Modelling tools & applications

ICAS-MoT

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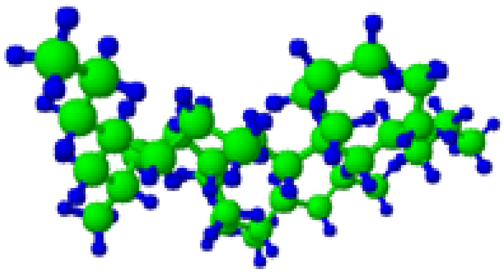
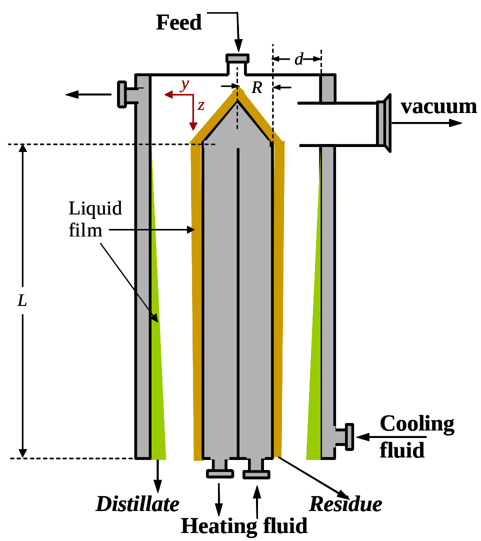
Overview

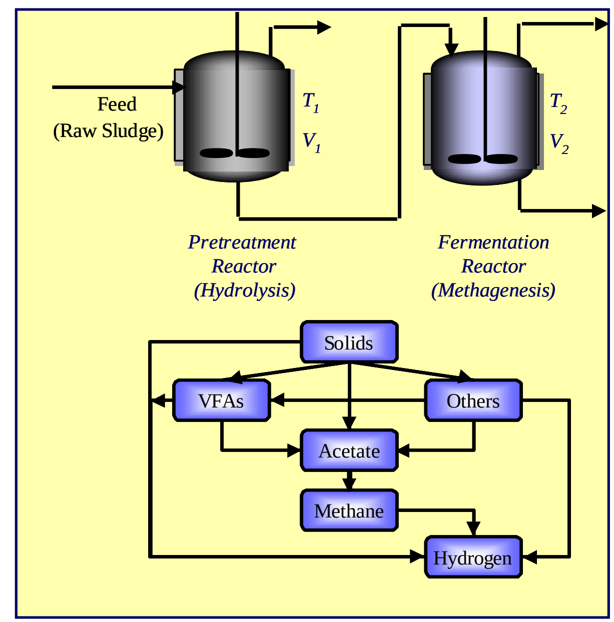
- Modelling concept (summary)
- Tool for model analysis & solution (MoT)
- Examples with MoT

Modelling concept - 1

For a given modelling task, generate (create) the mathematical model; analyze the model; solve the model; create a model object & finally use

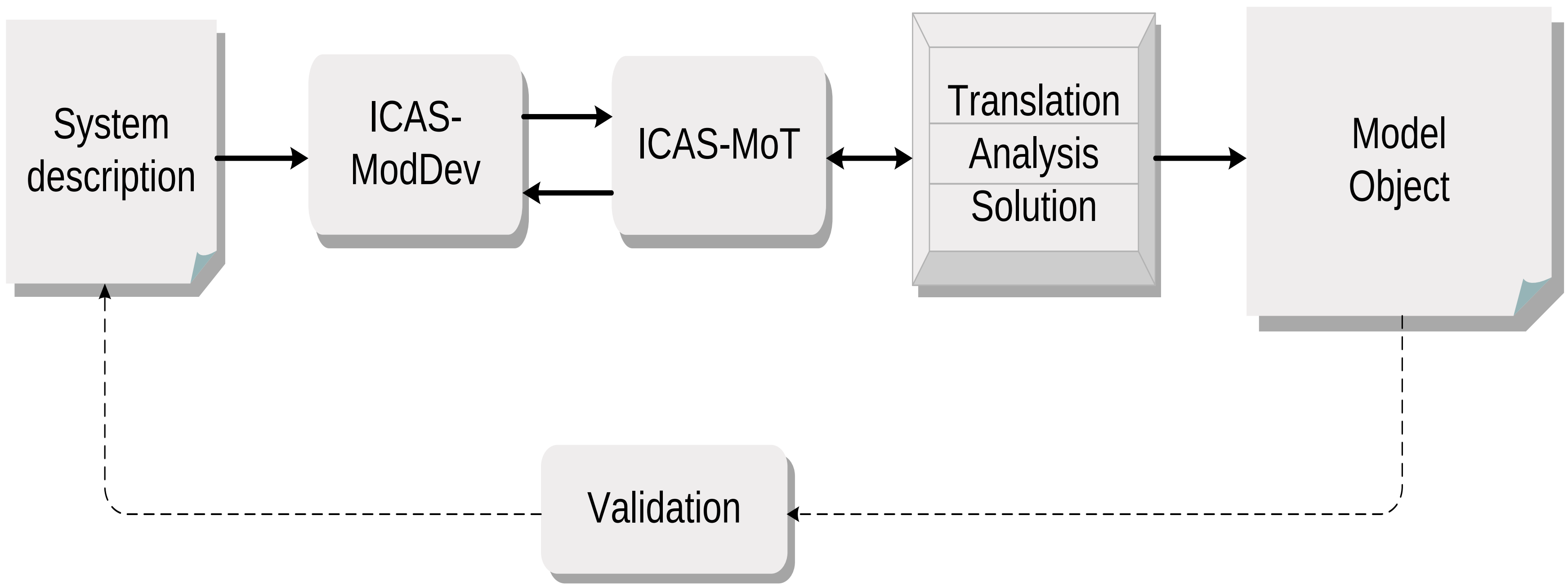




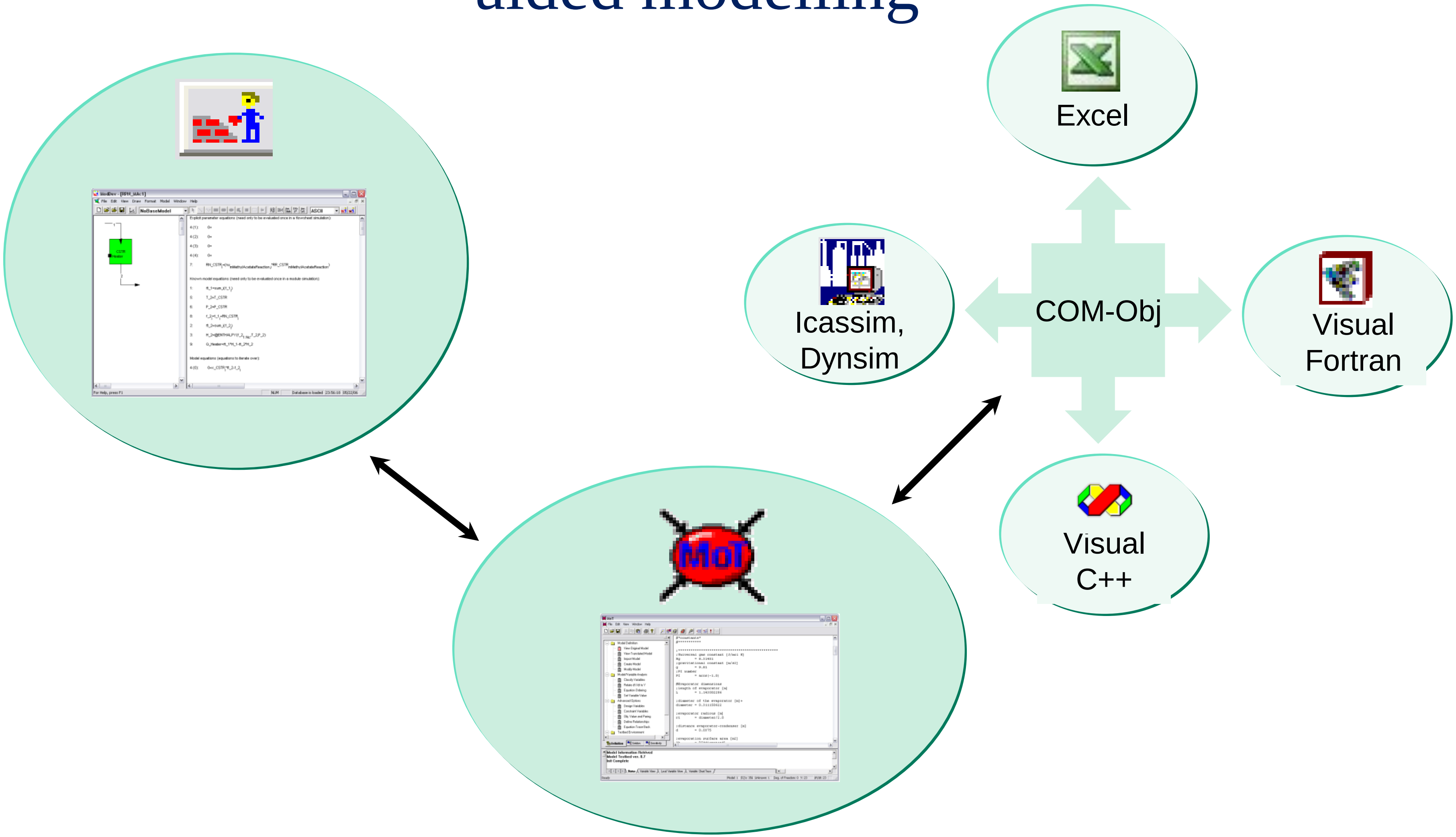


Modelling concept - 2

For a given modelling task, generate (create) the mathematical model; analyze the model; solve the model; create a model object & finally use

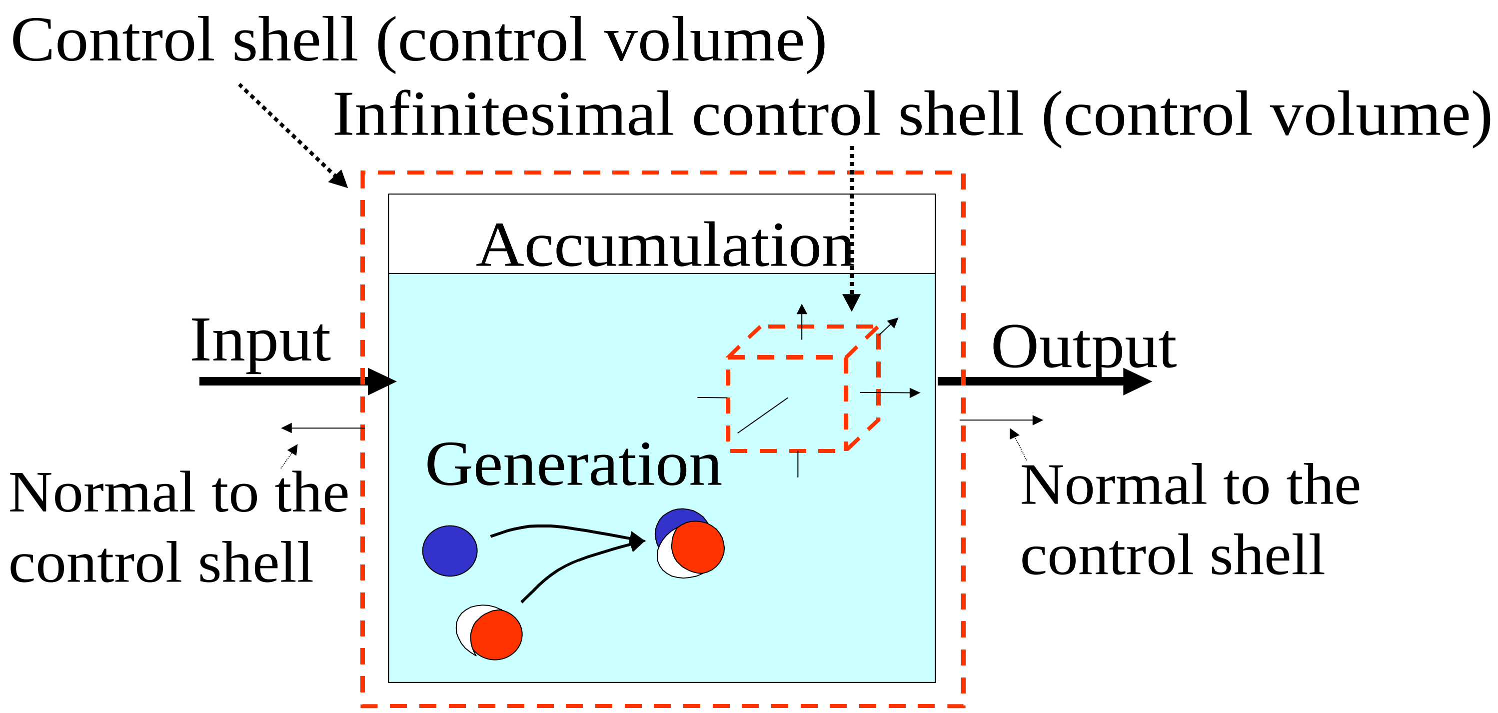


Modelling concept – 3: Integrated computer aided modelling



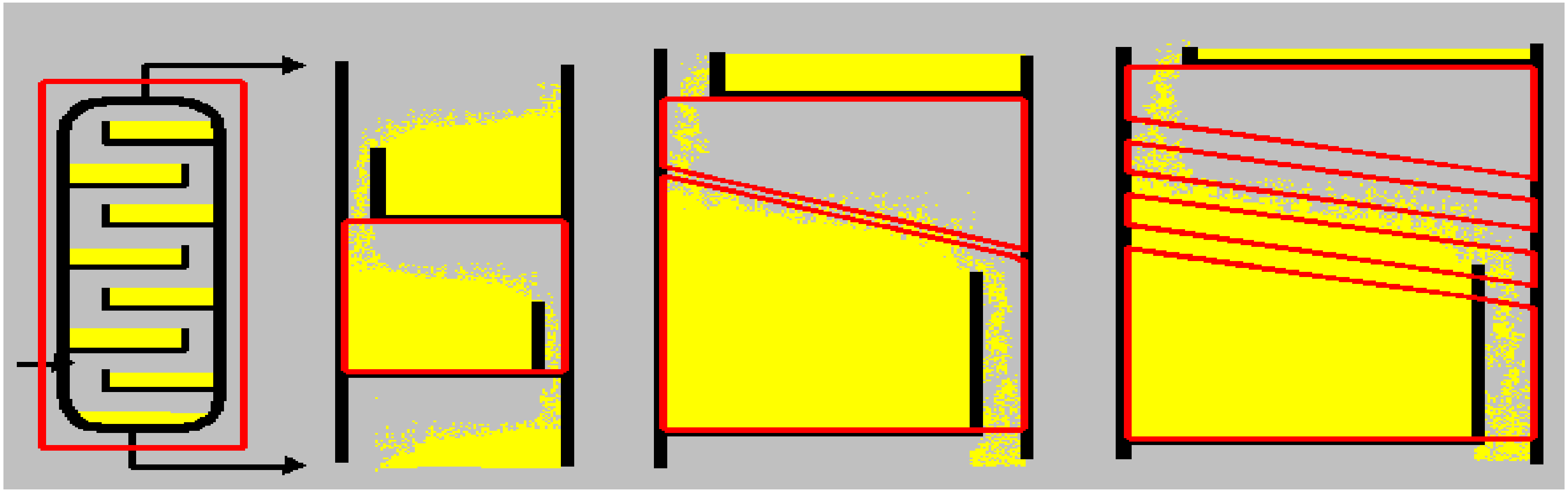
Tool for model generation: ModDev -1

Describe balance volume (control shell) & connection to surroundings; retrieve equations from model library; export model to MoT



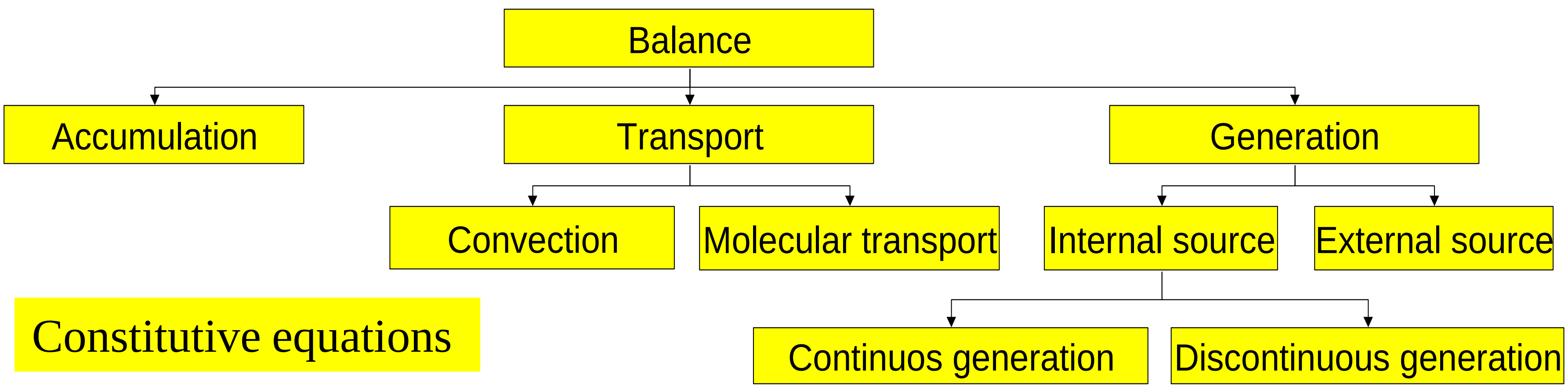
Tool for model generation: ModDev -2

Describe balance volume (control shell) & connection to surroundings; retrieve equations from model library; export model to MoT



Tool for model generation: ModDev -3

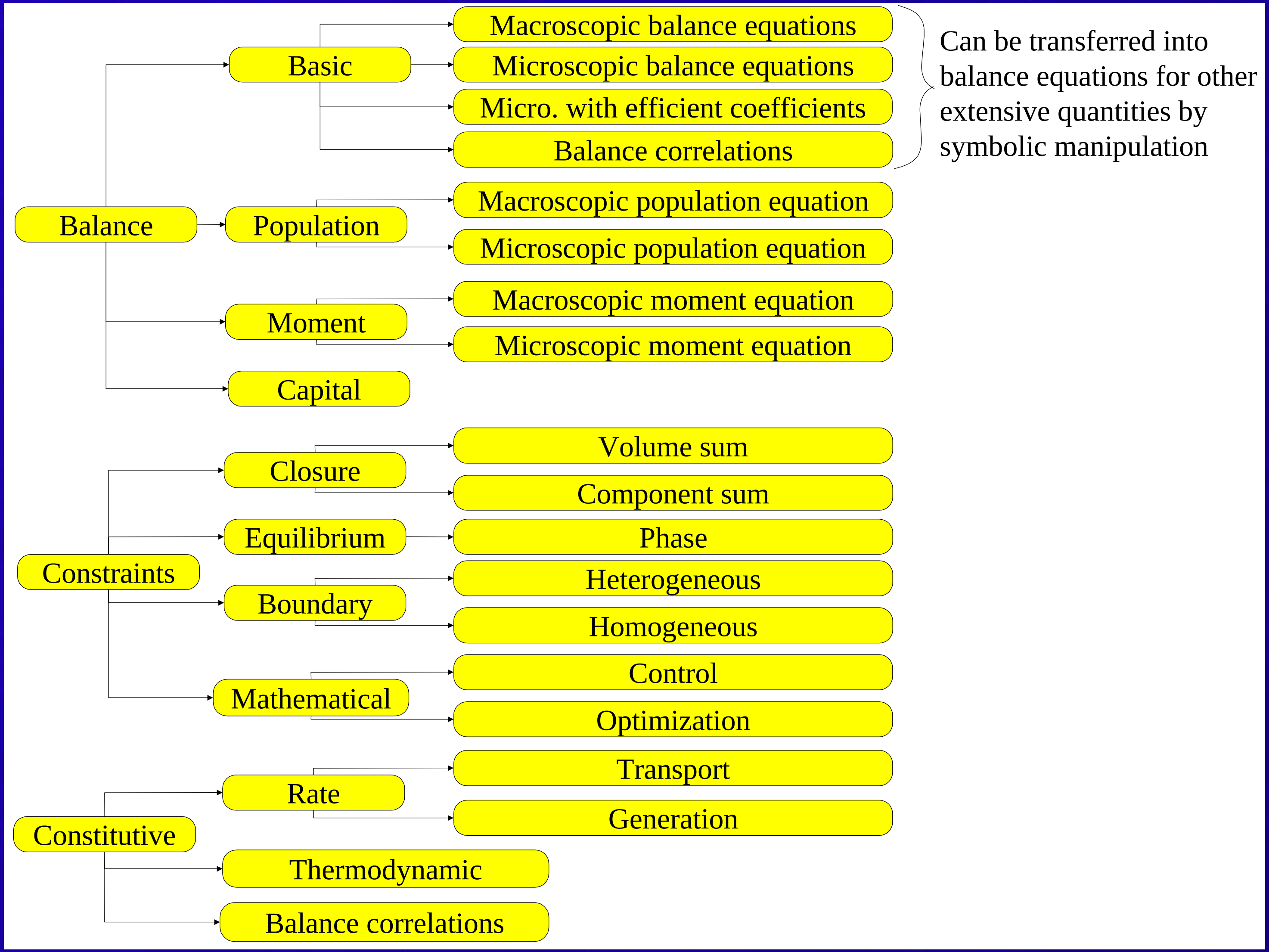
Describe balance volume (control shell) & connection to surroundings; retrieve equations from model library; export model to MoT



Constitutive equations

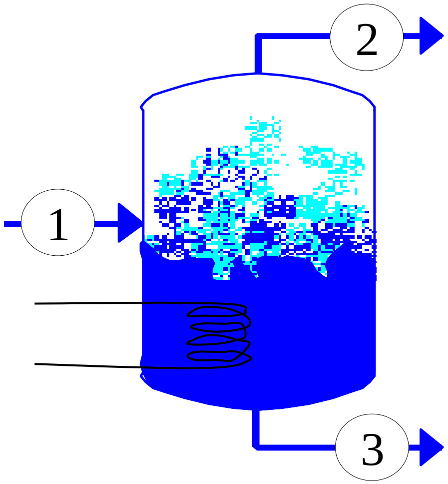
Conditional equations

Match problem description with Reference Models



Retrieve matched models otherwise build new models

Tool for model generation: ModDev - example



STREAM CONNECTION OBJECT
Name: *3*
Models for quantities:
Energy (enthalpy): H_3=@FUNC_E(2,$f_{3[]}$,T_3,P_3)
Models for the "from"-connection: *(equilibrium)*
Energy connection: $T_3=T_{flash}$
Momentum connection: $P_3=P_{flash}$

SHELL OBJECT
Name: *flash*
Assumed phase condition: *Calculate (VL)*
Equilibrium model: $0= f_{2i}/ ft_2 - K_{flash} * f_{3i}/ft_3$, @KEQ($T_{flash}$, P_{flash}, $f_{2[]}$, $f_{3[]}$, #K_{flash}), no accumulation, include mass & energy balance

SHELL CONNECTION OBJECT
Name: *heater*
Connection models:
Energy connection: $Q_{heater}=Q_{flash}$

Tool for model generation: ModDev - example

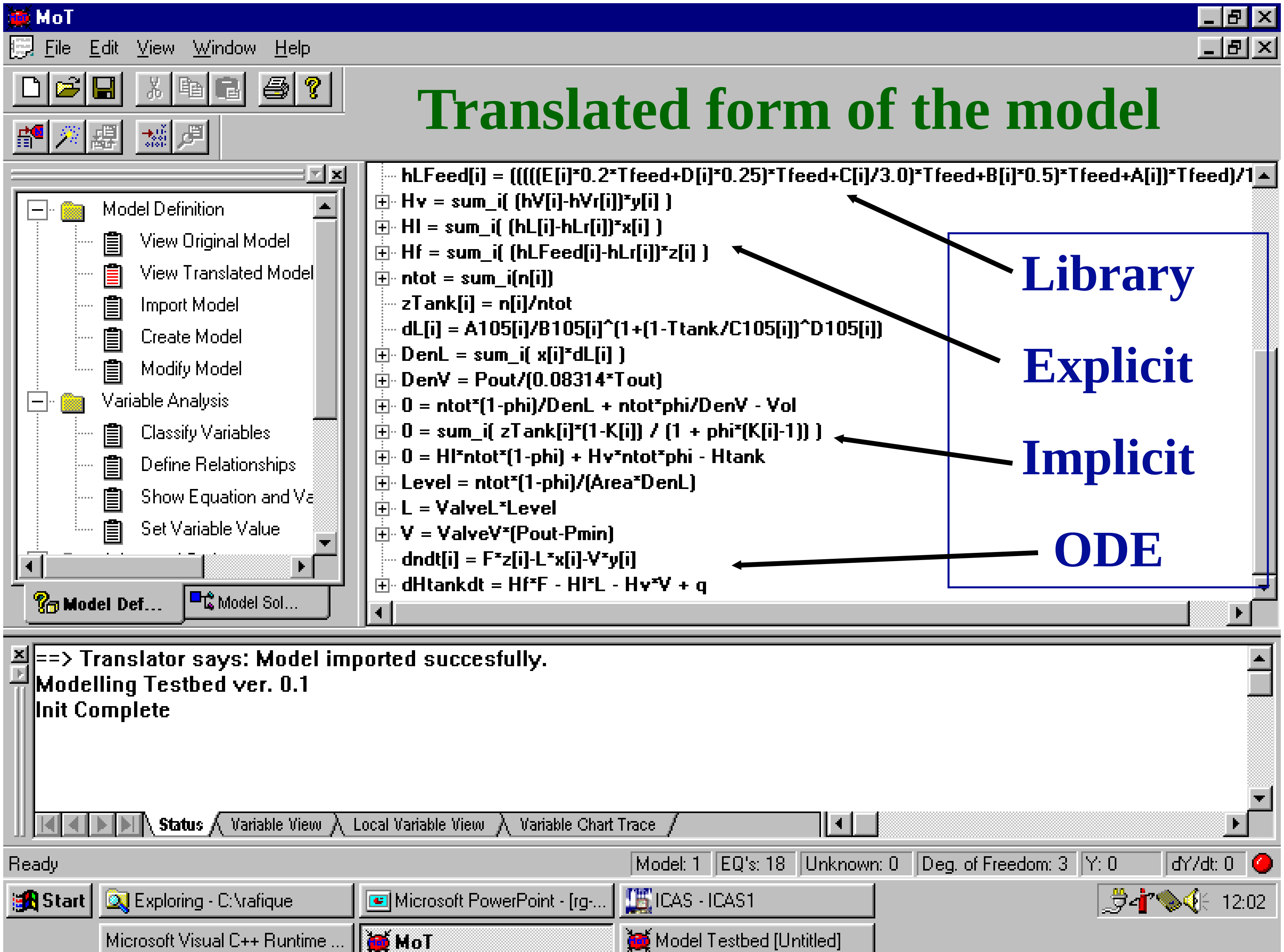
```
Tl = Tout
Pl = Pout
Ttank=Tout
Tv = Tl
Pv = Pl
ntot = sum_i(n[i])
zTank[i] = n[i]/ntot

#find k values
Psat[i] = (10^(DB_AntoineA[i] - DB_AntoineB[i]/(Tout-273.15+DB_AntoineC[i]) ))/760
K[i] = Psat[i]/Pout
x[i] = zTank[i]/(1+phi*(K[i]-1))
y[i] = x[i]*K[i]

#get the enthalpies
#hVap[i] = (Avap[i]*(1-(Tout/
#hV[i]=(((((E[i]*0.2*Tout+D[i]
#hVr[i]=(((((E[i]*0.2*Tref+D[
#hL[i] = (((((E[i]*0.2*Tout+D
#hLr[i] = (((((E[i]*0.2*Tref+
```

Model equations written in ASCII-text is exported to MoT

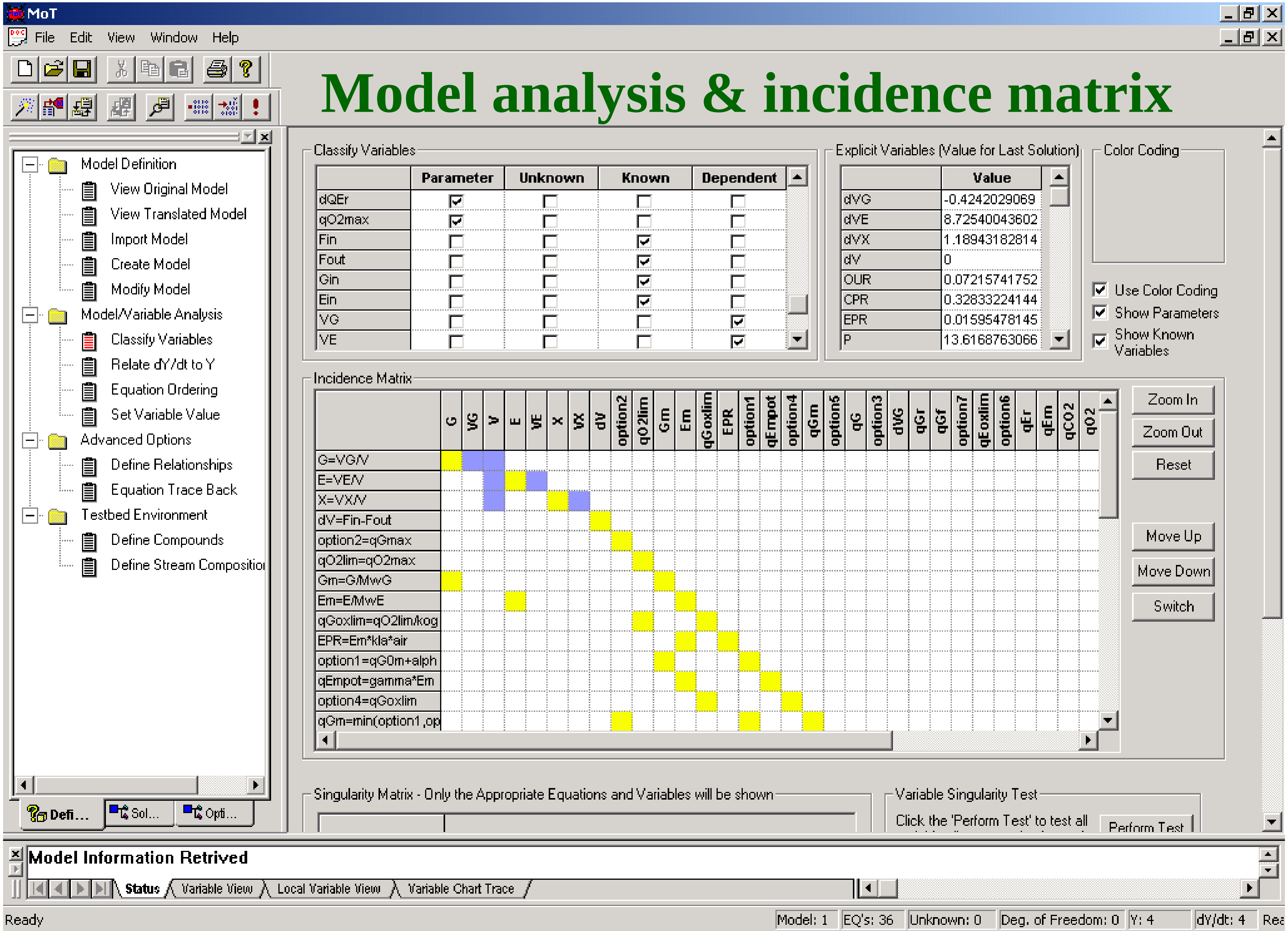
```
#get the densities
#dL[i] = A105[i]/B105[i]^(1+(1-Ttank/C105[i])^D105[i])
dL[i] = ADippr101[i]/BDippr101[i]^(1+(1-Ttank/CDippr101[i])^DDippr101[i])

DenL = 1 / sum_i( x[i]/dL[i] )
DenV = Pout/(0.08314*Tout)

#rachford rice
0 = ntot*(1-phi)/DenL + ntot*phi/DenV - Vol
0 = sum_i( zTank[i]*(1-K[i]) / (1 + phi*(K[i]-1)) )
Level = ntot*(1-phi)/(Area*DenL)
L = ValveL*Level
V = ValveV*(Pout-Pmin)
Hv = sum_i( (hV[i]-hVr[i]+hVap[i])*y[i] )
Hl = sum_i( (hL[i]-hLr[i])*x[i] )
0 = (Hl*ntot*(1-phi) + Hv*ntot*phi - Htank)/1000

#update holdups
dndt[i] = F*z[i]-L*x[i]-V*y[i]
dHtankdt = Hf*F - Hl*L - Hv*V + q
```

Note: all the model equations are not shown here

Tool for model analysis & solution: MoT



Tool for model analysis & solution: MoT



Eq. No.	Equation		Number of equations
1	$\ln\varphi_i = b_{ci}(Z-1) - \ln(Z-B) - A/B\,(2a_{ci}^{0.5} - b_{ci})\ln(1+B/Z)$	$i=1,NC$	NC
2	$a_{ci} = (\alpha_i^{0.5} T_{ci}/P_{ci}^{0.5})/\Sigma_j(x_j\,\alpha_j^{0.5} T_{cj}/P_{cj}^{0.5})$	$i=1,NC$	NC
3	$b_{ci} = (T_{ci}/P_{ci})/\Sigma_j(x_j\,T_{cj}/P_{cj})$	$i=1,NC$	NC
4	$Z^3 - Z^2 + Z(A - B - B^2) - AB = 0$		1
5	$A = aP/(RT)^2$		1
6	$B = bP/(RT)$		1
7	$a = \Sigma_i x_i \Sigma_j x_j\ a_{ij}$	$i=1,NC; j=1,NC$	1
8	$b = \Sigma_i x_i\ x_j b_{ij}$	$i=1,NC; j=1,NC$	1
9	$a_{ij} = (a_i a_j)^{k}(1-k_{ij})$	$i=1,NC; j=1,NC$	$NC*NC$
10	$b_{ij} = (b_i + b_j)/2$	$i=1,NC; j=1,NC$	$NC*NC$
11	$a_i = \psi_A\,\alpha_i(T)(R^2 T_{ci}^2/P_{ci})$	$i=1,NC$	NC
12	$b_i = \psi_B(RT_{ci}/P_{ci})$	$i=1,NC$	NC
13	$\alpha_i(T) = [1 + m_i(1 - T_{Ri}^{0.5})]^2$	$i=1,NC$	NC
14	$m_i = 0.48 + 1.574\,\omega_i - 0.176\,\omega_i^2$	$i=1,NC$	NC
15	$T_{Ri} = T/T_{ci}$	$i=1,NC$	NC
Total number of equations = $5 + 8NC + 2NC*NC$			
Total number of variables = $10\ [T, P, R, \psi_A, \psi_B, a, b, A, B, Z] + 12NC\ [x, T_c, P_c, \omega, T_R, \alpha, m, a, b, a_n, b_n, \varphi] + 3NC*NC[a, b, k] = 10 + 12NC + 3NC*NC$			

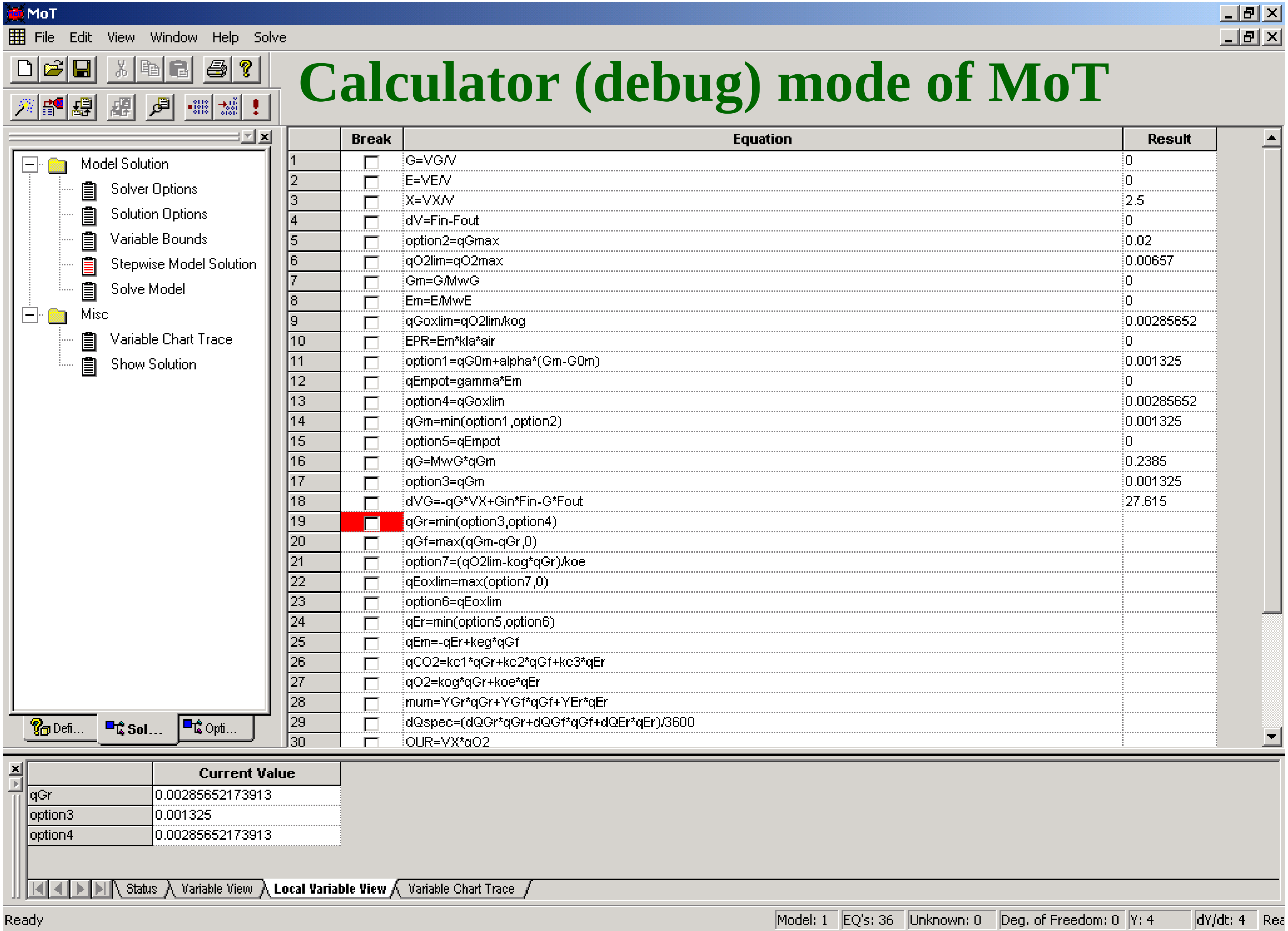
Table 2d: Incidence matrix of SRK EOS property model equations.

Eq.	Unknown Variables														
	T_r	m	α	$\underline{b}$	$\underline{a}$	$\underline{\boldsymbol{b}}$	$\underline{\boldsymbol{a}}$	a	b	B	A	Z	$\underline{b}_r$	$\underline{a}_r$	$\underline{\varphi}$
15	*														
14		*													
13	*	*	*												
12				*											
11			*		*										
10				*		*									
9					*		*								
7							*	*							
8						*			*						
6									*	*					
5								*			*				
4[1]										*	*	*			
3													*		
2			*											*	
1										*	*	*	*	*	*

[1]: requires the solution of a cubic equation in Z

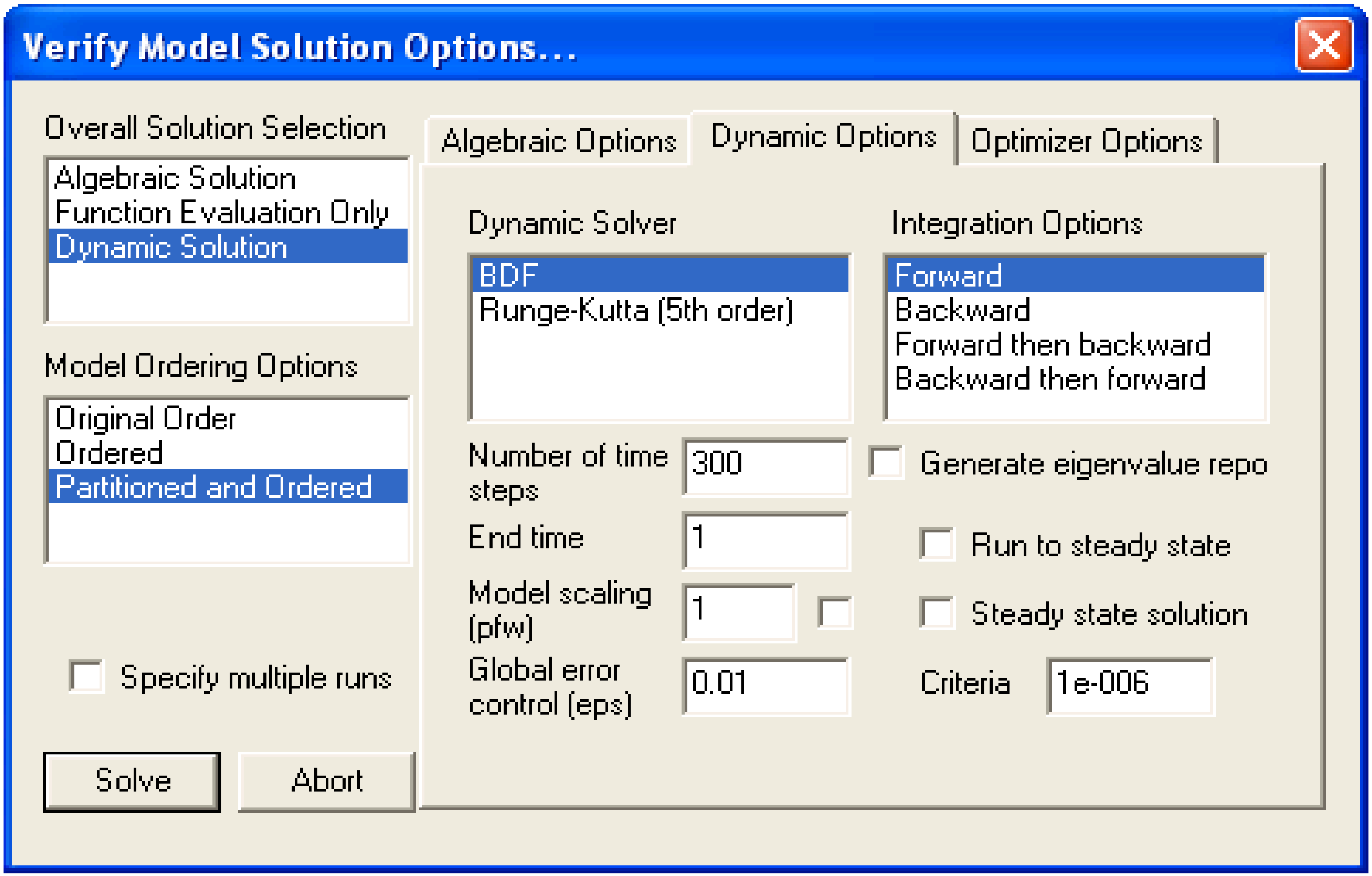
Tool for model analysis & solution: MoT

Calculator (debug) mode of MoT



Tool for model analysis & solution: MoT

Select the appropriate solver options



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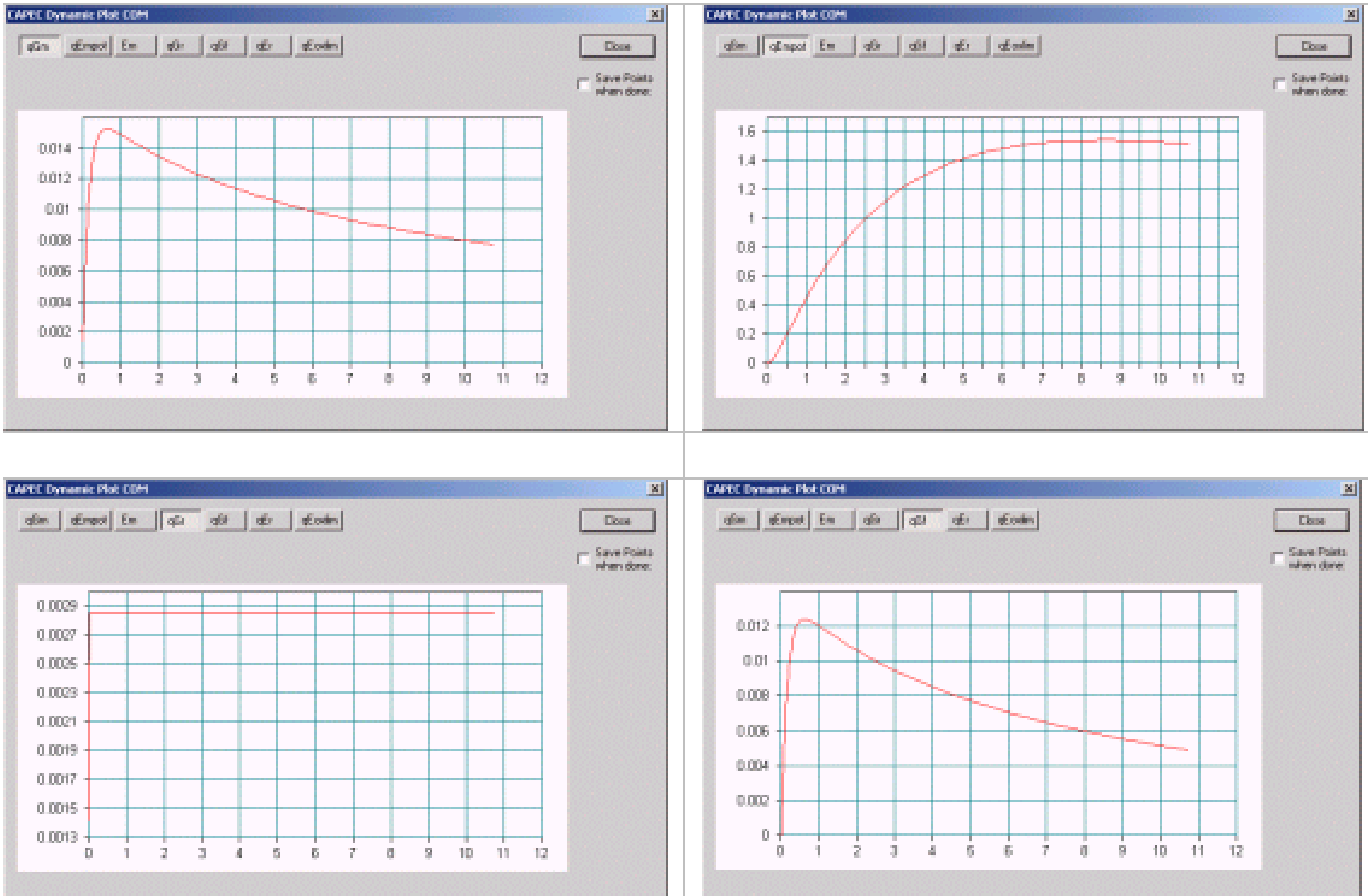
Tool for model analysis & solution: MoT

Visualization of simulation results



Use of MoT model-objects

- Run MoT models on a stand-alone basis
- Run MoT models from a simulator (export MoT models to ICAS or other simulation engines)
- Run Mot models from external software environments (for example, EXCEL)
- Create customized simulator!

Modelling exercise – MoT

Run MoT model objects from EXCEL

Note: It is necessary to first execute ComMOT.exe and then open the supplied EXCEL-macro (MoT_Model_Interface.xls)