# **Computer Aided Modeling Tool – ModDev**

**Tutorial Examples. Part I** 

Marina Fedorova, Rafiqul Gani CAPEC Department of Chemical Engineering Technical University of Denmark DK-2800 Lyngby, Denmark

#### 1. Introduction

This tutorial concentrates on the basic features of ModDev in order to guide the user through the different steps of the model generation procedure followed in ModDev. Simple examples are only considered here.

The model generation procedure followed in ModDev consists of providing descriptions of the process (to be modeled) in terms of shells, streams and connections. Based on the descriptions, ModDev generates the corresponding equations. In case the corresponding equations of a shell/stream/connection are not available, ModDev allows the user to define new equations.

The computer aided modeling tutorial is divided into two parts. Part I only deals with generation of the process model equations while part II deals with model analysis and code-generation.

#### 2. Process Modeling with ModDev

Before starting with the first example, let us first review the various features available in ModDev and how to start with ModDev in ICAS. Figure 1 shows the screen when ICAS is started.



Figure 1: Starting screen in ICAS

You can choose "ModDev" from task manager or click on the button "Model Development" on main ICAS screen. Figure 2 highlights the various tools available in the starting screen of ModDev.



Figure 2: Starting screen of ModDev with available tools highlighted.

We will start every example from this screen (minus the model and equations shown in figure 2) and generate our own process model. There are 5 detailed examples starting from a simple steady state tank mixer and ending with a dynamic reactor where the reaction is defined through a kinetic model.

# 2.1 Tutorial example 1 – Steady state tank (mixer)

In this example, we have 2 streams coming in and one stream going out. We will perform both mass and energy balance.

<u>Step1: Describe the process through a flow diagram</u> - Draw a shell connected by the inlet streams and one outlet stream. This is the necessary description of the shell (tank), streams (inlet/outlet) and connection (shell-stream). As the shells and streams are drawn, the default component mass balance and energy balance equations come on the right half of the screen (fig. 3).

🛃 ModDev - ModDev1	
File Edit View Draw Format Model Window	Help
🗅 🖻 🖨 🔛 🔽 NoBaseModel	
🔁 ModDev1	
	Model equations (equations to iterate over):
	1: 0=f_1;+f_2;-f_3;
ll	2: 0=ft_1*H_1+ft_2*H_2-ft_3*H_3
Shell1 💶 3	
2 <b>b</b>	

Figure 3: Describing of the process.

<u>Step2: Describe the shell</u> – Double click on the shell to enter the "shell description" tool (fig. 4). For this simple model, the default equations for mass and energy balance are acceptable. Therefore, no further action is needed. Exit by clicking on "close".

<b>ModDev-ModDev1</b> File Edit View Draw Format Model W	Vindow Help		
D 🗃 🖨 🖬 🔛 NoBaseMode	:I 🔹 🖡 💊 🗖 🗖	🕒 🛋 🔳 📖 🖨 🔣 KB 🕅 Start Start	e X <sup>x</sup> = Vor. X <sup>x</sup> Set ASCII
ModDev1	Model equal 1: 0= 2: 0= description	tions (equations to iterate over): =f_1 <sub>1</sub> +f_2 <sub>i</sub> -f_3 <sub>i</sub> =ft_1*H_1+ft_2*H_2-ft_3*H_3	×
Shell	e: Shell ams: Shell connections: ams: Shell connections: ams: Shell connections: bipersive state Homogeneous Pseudo homogeneous Distributed particulated (population Distributed particulated (population Distribution function Biubstitute equation of continuity in nass based balance equations bise substantial derivatives in the bialance equations	Lumped / distributed system  Macroscopic balance (lumped)  Macroscopic balance (distributed)  Phase condition  Iquid  Equilibrium models  Viscous fources Gravity field Fressure field Other heat source  Associated variable group NoVariableGroup Name of variable group in base model	Geometric description Components Reactions Mass balance Component balance Energy balance Variables Variables Related variables Other models Get holdup values Description Reset specifications
Numt	per of repetitions (0 if defined in prob	lem definition)	Close

Figure 4: Describing of the shell.

<u>Step3: Describe streams</u> – Double click on stream 1 to enter the "stream description" tool (fig. 5).

ModDev - ModDev1			
File Edit View Draw Format Model Window Help			
D 🖻 🖻 🖳 🔽 NoBaseModel 🛛 💌 📐	↘৵∎៙៙⊈▮	■ 🗔 🖨 KB 🛙	X=1 Var. X-X= Var. State X <sup>#</sup> Set ASCII
🔁 ModDev1			
	Model equations (equations)	ins to iterate over):	
	1: 0=f_1,+f_2,-f_3	3,	
	2: 0=ft_1*H_1+ft_	_2*H_2-ft_3*H_3	
s			×
Shell1 — Name: 1	Associa	ated variable group	NoVariableGroup 💌
Base model .	Name o in base	of variable group model	
From phase condition C Gas C Liquid C Solid C Calculate	Phase condition equal to the from connection Equilibrium mo	on 🔽	To phase condition — C Gas C Liquid C Solid C Calculate
Surroundings	Overall		Shell1
Connection location		M	Connection location
Components	Component - Concentration	Temperature drop	Variables
Reactions	Energy - Temperature	Pressure drop	Related variables
Description	Momentum - Pressure	Other models	Get stream values
Number of repetitions (if	specified later, give 0): 1	-	Reset specifictions
🔲 Known stream (all ur	nknown variables associated w	ith the stream are se	et to known) Close

Figure 5: Shell description tool.

Introduce new variables by clicking on "variables". Search for temperature and select it as a variable for addition. In the same manner, add also pressure as a variable (fig. 6).

ModDev - ModDev1	
File Edit View Draw Format Model Window Help	
D 📽 🛱 🛃 🔽 NoBaseModel 💿 🖹 📐 🗠 🗖 🖢	
T ModDev1	
Model eq 1: 2: Stream	Jations (equations to iterate over): 0=f_1¦+f_2¦-f_3¦ 0=f_1'H_1+ft_2'H_2-ft_3'H_3 ➤
Shell1 Name: 1	Associated variable group NoVariableGroup
Add/delete variables manual     Add/delete variables manual     Defined variable types     FilonenkoPressure.DiopCoefficier     Pressure_Absolute     Pressure_Bubble     Pressure_Dubble     Pressure_Dubble     Pressure_DintensionLess     Pressure_DimensionLess     Pressure_DimensionLess     Pressure_Pa     Pressure_Saturation_pureComponent     Pressure_Saturation_m     Pressure_Saturation_PareComponent     Pressure_Saturation_PareComponent	y to 1

Figure 6: Selection of additional variables.

Close the "variables" window with clicking on "Close". Click on "energy-temperature" (on the stream description window – see fig. 5) to introduce a model for enthalpy as a function of temperature (for the simple example, we will ignore the effect of pressure). Figure 7 shows the screen shot at this stage.

Close the "model search" tool. Search for the model in "Enthalpy" -> "Enthalpy\_Mole" -> "Pure component" -> "DIPPR100".



Figure 7: "Add/delete models" tool plus associated tools – "model definition" and "model search".

Select "Liquid" with clicking on it. The correlation will be shown under "Local model equations". Now drag down the "Model definition" tool and click on "add model" in the "add/modify/remove models" tool (fig. 8).



Figure 8: Model definition for stream 1.

Exit by clicking on "close" in the "add/modify/remove models" tool. Note that it is not possible to exit from "model definition" when "add/modify/remove models" is still active. Close the window for description of Stream 1. Now the main screen will show the enthalpy correlation for components in Stream 1 (fig. 9).



Figure 9: Main screen after describing of stream 1.

Repeat the above procedure for streams 2 and 3. Figure 10 shows the main screen after describing of all streams.



Figure 10: Main screen after describing of all streams.

We want to make the temperature and pressure of stream 3 the same as that of the tank. So, for stream 3, click on green rectangle on the main "Stream description" tool. This will open window "Transported matter" between Shell and Stream 3 (fig. 11). Click on "Energy" button to open tool for describing the connection between Shell and Stream 3.



Figure 11: "Transported matter" tool for stream 3.

From drop-down list of model types choose "Intensive property value continuous across the interphase (automatic choice of property)". And in list of properties - "Temperature". Add suggested model clicking on corresponding button (fig. 12). Then close the tool "Model suggestions".

Stream	2+CDippr100_Liq,/3*TT_1^3+DDippr100_Liq,/
Name:	Model suggestions - model equations used to describe the connection: Shell1 -> 3
Base model	Model type:
- From phase	Intensiv property value continuous across the interphase (automatic choise of property)
C Gas	Property Property Fixed value
Liquid	
C Solid C Calcul	List only properties used in the current equation system in the property combo-boxes M Include boundary
	Generated model suggestions
Shell1	Temperature(3)=Temperature(ShellT)
Connection	
	Add Remove Interchange Reset suggestion models
Compon	
Reacti	
Descrip	
Number of rep	Use symbols Add transport coefficient models Modify/add/delete added model equations Close
🔲 Known stru	

Figure 12: Describing connection between shell and stream 3 – Temperature.

Click on "Momentum" at "Transported matter" tool. Pick the same Model type as before, and "Pressure" as a property. Add suggested model equation (fig. 13).

Stream	X
Name:	Model suggestions - model equations used to describe the connection: Shell1 -> 3
Base model	Model type:
- From phase	Intensiv property value continuous across the interphase (automatic choise of property)
C Gias	Property Property Fixed value Pressure
C Solid	List only properties used in the current equation system in the property combo-boxes 🔽 Include boundary
L	Generated model suggestions
Shell1	Pressure{3}=Pressure{Shell1}
Connection	
	Add Remove Interchange Reset suggestion models
Compon	
Reacti	
Descrip	
Number of rep	Use symbols Add transport coefficient models Modify/add/delete added model equations Close
🔲 Known str	· · · · · · · · · · · · · · · · · · ·

Figure 13: Describing connection between shell and stream 3 – Pressure.

At this point, on the main "ModDev" screen, 7 equations will be shown (see figure 14).

ModDev - ModDev1	
File Edit View Draw Format Model Window Help	
D B B L NoBaseModel	
H ModDev1	
	Model equations (equations to iterate over):
	1: Hi_1;=ADippr100_Liq,*TT_1+BDippr100_Liq,/2*TT_1^2+CDippr100_Liq,/3*TT_1^3+DDippr100_Liq,/4*TT_1^4+EDippr100_Liq,/5*TT_1^5
	2: Hi_2=ADippr100_Liq,*TT_2+BDippr100_Liq,/2*TT_2^2+CDippr100_Liq,/3*TT_2^3+DDippr100_Liq,/4*TT_2^4+EDippr100_Liq,/5*TT_2^5
	3: HL_3=ADippr100_Liq,*TT_3+BDippr100_Liq,/2*TT_3*2+CDippr100_Liq,/3*TT_3*3+DDippr100_Liq,/4*TT_3*4+EDippr100_Liq,/5*TT_3*5
Shell	4: T_3=T_Shell1
	5: P_3=P_Shel/1
	6: 0=f_1;+f_2;-f_3;
	7: 0=ft_1*H_1+ft_2*H_2-ft_3*H_3

Figure 14: Model equations after streams have been described.

<u>Step4: Definition of "closure equations"</u> – The model is not yet complete since there are several terms on the right hand side of equation 7 which have not been defined but which are not independent equations. These equations are termed as "closure equations" or constraints. In order to define them, double click on the stream (for example, stream 1), select "related variables" on the "stream description" tool and then add the "mass" and "energy" related constraints. An example is shown in figure 15.

Add/modify/remove model equations used to describe the	object 1
Added model equations 🔽 Use syr	nbols Object indices
H_1=sum_i(Hi_1[i]*f_1[i])/ft_1 ft_1=sum_i(f_1[i])	
	Component indices
	i <u> </u>
	Reaction indices
Add model Remove model(s) Interchange model Modify model 0	
Related variables within the object 1	
Possible constraint equations	Closure equation type
Possible constraint equations	Closure equation type Property related closure constraints C Geometric closure constraints C Muse C Securities
Possible constraint equations	Closure equation type Closure equation type C Property related closure constraints C User defined closure equations C User defined closure equations C User defined closure equations C User defined closure equations
Possible constraint equations	Image: State of the state
Possible constraint equations	Image: Streen options       Closure equation type       Variable type         Image: Streen options       Image: Streen options       Maximum number of variables in closure
Possible constraint equations	Ols       Closure equation type         Image: Property related closure constraints       Image: Property related closure constraints         Image: Property related closure constraints       Image: Property related closure constraints         Image: Property related closure constraints       Image: Property related closure constraints         Image: Property related closure constraints       Image: Property related closure constraints         Image: Property related closure constraints       Image: Property related closure constraints         Image: Property related closure constraints       Image: Property related closure closure         Image: Property related closure constraints       Image: Property related closure closure         Image: Property related closure constraint that is not included in the current       Image: Property related closure closure closure         Image: Property related closure closure constraint that is not included in the current       Image: Property related closure closure closure         Image: Property related closure closu
Possible constraint equations	Ols       Closure equation type       Variable type         Image: Constraints       Image: Constraints       Image: Constraints         Image: Constraint of the constraints       Image: Constraints       Image: Constraints         Image: Constraint that is not included in the current       Image: Constraints       Image: Constraints         Image: Constraint that is not included in the current       Image: Constraints       Image: Constraints         Image: Constraint that is not included in the current       Image: Constants       Image: Constants         Image: Constant the constant parameters and universal constants       Image: Constants       Image: Constants         Image: Constant the constant parameters and universal constants       Image: Constants       Image: Constants         Image: Constant the constant parameters and universal constants       Image: Constants       Image: Constants         Image: Constant the constant parameters and universal constants       Image: Constants       Image: Constants       Image: Constants         Image: Constant the constant parameters       Image: Constants       Image: Constants       Image: Constants
Possible constraint equations  Use symbol Location of the constraint with the focus in the knoledgebase	Image: Show closure constraints       Variable type         Image: Closure equation type       Image: Closure constraints         Image: Closure closure constraints       Image: Closure closure constraints         Image: Closure closure constraints       Image: Closure closure closure closure         Image: Closure closure conversion constraints       Image: Closure closure closure         Image: Closure closure conversion constraints       Image: Closure closure         Image: Closure closure conversion constraints       Image: Closure closure         Image: Closure closure closure closure       Image: Closure closure         Image: Closure closure closure       Image: Closure closure         Image: Closure closure closure       Image: Closure         Image: Closure closure       Image: Closure         Image: Closure closure       Image: Closure         Image: Closure       Image: Closure         Image: Closure       Image: Closure         Image: Closure<
Possible constraint equations  Use symbol Location of the constraint with the focus in the knoledgebase Add variables to system	ols       Closure equation type       Variable type            • Property related closure constraints         • Geometric closure constraints         • User defined closure equations         • Units of measure conversion constraints         • Units of measure conversion constraints         • Energy • Other          Screen options       Maximum number of variables in closure         constraint that is not included in the current         Above, count constant parameters and universal constants         The two related properties must exist in the current equation system         Show closure constraints that are explicit in differenial dep, variables         Show closure constraints that are explicit in known variables         Model types to screen for in knowledge base         Definition

Figure 15: Tool for adding "closure equations"

Repeat this procedure for streams 2 and 3.

When "closure equations" for all three streams have been defined, a process model consisting of a total of 13 equations is generated. This is the steady state mass and energy balance model for a tank mixer where the effect of pressure is neglected. Figure 16 shows the final model equations.

ModDev - ModDev1		_ 8 >
File Edit View Draw Format Model Window Help		
🗅 🗃 🖨 🔛 NoBaseModel 🔹 🕅		
ModDev1		
	Model equations (equations to iterate over):	<u> </u>
	2: ft_1=sum_i(f_1;)	
	3: Hi_1,=ADippr100_Liq,*TT_1+BDippr100_Liq,/2*TT_1^2+CDippr100_Liq/3*TT_1^3+DDippr100_Liq,/4*TT_1^4+EDippr100_Liq,/5*TT_1^5	
1_ <b>_</b> _	1: H_1=surn_i(Hi_1_i^+(_1_))/tt_1	
Shell - 3-	5: ft_2=sum_((f_2)	
	6: Hi_2=ADippr100_Liq,*TT_2+BDippr100_Liq,/2*TT_2*2+CDippr100_Liq,/3*TT_2*3+DDippr100_Liq,/4*TT_2*4+EDippr100_Liq,/5*TT_2*5	
	4: H_2=sum_((Hi_2 <sup>+</sup> <sub>1</sub> , 2))/ft_2	
	8: ft_3=sum_i(f_3)	
	9: HL3;=ADippr100_Liq;*TT_3+BDippr100_Liq;/2*TT_3*2+CDippr100_Liq;/3*TT_3*3+DDippr100_Liq;/4*TT_3*4+EDippr100_Liq;/5*TT_3*5	
	7: H_3=sum_i(Hi_3*f_3)/ff_3	
	10: T_3=T_Shell1	
	11: P_3=P_Shel1	
	12: $0=f_{-1}+f_{-2}-f_{-3}$	
	13: 0=tt_1*tt_1+tt_2*tt_2-tt_3*tt_3	
11		

Figure 16: process model for a steady state tank mixer

Note that this tutorial stops at the model generation step. Before a code is generated for connection to a solver, it is necessary to analyze the model equations (see part II of the tutorial examples).

<u>Step5: Saving of a generated model</u> – Select "file" on the tool-bar and then "save as". As name, give any preferred name. As part of this tutorial, the same model file is enclosed and it is called model1a.mdl (note that the extension will always be mdl).

### 2.2 Tutorial example 2 – Dynamic tank mixer model with negligible energy holdup

We start with the previous model (model1a.mdl) as the base model and add/change the process description. Since we would like a dynamic model, equation 12 is not acceptable. We need to add an "accumulation" term.

<u>Step1: Change component balance equation</u> – Double click on the shell to enter the "shell description" tool. Click on "component balance", select "accumulation" in the "component balance" tool and exit by clicking on "close" in the "component balance" tool (fig. 17). This will add a molar hold-up term to the left-hand side of equation 12 (replacing the "0" from the steady state version). The molar hold-up term will now have to be related to the flow-out of the tank (stream 3). This is done in the next step, before exiting from the "shell description" tool.

Shell descriptio	n			×
Name: Sh	ell1	Lumped / distributed system Macroscopic balance (lumped)	Geome	tric description 5*TT_1^5
Base model -		C Microscopic balance (distributed)	Co	mponents
Streams:	Shell connections:	Phase condition	R	leactions
1		liquid	Ma	ss balance
3		Equilibrium models	Compo	onent balance 5*TT_2^5
- Nienareiva etal	·			
Component bala	ance specifications			×
Bal./Cor. Balance C Correlation	Extensiv basis	Calculate total input Calculate total output Accumulation		Close
Holdup size	MoleNumber		-	Quantity - Concentration
Flow size	MoleFlow		•	Flux model
Correlated size	MoleFraction		V	Correlation model
Number of repeti	tions (0 if defined in prol	blem definition)		Llose

Figure 17: Changing of component balance equation.

<u>Step2: Relate molar hold-up to stream 3 flow</u> – Click on "other models" and double click on "rootmodel", "geometric", "length", "height", "fluidheight" and single click on "MoleNumber\_Total" to generate the corresponding liquid level model equation (as shown in figure 18). The model is added by clicking on "add model" on the "add/delete models" tool.

Add/modify/remove model equations used to	describe th	e object She	1				×
Add/modify/remove model equations used to Added model equations Height_Shel1=nt_Shel1/(ct_Shel1*Area_Shel1)	v describe th	e object She ymbols Obj Inde Con Inde	II1 ect indices ex keywords aponent indice ex keywords	Indices			
Add model         Remove model(s)         Interchange model           Model definition (ModDef)         Interchange model         Interchange model	Modify model	Close	action indices <sup>=</sup> ex keywords				
Model name MoleNumber_Total	Parent model	equations			<u> </u>	Include paren	t models
PhaseEquilibrium     Geometric	I ocal model e	quations Mod	ify local molel :	equations Vie	w structure of	local model er	Juations 6
	Height=nt/(ct	*Area);					
⊡ Length		al equations		dd iacluded m	odels too 🗖	Select include	
i⊟ Height I⊟ FluidHeight Masshumber Totu		el equations			00010100	Selectificidat	
Massivunibe_Tok MoleNumber_Tota Volume_Area	[r	iclude selected	i model	-	[ <b>.</b>		
Adius	Add child Delete	Add before Rename	Add after Description	Heferences	Edit variable symbols	types C	iose irch tool

Figure 18: Add the equation for liquid height in the tank.

The next step is to relate the liquid height to the flow out (stream 3). To do this, double click on stream 3 and then click on "other models" in the "stream description" tool. This will again start the "add/delete models" tool with "model definition" and "model search" tools. The path to finding the level-flow model is shown in Figure 18 ("Rootmodel" -> "Transport" -> "InterPhase" -> "Mass" -> "ValveConnection" -> "MoleFlow" -> "Hight"). Note that before clicking on "add model" in "add/delete models" tool, define index keyword "from" as "shell1" (shown in figure 19).



Figure 19: Addition of level-flow equation.

Before leaving the "add/delete models" tool, the equation relating the total flow out from stream 3 to the component flows for stream 3 needs to be generated. The path for finding this equation is shown in figure 20. As in the total flow equation, before clicking on the "add model", the "from" index should be specified as "shell1" on the "add/delete models" tool.

	l to describe th	ie object 3				
Added model equations	🔽 Use s	wmbols E.	ject indices —			
ft 3=Alpha 3*sgrt(Height Shell1)		- Inc	lex keywords	Indices		
f_3[i]=x_Shell1[i]*ft_3		3		3		
		to		3		<u> </u>
		fro	m	Shell1		<b>•</b> •
		- Co	mponent indice	s		
		Inc	lex keywords	Indices		
		i		li		
						<b>•</b> •
		Be	action indices			
		Inc	lex keywords	Indices		
						T _
And model Bernows model(s) [ Justice house model	المتحصين والمحاط ألما	Classel				
Add model Remove model(s) Interchange mod	ier modily moder					
		_				
Model definition (ModDer)						
Model name Molefraction (Specific phase)	Parent model	equations				parent models
MolecularWeight Mea						<u> </u>
SurPlusEromBeaction						<b>T</b>
E Component	1					
E Gradient				a fre		
E MoleFlow	Local model e	quations <u>Mo</u>	dify local molel	equations   Viev	w structure of local m	odel equations
Molariry	f{to}[i]=x{from	}{phase}[i]*ft{t	:0};			<u> </u>
Molaliny						
Molefraction						· · · · · ·
			_		_	
Moletraction IS	Included mod	el equations	🖂 📈 A	vdd included ma	odels too 🔽 Select	include model:
MoleNumber	- moladed mod					
Molefraction (\$ MoleNumber MoleFlow						<b>A</b>
Molefraction [5 						*
Molefraction (\$ MoleNumber MoleFlow DifferenceInMolari MassTraction						×
Moleffaction IS MoleFlow DifferenceInMolari MassFraction FF- Molaritu		iclude selecte	d model	4		× ×
MoleFlacton IS     MoleFlow     MoleFlow     MoleFlow     DifferenceInMolari     MassFraction     Molarity     P     Molerity	Add child	nclude selecte Add before	d model Add after	References	Edit variable types	Close

Figure 20: Addition of component flow equation.

At the end of this step, three equations are added, the first relates the total molar holdup of liquid to the height of the liquid (introducing tank geometric parameters), then the height is related to the total flow out (stream 3) and then the total flow is related to the component flow. Two additional terms - total molar liquid holdup and liquid mole fraction in the tank – are introduced by the three new

equations. These additional terms are dependent on the other variables and therefore need "closure equations".

Finally, after adding the above three equations, ModDev gives a warning that two equations have same explicit variables. This means that one of the equations have to be removed.

Examining the model equations on the main ModDev screen shows that the two equations both have the total flow out from stream 3 as the unknown variable (on the left hand side of the equation). One of these equations need to be removed – that is,

$$ft_3 = sum_3(f_3_i)$$

A1

A3

need to be deleted. Addition of the necessary "closure equations" and deletion of the above equation is done in the next step (step 3).

<u>Step3: Addition and deletion of "closure equations"</u> – click on the shell and then select "model" in the tool-bar. From the "model" window items, select "closure equations" as shown in figure 21. From the "closure equations" tool, remove the Eq. A1 from the list of closure equations and add the following equations,

$x_Shell1_i = n_Shell1_i / nt_Shell1$	A2

 $nt_Shell1 = sum_i(n_Shell1_i)$ 



to the list of added closure equations (as shown in figure 22).

Figure 21: Selection of "closure equations" from tool-bar.

Add/modify/remove model equations to	×
Added model equations	Component indices     Component indices
n_Shell1=sum_(n_ShellT[i])	Index keywords Indices
Add model Remove model(s) Interchange model Modify model Close	
Closure constraints	
Possible constraint equations n(Shell1)[i]=x(Shell1)[i]*nt(Shell1)	Closure equation type Property related closure constraints Closure constraints Closure constraints Closure defined closure equations Closure equation type Closure equation type
	Screen options Maximum number of variables in closure constraint that is not included in the current
	Above, count constant parameters and universal constants The two related properties must exist in the current equation system Show closure constraints that are explicit in explicit variables
Location of the constraint with the focus in the knoledgebase	Show closure constraints that are explicit in differenial dep.variables Show closure constraints that are explicit in known variables

Figure 22: Addition and removal of closure equations.

Exit from the "closure equations" tool and now the warning will disappear and we will have a dynamic tank model with 17 equations as shown in figure 23.

ModDev - [ModDev1]		
File Edit View Draw Format Model Window	Help	
D 🖻 🖻 🖳 🔽 NoBaseModel 🔍		
	Model e	quations (equations to iterate over):
	2:	ft_1=sum_i(f_1;)
	3:	Hi_1;=ADippr100_Liq;*TT_1+BDippr100_Liq;/2*TT_1^2+CDippr100_Liq;/3*TT_1^3+DDippr100_Liq;/4*TT_1^4+EDippr100_Liq;/5*TT_1^5
	1:	H_1=sum_i(Hi_1^f_1)/ft_1
a	5:	ft_2=sum_((f_2)
	6:	Hi_2;=ADippr100_Liq,*TT_2+BDippr100_Liq,/2*TT_2*2+CDippr100_Liq,/3*TT_2*3+DDippr100_Liq,/4*TT_2*4+EDippr100_Liq,/5*TT_2*5
1,	4:	H_2=sum_i(Hi_2^+f_2)/ft_2
2	10:	Hi_3=ADippr100_Liq,^TT_3+BDippr100_Liq,/2*TT_3*2+CDippr100_Liq,/3*TT_3*3+DDippr100_Liq,/4*TT_3*4+EDippr100_Liq,/5*TT_3*5
	11:	T_3=T_Shelf1
	12:	P_3=P_Shell1
	14:	nt_Shell1=sum_i(n_Shell1;)
	13:	x_Shelf1;=n_Shelf1;ht_Shelf1
	15:	Height_Shell1=nt_Shell1/(ct_Shell1*Area_Shell1)
	8:	ft_3=Alpha_3*sqrt(Height_Shell1)
	9:	f_3=x_Shell1_ftf_3
	7:	H_3=sum_i(Hi_3 <sup>+</sup> f_3)/ff_3
	16:	\$(n_Shell1 <sub>i</sub> )=f_1+f_2-f_3
	17:	0=tt_11t_1+tt_21t_2-tt_31t_3

Figure 23: Dynamic model for a tank mixer with negligible energy holdup.

<u>Step4: Save the model</u> – Before exiting from ModDev or starting another problem, save the model under the "save as" option. In the files corresponding to this tutorial, the file model1b.mdl corresponds to this model.

#### 2.3 Tutorial example 3 – Dynamic tank with mass and energy holdup

We start with the model from example 2 as the basis. We only need to add the energy holdup and related equations. Open ModDev with the model1b.mdl file.

<u>Step1: Add energy holdup</u> – Double click on the shell and then select "energy balance". In the "energy balance" tool, select "accumulation" and exit (fig. 24).

Shell description Name: Shell1 Base model	C Macroscopic balance	stem Geometric de e (lumped) Compon : (distributed) Compon	ents	
Streams: Shell conner 1 2 3 Dispersive state Homogeneous	Ctions: Phase condition	Reaction Mass ball Component sible fluid	ons 5 balance ^5	
Energy specifications				×
Bal./Cor. Extensiv base	is Calculate total output Calculate total input	Accumulation     Accumulation in wall     Accumulation in particle	Close	
Holdup size Enthalpy_Tota	al		💌 Quantity - Tempe	erature
Flow size MoleFlow_Tot	tal*Enthalpy_Mole		Flux mode	
Correlated size Temperature			Correlation m	odel

Figure 24: Energy specification for shell.

<u>Step2: Relate the stream 3 enthalpy to the tank liquid enthalpy</u> – double click on stream 3 and select "other models". Select the model in way "Rootmodel" -> "Quantity" -> "Enthalpy" -> "Enthalpy\_Mole" -> "EqualEnthalpy" (fig. 25).

ModDev will now give a warning that the same explicit variable appears in two equations. This means one closure equation must be removed. Also, the shell enthalpy needs to be related to the total enthalpy through a closure equation.

Add/modify/remove model equations use	l to describe the	object 3					×
Added model equations [ft_3-Alpha_3*sqt[Height_Shell1] f_3[]=x_Shell1[]ft_3 H_3=H_Shell1	Vise sy	mbols Ubj Ind G Ind Ind Ind Ind	ect indices ex keywords n nponent indice ex keywords ex keywords	Indices 3 3 Shell1 Indices i Indices			• • • • •
Add model Remove model(s) Interchange mod	lel Modify model   I						]_
Model name     EqualEnthalpy       ⊕     Temperature_Absolute       ⊕     Heat capacity       ⊕     Enthalpy       ⊕     Enthalpy       ⊕     Enthalpy       ⊕     Enthalpy_Mole       □     Enthalpy_Model       □     U+PV       □     CordT       ⊕     Enthalpy_Mass       ⊕     Enthalpy_Total       ⊕     Enthalpy_Total       ⊕     Enthalpy_Total       ⊕     Enthalpy_Total	Parent model eq	equations <u>Moc</u> equations <u>Moc</u> iPhase\Energ idude selecter Add before	ify local molel IV A gy\Equal inten I model Add after	equations View Add included m siv pr H{to}=H I References	w structure o odels too (from); Edit variab	Include parent m filocal model equination Select include m le types Closs	indels
i ⊡ Vaporization	- Delete	Rename	Description	🔽 Use	symbols	Show searc	h tool

Figure 25: Addition of equation relating stream and shell enthalpies.

<u>Step3: Addition and removal of closure equations</u> – Highlight the shell and enter the "closure equations" tool as shown in figure 21. Add equation A4 and remove equation A5 as shown in figure 26.

add/modify/remove model equations to model1b	X
Added model equations       Image: Construction of the symbol         Added model equations       Image: Construction of the symbol         x_Shell[Tip]=n_Shell[Tip]/nt_Shell1       Image: Construction of the symbol         nt_Shell = sum_(int_2)[n_1^2, 2[n_1/nt_2]       Image: Construction of the symbol         H_1 = sum_(int_1)[n_1^2, 1[n_1/nt_1]       Image: Construction of the symbol         H_1 = sum_(int_1)[n_1^2, 1[n_1/nt_1]       Image: Construction of the symbol         H_2 = sum_(int_1)[n_1^2, 1[n_1/nt_1]       Image: Construction of the symbol         H_1 = sum_(int_1)[n_1^2, 1[n_1/nt_1]       Image: Construction of the symbol         H_2 = sum_(int_1)[n_1^2, 1[n_1/nt_1]       Image: Construction of the symbol         H_2 = sum_(int_1)[n_1^2, 1[n_1/nt_1]       Image: Construction of the symbol         Add model       Remove model(s)       Interchange model         Add model       Remove model(s)       Interchange model	object indices     Indices       Index keywords     Indices       Shell1     Shell1       Shell1     Shell1       Component indices     V       Index keywords     Indices       I     V       Reaction indices     Indices       Index keywords     Indices       V     V
Closure constraints	
Possible constraint equations I Use symbols n(Shell1)[i]=x(Shell1)[i]=nt(Shell1) Ht(Shell1)=H(Shell1)=nt(Shell1)	Closure equation type Property related closure constraints Geometric closure constraints User defined closure equations Units of measure conversion constraints Closure equations Closure equations Closure equations Closure equation type Closure equations Closure equation type Closure equations Closure equations Closure equations Closure equation type Closure equation type Closure equations Closure equations Clo
	Screen options Maximum number of variables in closure constraint that is not included in the current
Location of the constraint with the focus in the knoledgebase	Above, count constant parameters and universal constants The two related properties must exist in the current equation system Show closure constraints that are explicit in explicit variables Show closure constraints that are explicit in differential dep variables Show closure constraints that are explicit in known variables
Add variables to system	Model types to screen for in knowledge base Definition

Figure 26: Addition and removal of closure equations.

A4

A5

 $H_Shell1 = Ht_Shell1/ nt_Shell1$  $H_3 = sum_i(f_3[i]*Hi_3[i])$ 

Now the warning will disappear and we will have the full model. Note that this dynamic model considers the existence of only one phase, that is, liquid. The final model equations are shown in figure 27.

ModDev - [model1b]		
🔁 File Edit View Draw Format Model Window	elp	
D 🖻 🖨 🖳 NoBaseModel 🔍		
	Model equations (equations to iterate over):	
	2: ft_1=sum_i(f_1)	
	3: Hi_1_=ADippr100_Liq_*TT_1+BDippr100_Liq_/2*TT_1^2+CDippr100_Liq_/3*TT_1^3+DDippr100_Liq_/4*TT_1^4+EDippr100_Liq_/5*TT_1^5	
	1: H_1=sum_i(Hi_1^*f_1;)/ft_1	
· · · · · · · · · · · · · · · · · · ·	5: ft_2=sum_i(f_2)	
<b>►</b>	6: Hi_2_=ADippr100_Liq, <sup>4</sup> TT_2+BDippr100_Liq, <sup>2</sup> *TT_2^2+CDippr100_Liq, <sup>3</sup> *TT_2^3+DDippr100_Liq, <sup>4</sup> *TT_2^4+EDippr100_Liq, <sup>5</sup> *TT_2^5	
1, <b>&gt;</b>	4: H_2=sum_i(Hi[2;*[2])/ft_2	
2	10: Hi_3j=ADippr100_Liq,*TT_3+BDippr100_Liq,/2*TT_3^2+CDippr100_Liq,/3*TT_3^3+DDippr100_Liq,/4*TT_3^4+EDippr100_Liq,/5*TT_3^5	
	11: T_3=T_Shel1	
	12: P_3=P_Shel1	
	14: nt_Shel/1=sum_i(n_Shel/1;)	
	13: ×_Shell1,=n_Shell1,ht_Shell1	
	15: H_Shell1=Ht_Shell1.ht_Shell1	
	9: H_3=H_Shell1	
	16: Height_Shell1=nt_Shell1/(ct_Shell1*Area_Shell1)	
	7: ft_3=Alpha_3*sqrt(Height_Shel/1)	
	8: f_3;=x_Shel1;*tt_3	
	17: $(n_shell_i,t)=f_1+f_2-f_3$	
	18: \$(Ht_Shell1,t)=tt_1*H_1+tt_2*H_2-tt_3*H_3	

Figure 27: Dynamic tank mixer model with mass & energy holdup.

<u>Step3: Save the model</u> – Save this model before starting a new problem or exiting from ModDev. Use the "save as" option. In the files corresponding to this tutorial, the file model1c.mdl corresponds to this model.

#### 2.4 Tutorial example 4 – Tank with reaction (CSTR)

For this example, any of the above three models can be used. For simplicity, model1a.mdl will be used. Models model1b.mld and model1c.mdl will need exactly the same steps. In the first example, a stoichiometric reaction with specified degree of reaction will be used. In the second example, a kinetic model will be used. The starting point is model1a.mdl – start ModDev by openning the file model1a.mdl.

<u>Step1: Add the reaction term</u> – Double click on the shell and click on "reactions" in the "shell description" tool. In the "reaction" tool, double click on "root" until "stoichiometric" is shown. Type a name for the reaction and click on "add child" and then click on "modify stoichiometry". Fill out the reaction details as shown in figure 28. Back on the "reaction" tool, select for "add the current reaction" as shown in figure 29.

Define/modify/delete/add/remove reactions in	n the shell give	en by: Shell1			×
Defined reactions		Reaction name	•	Rea	action index
⊡ Root		reaction		Sto	pichiometric
🚊 Stoichiometric		,	1	÷.	
reaction		Add child	Add b	efore	Add after
Electrochemical		Rename	Del	ete	Description
		14 IV 1 1 1		1.1 17	12.00.00
Heterogeneous		Modify stoichi	ometry	Modify	kinetic model
Components in the reaction: reaction					×
List of Components (click to add/remove component to/fro	om the aridhox)				
HYDBOGEN.SULFIDE H2S	7783.06	1			
HYDROGEN-SELENIDE H2Se	7783-07-	5			-
HYDROGEN-CYANIDE CHN	74-90-8	-			
HYDROGEN H2	1333-74-0	)			
HYDRUGEN-(para) H2	1333-74-0	J			
HYDROGEN-BROMIDE BIH	7647-01-0	-0 1			
HYDROGEN-FLUORIDE FH	7664-39-3	3			
HYDROGEN-IODIDE HI	10034-85	-2			
HYDROGEN-PEROXIDE H202	7722-84-1	l			
Sodium-hydrogen-phosphate NaH2P04	-387				
Potassium-dihydrogen-phosphate KH2PU4	-394				-
Porassium-hudrodensuirare NH5114	431				
Search for component				01-3	
Search on name     Component     OCTANE				5(0)	c. Loer.
Search on formula				,	
C Search on casno     INFORME			-2	-	
Search string: HYDRUGEN					
hydrogen					
Reactants	Products				
2 C4H10	C8H18 + H2				
Mass balance over the reaction: 0.000879999999999		0	llose		
1			-	_	

Figure 28: Reaction definition

Define/modify/delete/add/remove reactions in the shell give	en by: Shell1			×
Defined reactions ⊡ Root	Reaction name reaction	•	Rea  Sto	action index bichiometric
	Add child	Add after		
in Electrochemical	Rename Delete De		Description	
	Modify stoichi	ometry	Modify	kinetic model
Reforming reactions	Set default	value of	kinetic	parameters
	V	/iew enti	ire mod	el
i± AmmoniaProcuction				
				l II
J Beactants Products			<b>I</b> •	Use symbols
2 C4H10 C8H18 +	H2			
Kinetic models (parent)	Lílocal)	5	linelu	aleboal models
	(1000)		mola	
Reaction included in the shell given by: Shell1				
reaction	Ado	d reactio	n to Sh	ell1
	Remov	/e reacti	on from	Shell1
	Other models	or mode	ls for u	ndefined reac.
Do the system contain unspecified reactions	Modify kinetic	model o	of sel, re	ac. Close

Figure 29: Adding reaction to the current system.

<u>Step2: Define equation for degree of reaction</u> - Exit from the "reaction" definition tool and click on "other models". This will open the "add/delete models" tool. Follow the path "Rootmodel" -> "Reaction" -> "KineticModel" -> "Stoichiometric" -> "DegreeOfReactionOfEveryReaction" (as shown in figure 30) to choose the degree of reaction equation. Note that before clicking on "add model", the "from" index should be set to 3 indicating the component flow from stream 3.



Figure 30: Defintion of degree of reaction.

Exit from the "shell description" menu. The final version of the model is shown in the main screen of ModDev (see figure 31).

ModDev - [model1a]		
🛒 File Edit View Draw Format Model W	w Help	
🗅 🗃 🖨 🔛 🔽 🛛 NoBaseModel		
	todel equations (equations to iterate over):	
	: ft_1=sum_i(f_1;)	
	: Hi_1=ADippr100_Liq,*TT_1+BDippr100_Liq,/2*TT_1^2+CDippr100_Liq,/3*TT_1^3+DDippr100_Liq,/4*TT_1^4+EDippr100_Liq,/5*TT_1^5	
	: H_1=sum_i(Hi_1^f_1)/ft_1	
	: ft_2=sum_i(f_2)	
	: Hi_2=ADippr100_Liq,*TT_2+BDippr100_Liq,/2*TT_2*2+CDippr100_Liq,/3*TT_2*3+DDippr100_Liq,/4*TT_2*4+EDippr100_Liq,/5*TT_2*5	
1	: H_2=sum_i(Hi_2 <sup>*</sup> t_2)/ft_2	
Shell1 3	: ft_3=sum_((f_3)	
2	: Hi_3=ADippr100_Liq,*TT_3+BDippr100_Liq,/2*TT_3*2+CDippr100_Liq,/3*TT_3*3+DDippr100_Liq,/4*TT_3*4+EDippr100_Liq,/5*TT_3*5	
	: H_3=sum_i(Hi_3,*f_3)/ft_3	
	0: T_3=T_Shell1	
	1: P_3=P_Shel1	
	2: RR_Shell1 <sub>m</sub> =alpha_Shell1 <sub>m</sub> *f_3 <sub>Key(m)</sub>	
	3: 0=t_1,+t_2,-t_3,+RN_Shell1	
	4: 0=tt_1'H_1+tt_2'H_2-tt_3'H_3	

Figure 31: Steady state tank-reactor model

Note that adding the same set of equations to the dynamic tank models, generates the corresponding dynamic CSTR models (one phase systems).

Save this model as model2a-r.mdl

# 2.5 Tutorial example – Tank-reactor model where kinetic model is included

The starting point again is the steady state tank model (for simplicity). Enter the "reaction" tool, double click on the root, the "homogeneous" and the "MethylAcetateReaction". Figure 32 shows the "reaction" tool with the various selected options. Click "Modify kinetic model of sel. reac." to define it. Figure 33 shows the details of the predefined kinetic model.

Define/modify/delete/add/remove reactions in the shell give the	ven by: Shell1		×
Defined reactions	Reaction name MethylAcetate	Reaction M	action index ethylAcetateRe
Electrochemical	Add child	Add after	
⊡ Homogeneous COoxidation	Rename	Delete	Description
MethylAcetateReaction	Modify stoichi	ometry Modif	y kinetic model
Heterogeneous     Heterogeneous     Heterogeneous	Set default	value of kineti	e parameters
. ShiftReactions	\\	/iew entire mod	lel
⊞… Combustion ⊞… AmmoniaProduction			
, Reactants Products			Osc symbols
CH40 + C2H402	? + H2O		
Kinetic models (parent) 🔽 Include parent models Kinetic mode	el (local)	🔽 Inclu	ide local models
			A V V
Beaction included in the shell given by: Shell1			
MethylAcetateReaction	Ade	d reaction to SI	hell1
	Remov	ve reaction from	n Shell1
	Other models	or models for u	indefined reac.
Do the system contain unspecified reactions	Modify kinetic	model of sel. r	eac. Close

Figure 32: Selection of MethylAcetate Reaction.

Add/modify/remove model equations used t	o describe th	e object She	ell1			×
Added model equations RRForward_Shell1(m]=Vt_Shell1'RKforward_Shell1 RRBackward_Shell1(m]=Vt_Shell1'RKbackward_S RR_Shell1(m]=RRForward_Shell1(m)-RRBackward_ RKforward_Shell1(m]=A1(m)*exp(Ea1(m)/(Rg*T_Sh RKbackward_Shell1(m)=A2(m)*exp(Ea2(m)/(Rg*T_	ymbols Ob d_Shell ackwarc	ject indices ex keywords mponent indice lex keywords action indices	Indices		<b>v</b> A <b>v</b> v <b>v</b> v	
Add model         Remove model(s)         Interchange model	Modify model	Close	lex keywords	Indices m		• • • •
Model definition (ModDef)						×
Model name     Arrhenius       ⊕-     BalanceCorrelations       ⊕-     Population       ⊕-     Reaction       ⊕-     KineticModel       ⊕-     Stoichiometric       ⊕-     HomogeneousReactions       ⊕-     Inversible	Parent model RRForward[n RRBackward RR[m]=RRFo	equations n]=Vt*RKforwa I[m]=Vt*RKbac rward[m]-RRB quations <u>Mo</u> o	rd[m] <sup>*</sup> XR_Forw :kward[m] <sup>*</sup> XR_ ackward[m]; tify local molel :	ard[m]; Backward[m]; equations   Views	Include	e parent models
Reversible     Beversible     Beversible     Beversible     Beversible     Beversible     Beversible     Constant     Beversible     Bev	Included mod Reaction\Re Add child	el equations actionRateCon nolude selecter Add before	▼ A nstant\Arrheniu d model Add after	Add included mod ISFor RKforward RKbackwa References E	lels too Select [m]=A1[m]*exp(-Ea ard[m]=A2[m]*exp(-E Edit variable types	include models
I →	Delete	Rename	Description	🔽 Use sy	ymbols 🔽 Shi	ow search tool

Figure 33: Kinetic model definition through the "model definition" tool.

Close "Reactions" tool and go to "Related variables" tool. Add suggested equation to the model (fig. 34). Figure 35 shows the final process model equations. The final model is saved as model3a-r.mdl.

Add/modify/remove model equations used	to describe the obje	ct Shell1		×	
Added model equations	Lise sumbols	- Object indices			
BN Shell1(i)-sum m(BB Shell1(m)*pu(i)[m])	It Ose symbols	Index keywords	Indices		
Triv_Sheirtij-sun_n(tri_Sheirtin) hutijinij		Shell1	Shell1		
				▼	
		Construction for the second			
		Lomponent indices-	Indices		
		li		<b>T</b> •	
		<u> </u>	-		
				<u> </u>	
		Reaction indices			
		Index keywords	Indices		
J		m	m		
Add model Bemove model(s) Interchange mode	el Modifu model Close			<b>T</b>	
Add filodol Fromove filodol(b) Filodoladige filodo	on modely model close				
Related variables within the object Shell1					
Possible constraint equations	🔽 Use symbols 🗖	Closure equation type-		Variable type	
		Property related close	sure constraints	All C Momentum	
		Geometric closure c	onstraints	C Harry C Committee	
		O User defined closure	e equations	C Mass C Geometric	
		O Units of measure co	nversion constraints	C Energy C Other	
		Screen options			
		Maximum number of variables in closure			
		constraint that is not inc	luded in the current		
		Above, count constant	parameters and univer	rsal constants 📃	
		The two related propert	ies must exist in the cu	irrent equation system	
Location of the constraint with the focus in the kn	oledgebase	Show closure constrain	ts that are explicit in ex to that are explicit in di	(plicit variables	
		Show closure constrain	ts that are explicit in kr	nereniaruep.variables	
1		Madal turnes to second (	rs and are explicit in Ki		
Add variables to system		model types to screen h	or in knowledge base	Definition	

Figure 34: Adding of closure equations.

ModDev - [model1a]				
1 File Edit View Draw Format Model Window Help				
D 🛎 🚔 🔛 🗠 NoBaseModel	• )			
	Model e	quations (equations to iterate over):		
1 Shell 3	2:	ft_1=sum_i(f_1)		
	3:	Hi_1;=ADippr100_Liq;*TT_1+BDippr100_Liq;2*TT_1^2+CDippr100_Liq;/3*TT_1^3+DDippr100_Liq;/4*TT_1^4+EDippr100_Liq;/5*TT_1^5		
	1:	H_1=sum_i(Hi_1^f_1)/ft_1		
	5:	ft_2=sum_i(f_2)		
	6:	HL2;=ADippr100_Liq;^TT_2+BDippr100_Liq;/2*TT_2^2+CDippr100_Liq;/3*TT_2^3+DDippr100_Liq;/4*TT_2^4+EDippr100_Liq;/5*TT_2^5		
	4:	H_2=sum_i(Hi_2^*f_2)/it_2		
	8:	ft_3=sum_i(f_3)		
	9:	HL3;=ADippr100_Liq;*TT_3+BDippr100_Liq;2*TT_3^2+CDippr100_Liq;/3*TT_3^3+DDippr100_Liq;/4*TT_3^4+EDippr100_Liq;/5*TT_3^5		
	7:	H_3=sum_i(Hi_3 <sup>*</sup> _3)/tt_3		
	10:	T_3=T_Shell1		
	11:	P_3=P_Shel1		
	15:	RKforward_Shell1_m=A1_m*exp(-Ea1_m/(Rg*T_Shell1))		
	12:	RRForward_Shell1 _m=Vt_Shell1 *RKforward_Shell1 _m*XR_Forward_Shell1 _m		
	16:	$RKbackward_Shell1_m = A2_m^*exp(-Ea2_m/(Rg^*T_Shell1))$		
	13:	RRBackward_Shell1_m=Vt_Shell1*RKbackward_Shell1_m*XR_Backward_Shell1_m		
	14:	RR_Shell1_=RRForward_Shell1RRBackward_Shell1_m		
	17:	RN_Shelfi_=sum_m(RR_Shelfi_m*nui,m)		
	18:	0=f_1;+f_2;-f_3;+RN_Shell1;		
	19:	D=ft_1'H_1+ft_2'H_2-ft_3'H_3		

Figure 35: CSTR model with reaction kinetics.

### 3. Other examples

The tutorial document "Computer Aided Modeling Tools: ModDev" contains a number of examples dealing with reactors with jacketed heating, flash, evaporator and distillation columns.