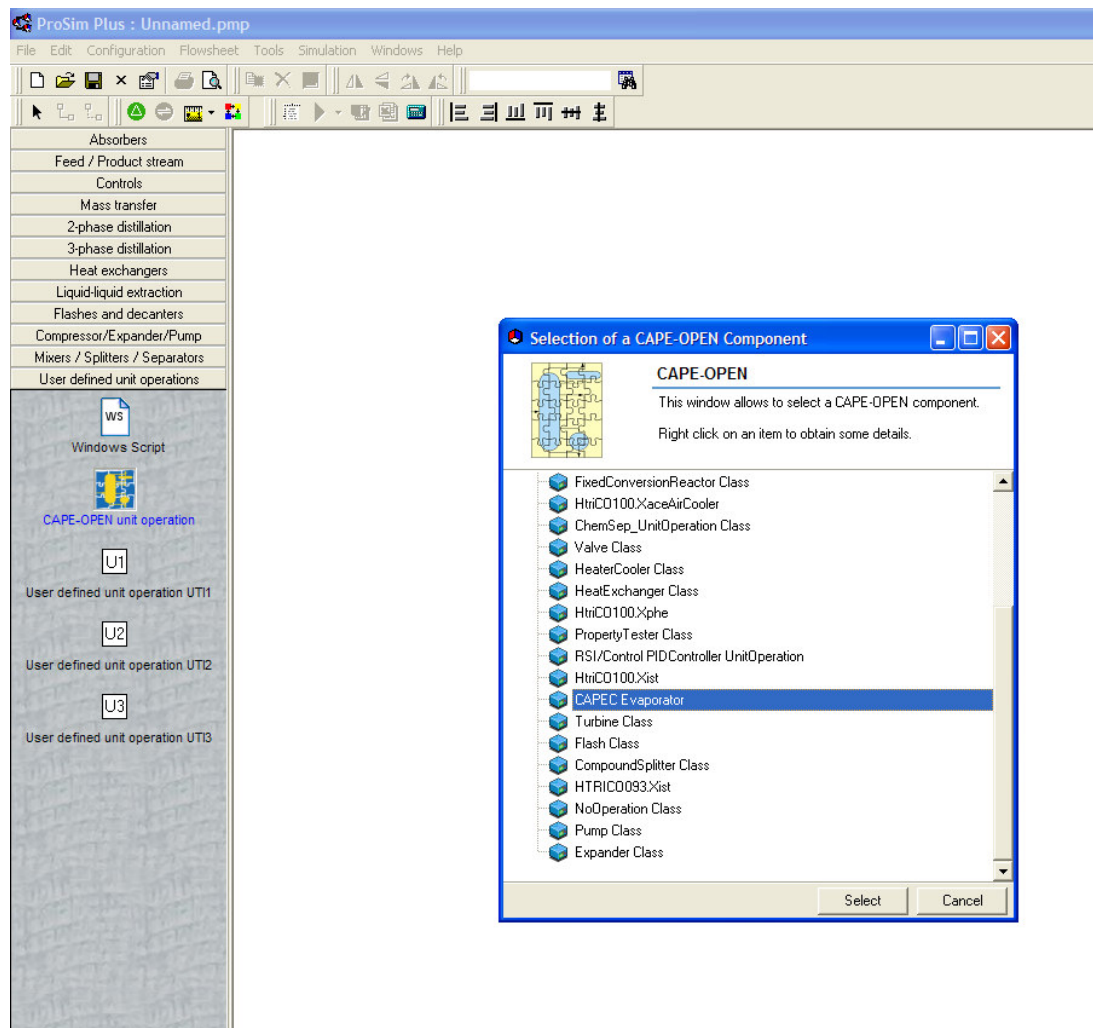
Licence informations



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All rights reserved.





The screenshot shows the ProSim Plus software interface. The main window is titled "ProSim Plus : Unnamed.pmp" and contains a menu bar (File, Edit, Configuration, Flowsheet, Tools, Simulation, Windows, Help) and a toolbar. On the left, there is a vertical toolbar with categories like Absorbers, Feed / Product stream, Controls, Mass transfer, 2-phase distillation, 3-phase distillation, Heat exchangers, Liquid-liquid extraction, Flashes and decanters, Compressor/Expander/Pump, Mixers / Splitters / Separators, and User defined unit operations. Below these are icons for Windows Script, CAPE-OPEN unit operation, and three user-defined unit operations (U1, U2, U3).

A dialog box titled "Selection of a CAPE-OPEN Component" is open in the center. It contains the following text:


CAPE-OPEN
This window allows to select a CAPE-OPEN component.
Right click on an item to obtain some details.

 Below the text is a list of components:

- FixedConversionReactor Class
- HtriCO100.XaceAirCooler
- ChemSep_UnitOperation Class
- Valve Class
- HeaterCooler Class
- HeatExchanger Class
- HtriCO100.Xphe
- PropertyTester Class
- RSI/Control PIDController UnitOperation
- HtriCO100.Xist
- CAPEC Evaporator** (highlighted)
- Turbine Class
- Flash Class
- CompoundSplitter Class
- HTRICO093.Xist
- NoOperation Class
- Pump Class
- Expander Class

 At the bottom of the dialog box are "Select" and "Cancel" buttons.

Edition of a CAPE-OPEN Component



CAPE-OPEN

This window displays some information about a CAPE-OPEN Component

URL Vendor: <http://www.prosim.net>

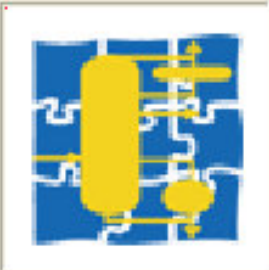
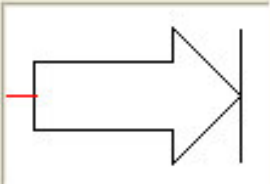
URL Help: <http://www.prosim.net>

Name	CAPEC Evaporator	
Description	<none>	
ClassID	{ABA99055-1FAE-4808-811F-C4256C4D63FF}	
ProgID	CAPECEvaporator.COUnit	
InProcServer32	V:\stardust project\capeopen\gani-evaporateur\CAPECEvapoUnit.dll	
Short description	CAPEC Evaporator	
Full description	CAPEC Evaporator : CAPE-OPEN Unit by ProSim and CAPEC	
Version	1.0.0.0	CAPE-OPEN version 1.0
About	Copyright© 2006 ProSim - CAPEC	

Close

Change the connections

Outlet connection port:	New stream	Inlet connection port:
<ul style="list-style-type: none"><input type="checkbox"/> CAPEC Evaporator<ul style="list-style-type: none"><input checked="" type="radio"/> Material Outlet #1<input type="radio"/> Material Outlet #2	<ul style="list-style-type: none"><input type="checkbox"/> Process outlet 1<ul style="list-style-type: none"><input checked="" type="radio"/> Process outlet	

Show only available connections

OK Cancel Apply

Thermodynamic calculator editor

Calculator actions and properties

Calculator Packages

- Show the package manager...
- Import a package...
- Build a package...
- Select a CAPE-OPEN package

Modifications

- Undo
- Redo

Services

- Calculate
- Export as a PSF file

Name
d-LIMONENE / WATER

Comments :

CAPE-OPEN

Calculator

This window helps you to define the context of your thermodynamic calculator

Compounds actions

Edition

- Import compounds...
- Edit this compound...
- Add a new compound
- Delete the selection
- Clone this compound
- Create pseudo-compounds...
- Temperature dependent properties...

Order

- Move this compound up
- Move this compound down

Compounds Packages

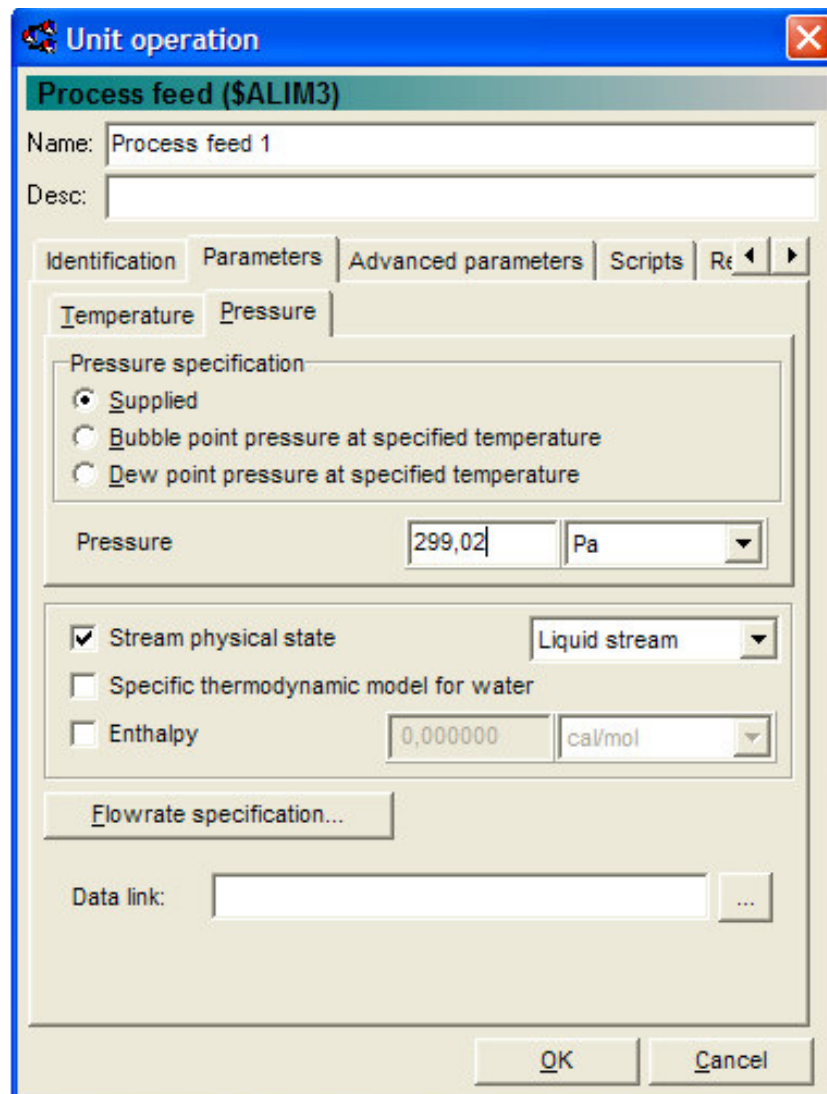
- Show the package manager...
- Import a package...
- Build a package with this list...

IUPAC Name	Registry Cas Number
d-LIMONENE	5989-27-5
WATER	7732-18-5

Comments :

Compounds | Model | Parameters

Ok Cancel



Unit operation

Process feed (\$ALIM3)

Name: Process feed 1

Desc:

Identification Parameters Advanced parameters Scripts Re ◀ ▶

Temperature Pressure

Pressure specification

- Supplied
- Bubble point pressure at specified temperature
- Dew point pressure at specified temperature

Pressure: 299,02 Pa

Stream physical state: Liquid stream

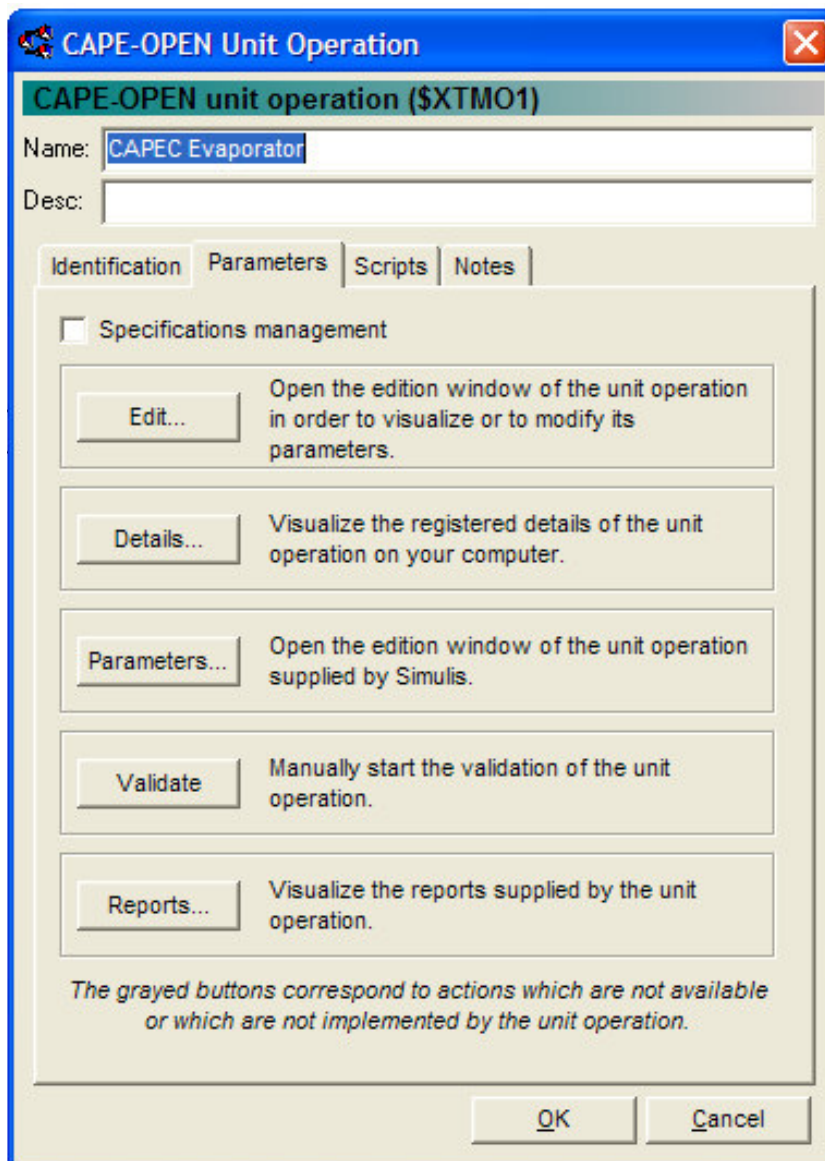
Specific thermodynamic model for water

Enthalpy: 0,000000 cal/mol

Flowrate specification...

Data link: ...

OK Cancel



The screenshot shows a software dialog box titled "CAPE-OPEN Unit Operation" with a close button (X) in the top right corner. The main title bar also includes a small icon. Below the title bar, the text "CAPE-OPEN unit operation (\$XTMO1)" is displayed. There are two input fields: "Name:" containing "CAPEC Evaporator" and "Desc:" which is empty. Below these fields are four tabs: "Identification", "Parameters", "Scripts", and "Notes". The "Identification" tab is selected. Under this tab, there is a checkbox labeled "Specifications management" which is unchecked. Below the checkbox are five rows of buttons with descriptions:

- Edit...**: Open the edition window of the unit operation in order to visualize or to modify its parameters.
- Details...**: Visualize the registered details of the unit operation on your computer.
- Parameters...**: Open the edition window of the unit operation supplied by Simulis.
- Validate**: Manually start the validation of the unit operation.
- Reports...**: Visualize the reports supplied by the unit operation.

At the bottom of the dialog, there is a note: "The grayed buttons correspond to actions which are not available or which are not implemented by the unit operation." Below this note are two buttons: "OK" and "Cancel".

CAPE-OPEN Unit Editor

Name	Description	Type	Mode
Length	Evaporator Length (m)	Real	Input
Diameter	Evaporator Diameter (m)	Real	Input

Value:

Parameters | Ports | Report

Ok

CAPE-OPEN Unit Editor

Connected object	Name	Description	Type	Direction
Input	Material Inlet #1	Material Inlet #1	Material	Inlet
Liquid Output	Material Outlet #2	Material Outlet #2	Material	Outlet
Vapor Output	Material Outlet #1	Material Outlet #1	Material	Outlet

Parameters | Ports | Report

Ok

CAPE-OPEN Unit Operation

CAPE-OPEN unit operation (SXTM01)

Name: CAPEC Evaporator

Desc:

Identification | Parameters | Scripts | Notes

Specifications management

Edit... Open the edition window of the unit operation in order to visualize or to modify its parameters.

Details... Validate the unit operation.

Parameters... Edit the parameters of the unit operation.

Validate Manually start the validation of the unit operation.

Reports... Visualize the reports supplied by the unit operation.

The grayed buttons correspond to actions which are not available or which are not implemented by the unit operation.

Ok Cancel

Validate

Validation successful.

Ok

Simulation progress

- Process feed 1
- CAPEC Evaporator

Simulation in progress
reading data
Checking data
Receiving calculation sequence
Simulation in progress

ProSim Plus : V:\stardust project\capeopen\gani-évaporateur\EvapoCAPEC0.pmp Modified

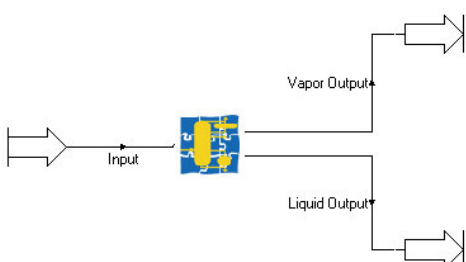
File Edit Configuration Flowsheet Tools Simulation Windows Help

Absorbers

Feed / Product stream

Process feed

Process outlet



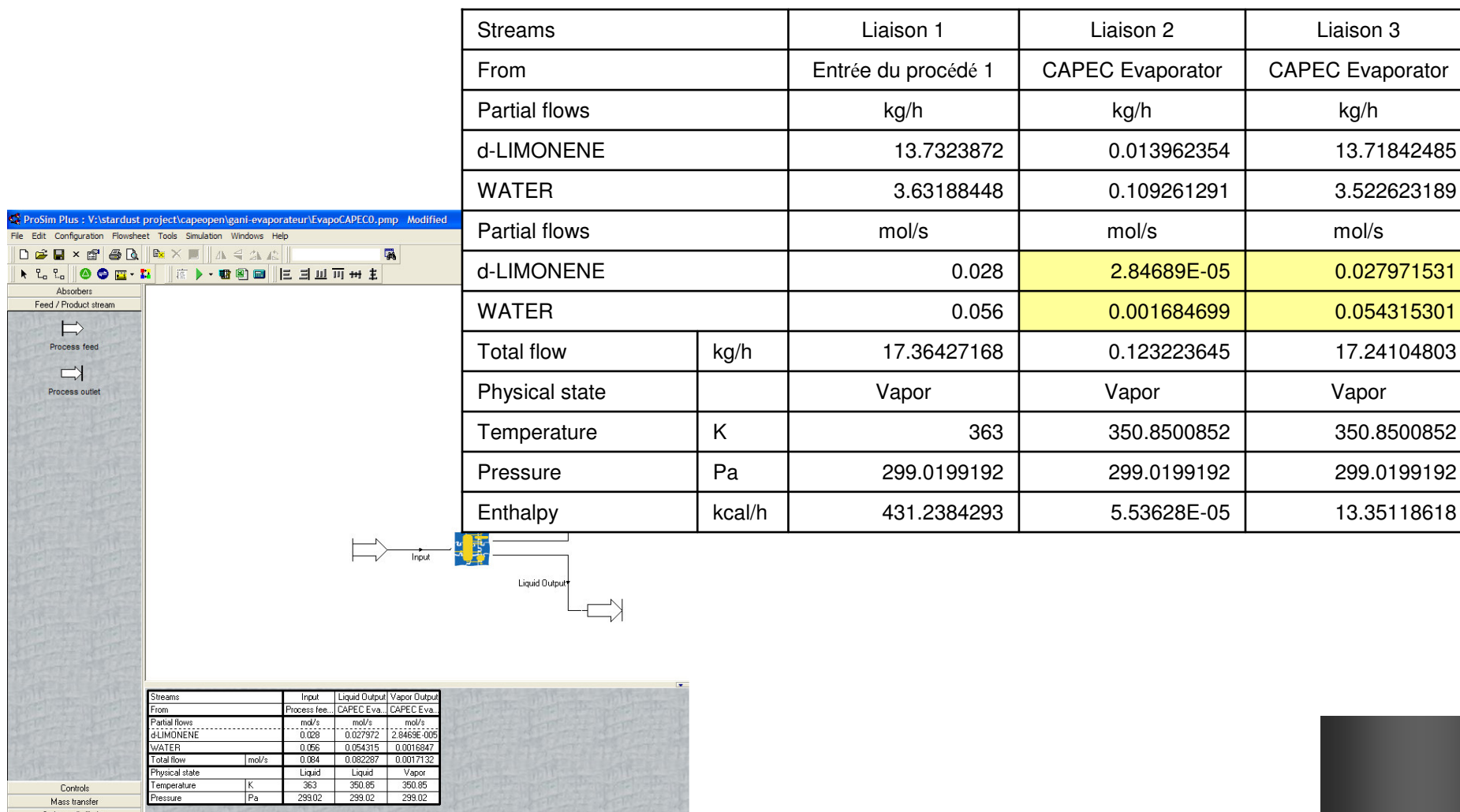
Streams	Input	Liquid Output	Vapor Output
From	Process fee...	CAPEC Eva...	CAPEC Eva...
Partial flows	mol/s	mol/s	mol/s
d-LIMONENE	0.028	0.027972	2.8469E-005
WATER	0.056	0.054315	0.0016847
Total flow	mol/s	0.084	0.082287
Physical state		Liquid	Liquid Vapor
Temperature	K	363	350.85
Pressure	Pa	299.02	299.02

Controls

Mass transfer

2-phase distillation

2. Short-Path Evaporator Model



- **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**