Computer Aided Modeling Tool – ModDev

Tutorial Examples. Part I

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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.

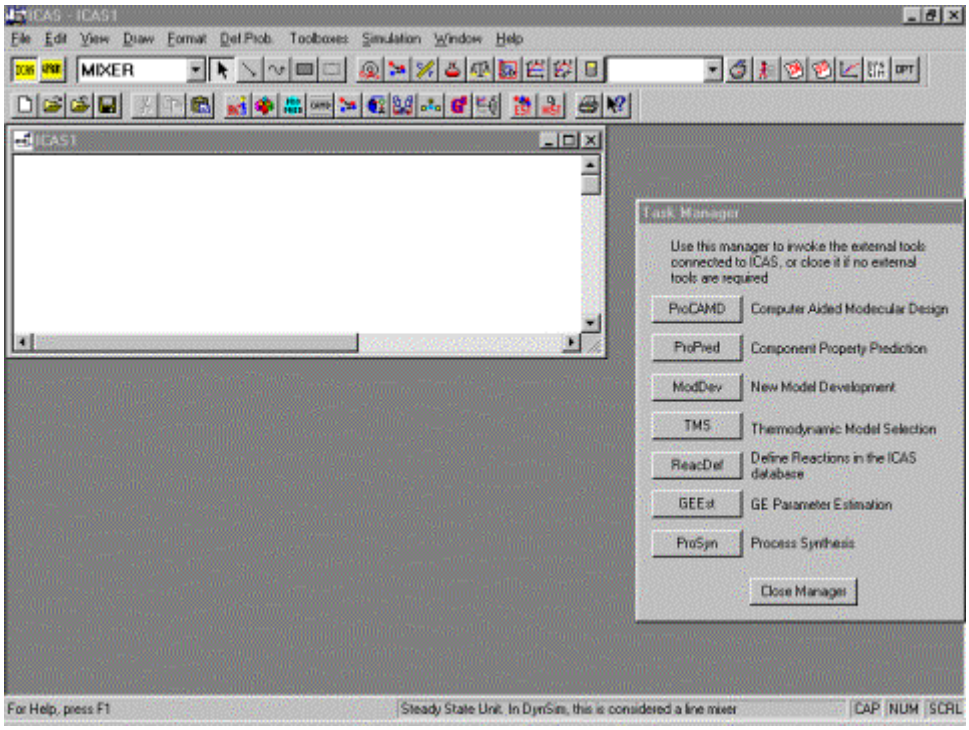

Figure 1: Starting screen in ICAS

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.

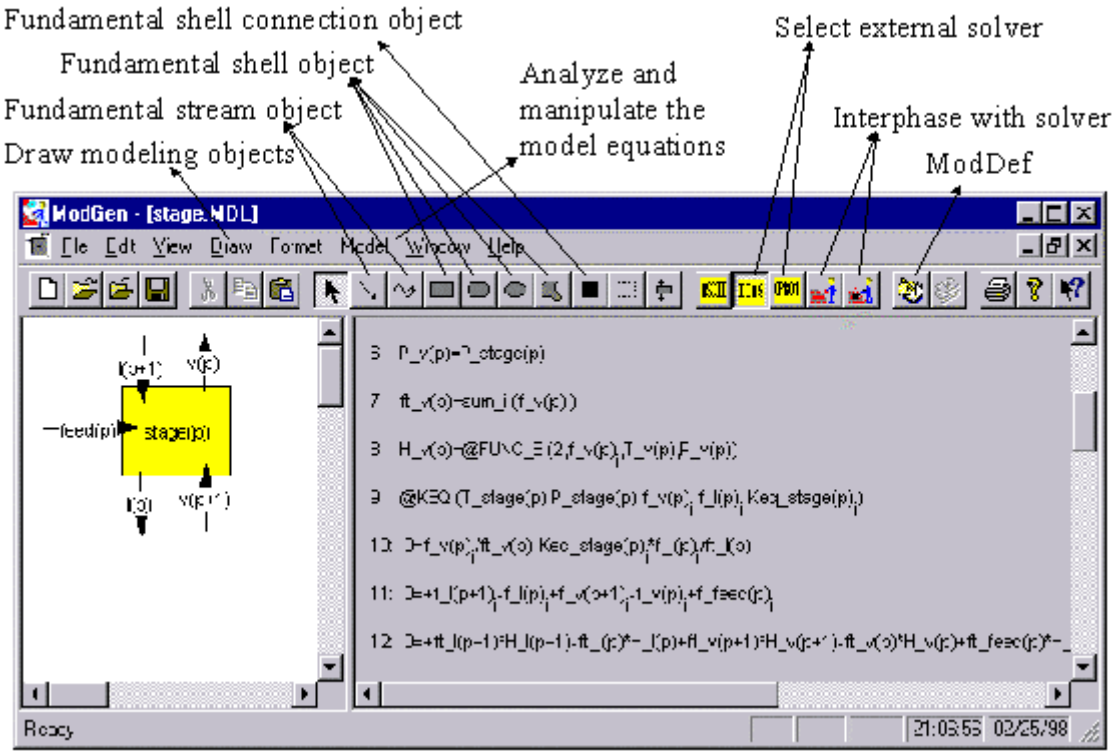

Figure 2: Starting screen of ModDev with available tools highlighted.

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.

Step1: Describe the process through a flow diagram - 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).

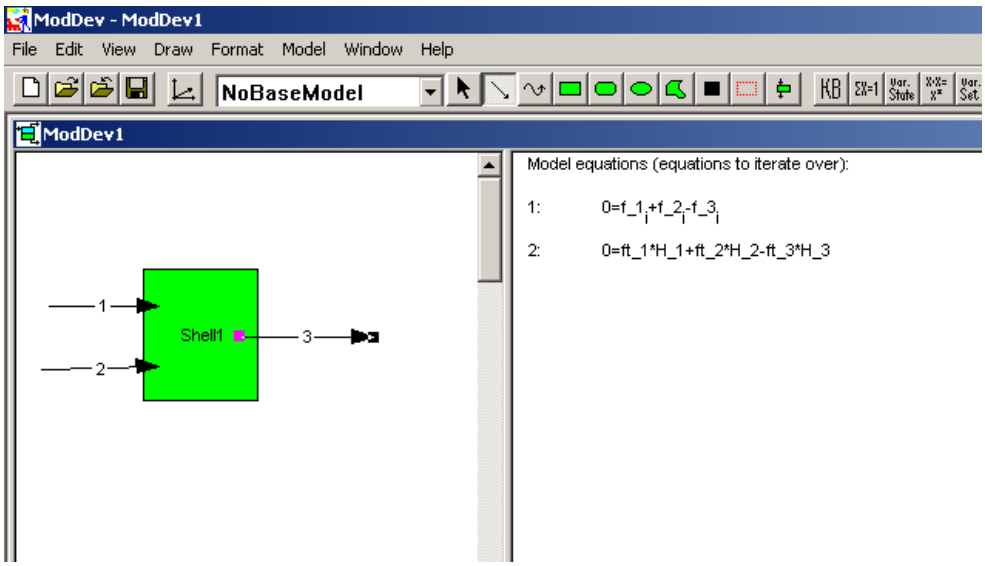

Figure 3: Describing of the process.

Step2: Describe the shell – 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".

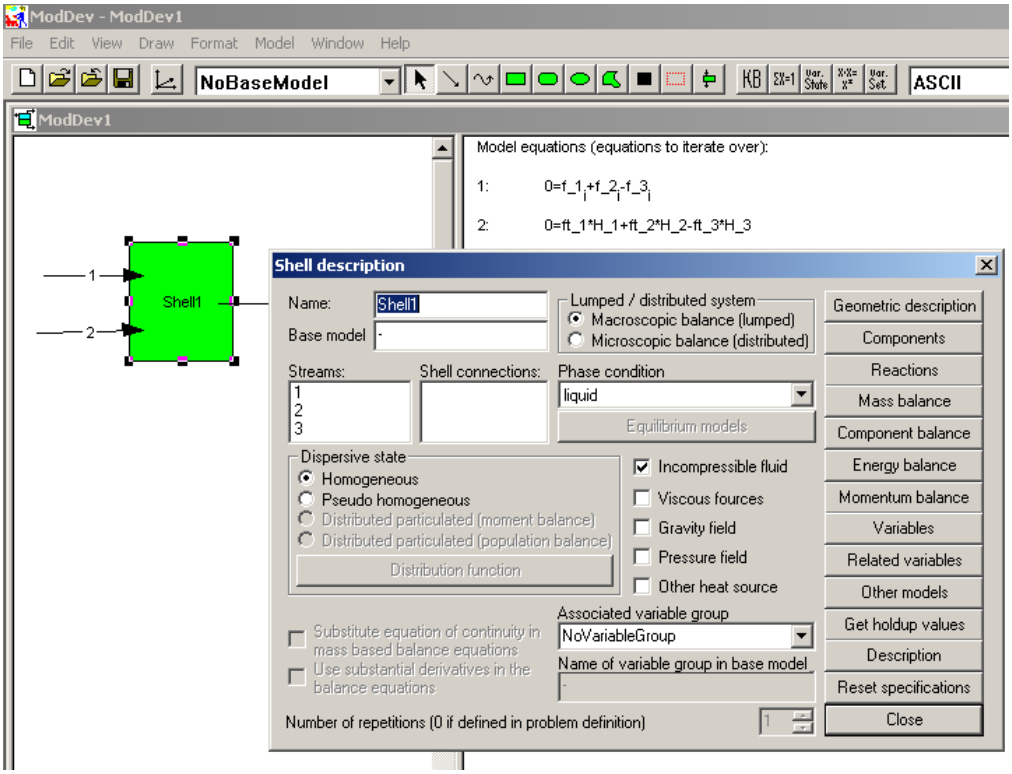

Figure 4: Describing of the shell.

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

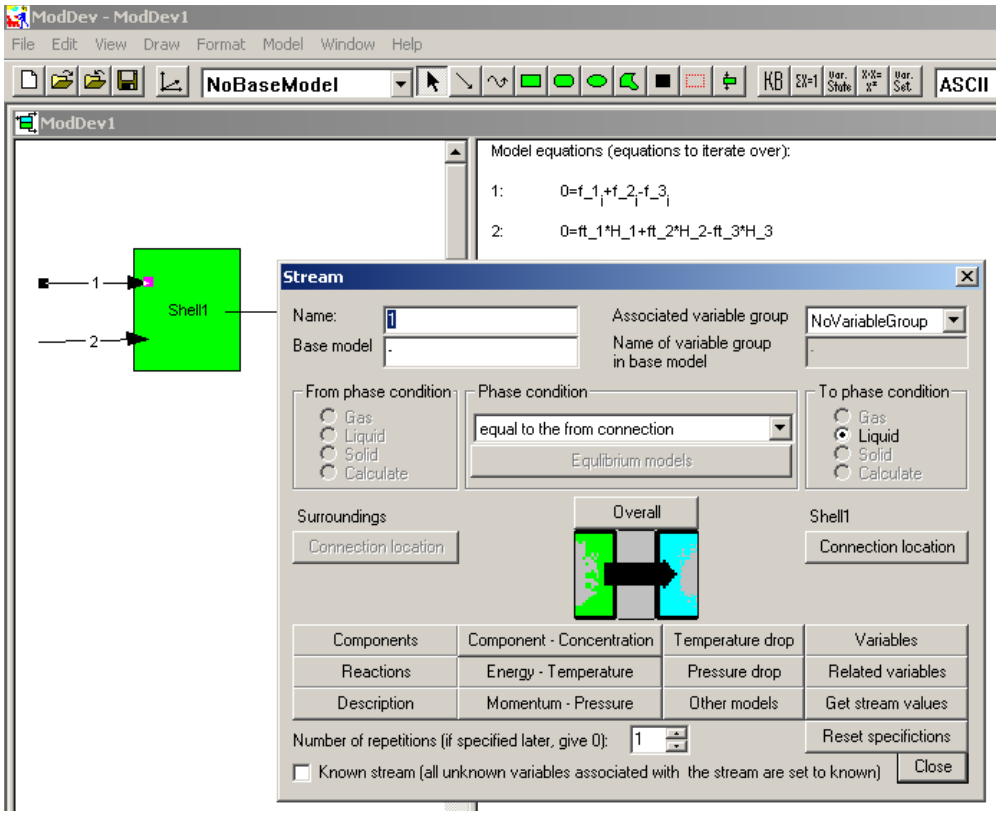

Figure 5: Shell description tool.

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).

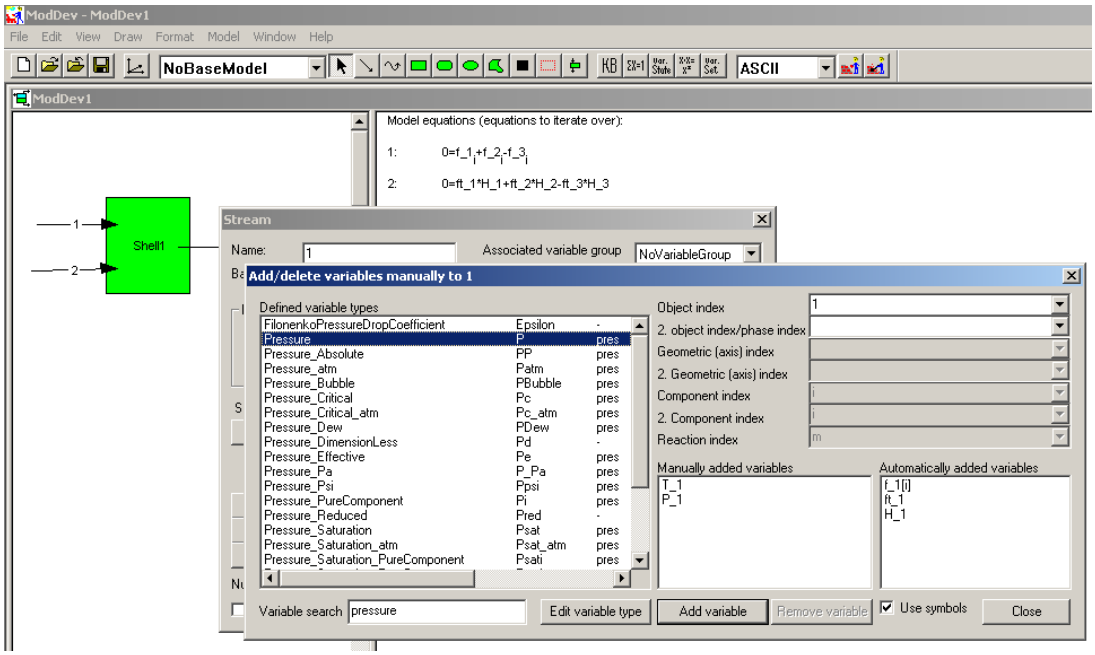

Figure 6: Selection of additional variables.

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”.

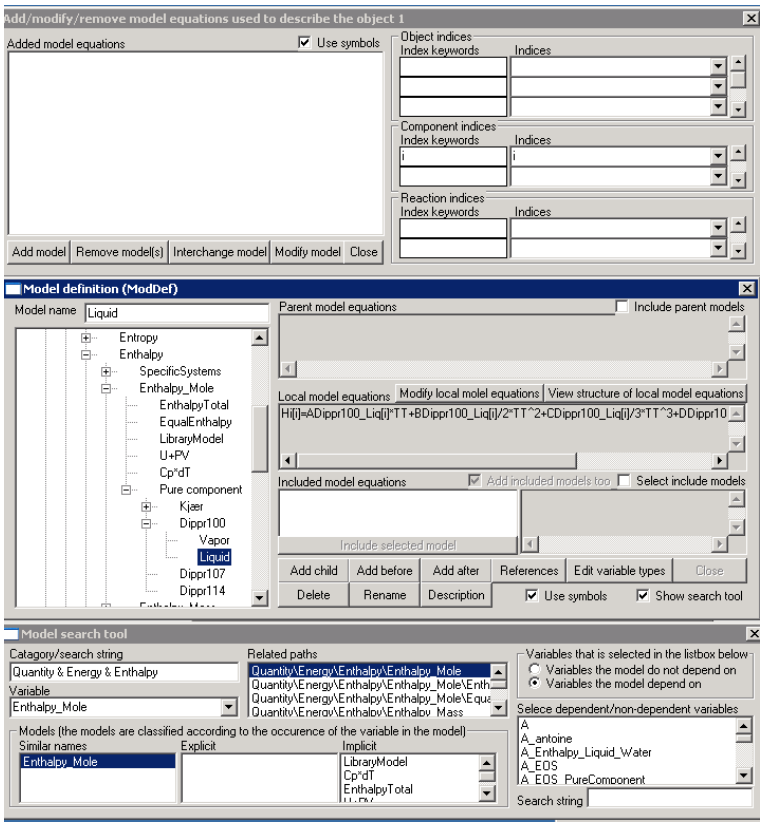

Figure 7: “Add/delete models” tool plus associated tools – “model definition” and “model search”.

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).

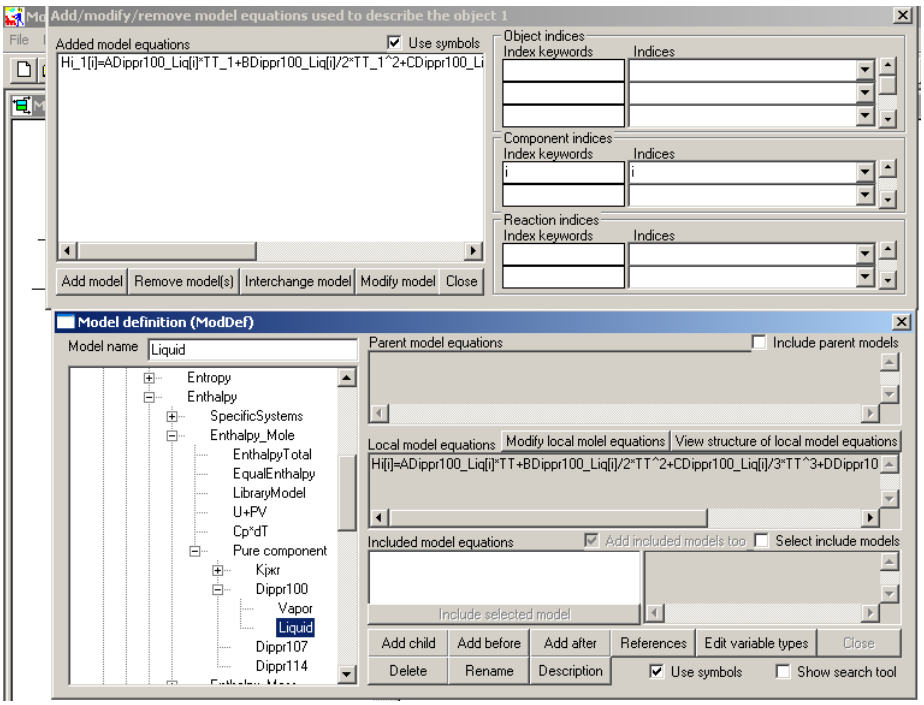

Figure 8: Model definition for stream 1.

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).

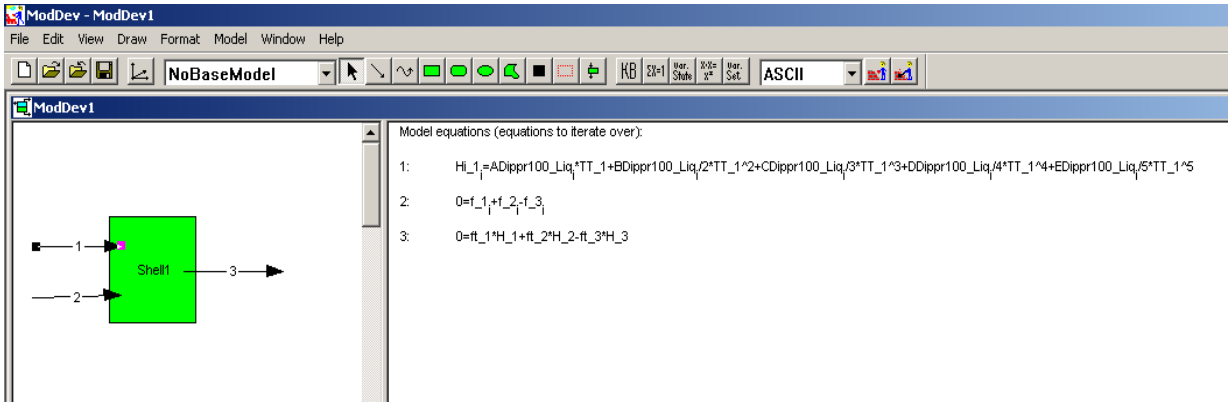

Figure 9: Main screen after describing of stream 1.

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

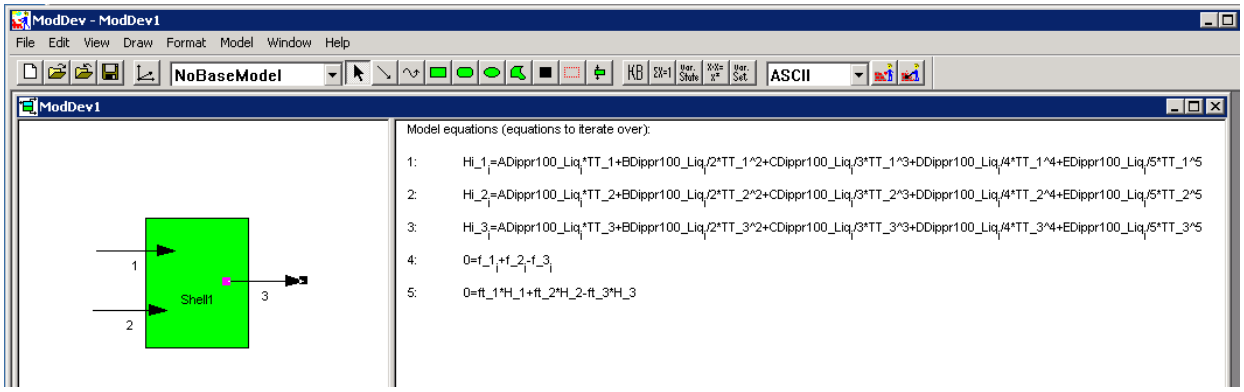

Figure 10: Main screen after describing of all streams.

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.

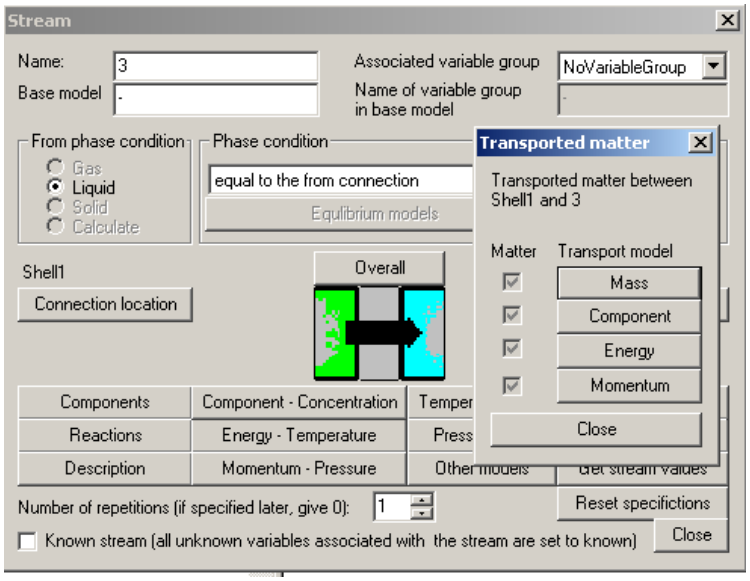

Figure 11: "Transported matter" tool for stream 3.

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".

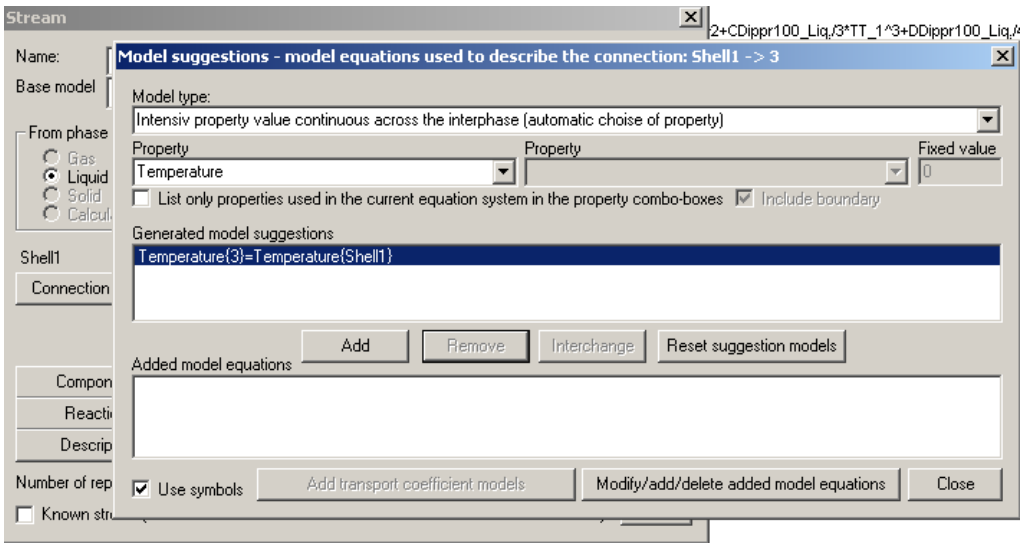

Figure 12: Describing connection between shell and stream 3 – Temperature.

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).

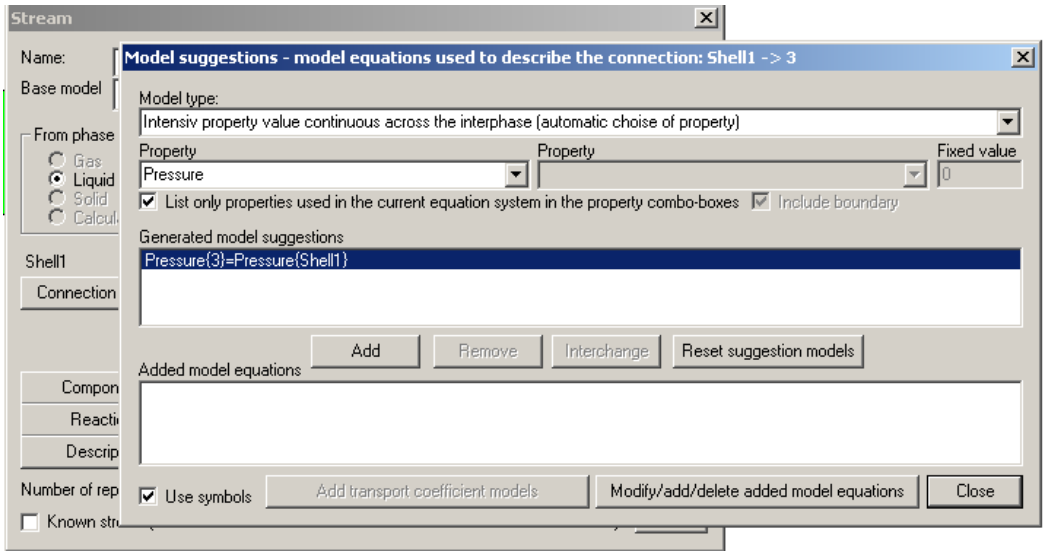

Figure 13: Describing connection between shell and stream 3 – Pressure.

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

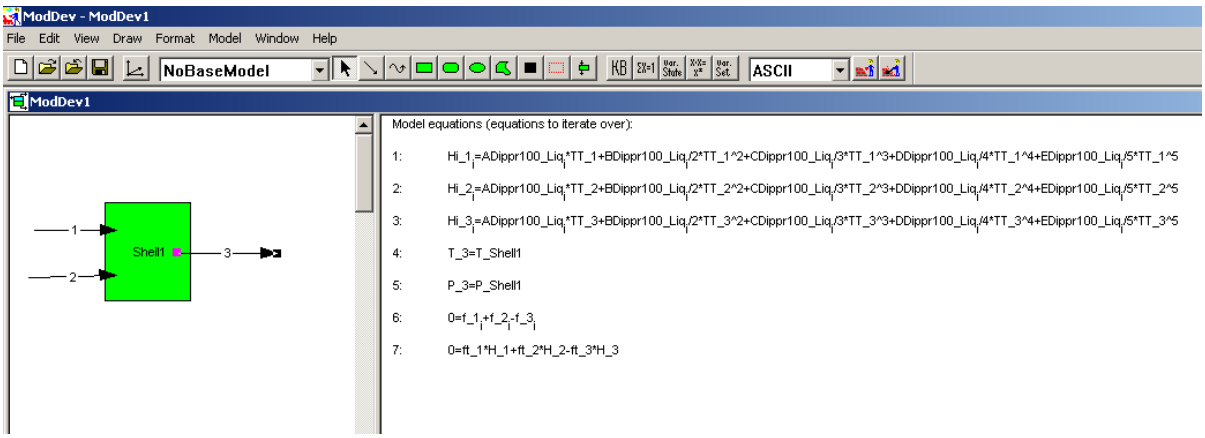

Figure 14: Model equations after streams have been described.

Step4: Definition of "closure equations" – 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.

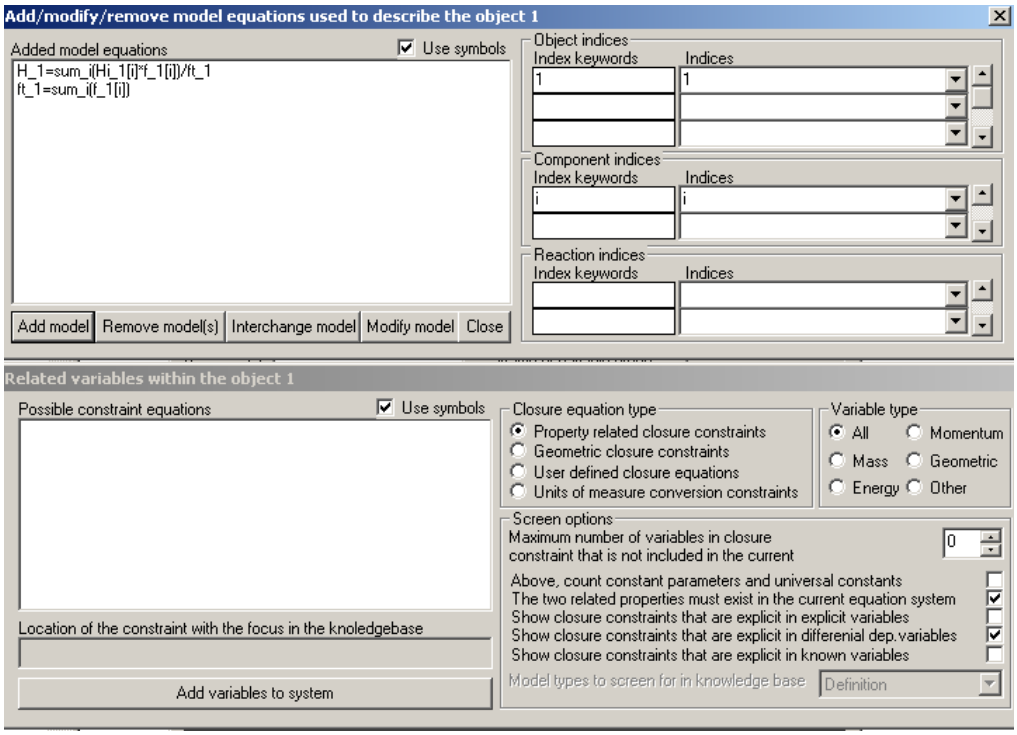

Figure 15: Tool for adding "closure equations"

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.

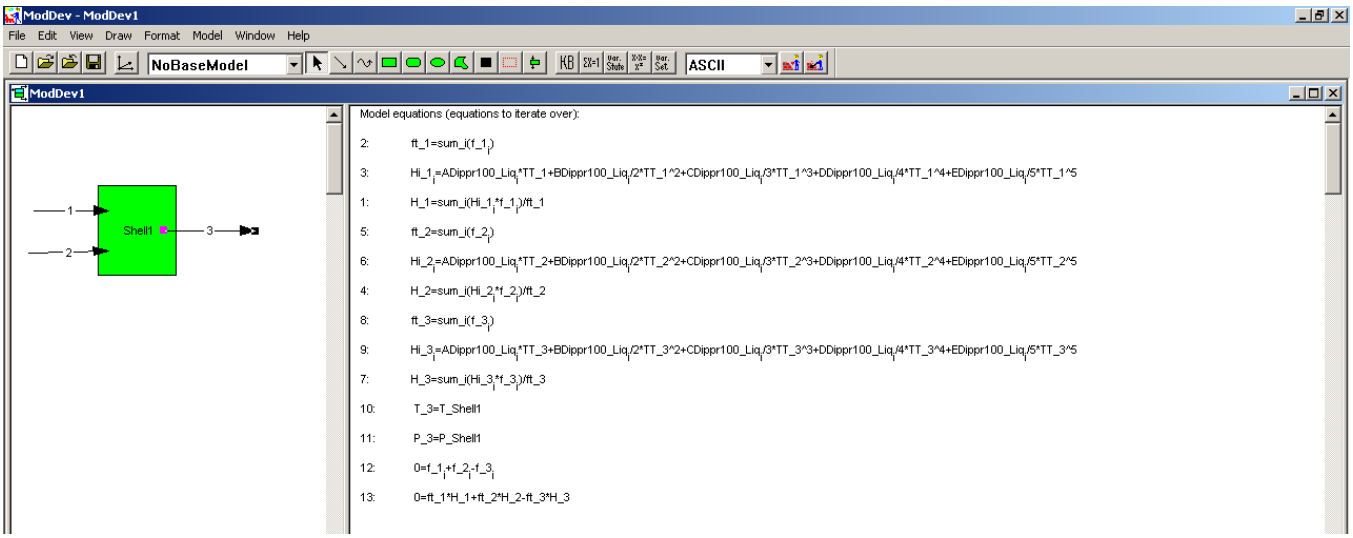

Figure 16: process model for a steady state tank mixer

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).

Step5: Saving of a generated model – 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.

Step1: Change component balance equation – 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.

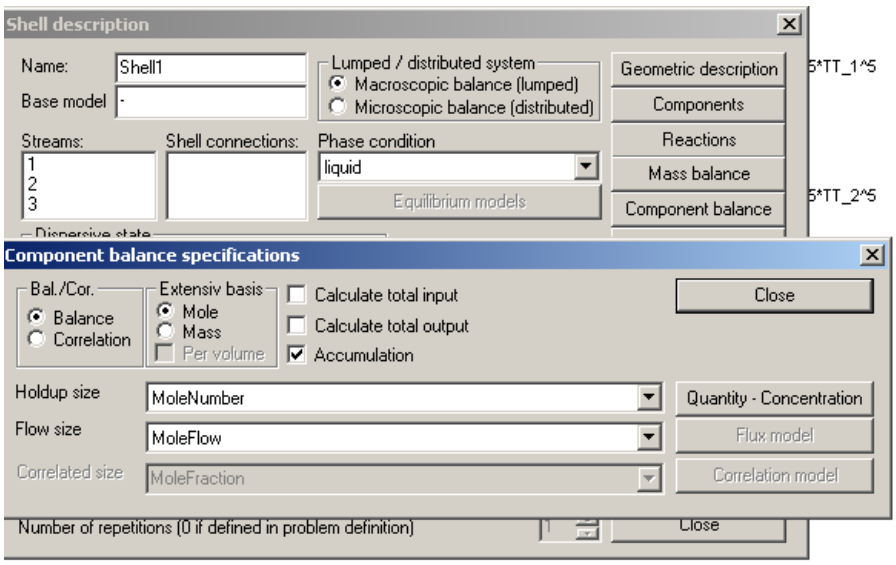

Figure 17: Changing of component balance equation.

Step2: Relate molar hold-up to stream 3 flow – 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.

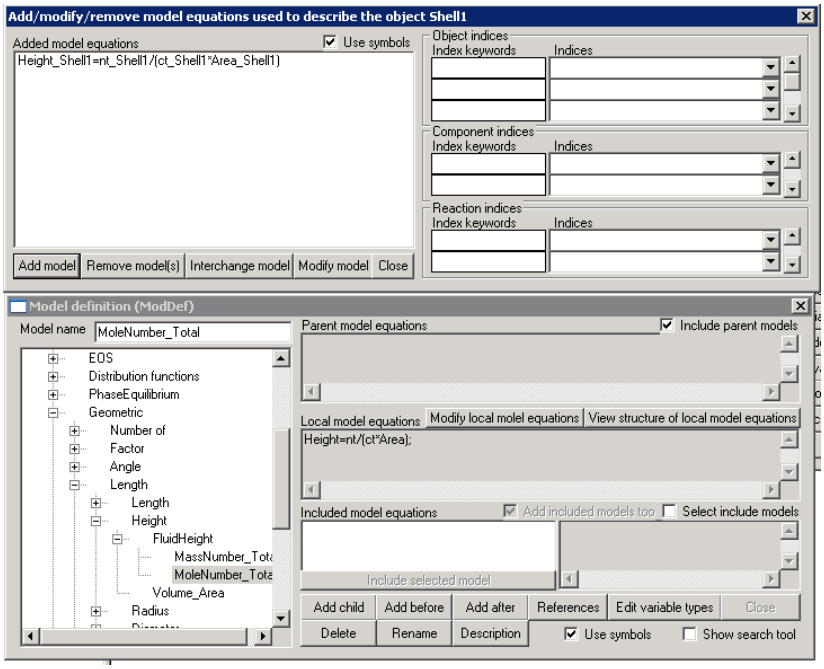

Figure 18: Add the equation for liquid height in the tank.

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).

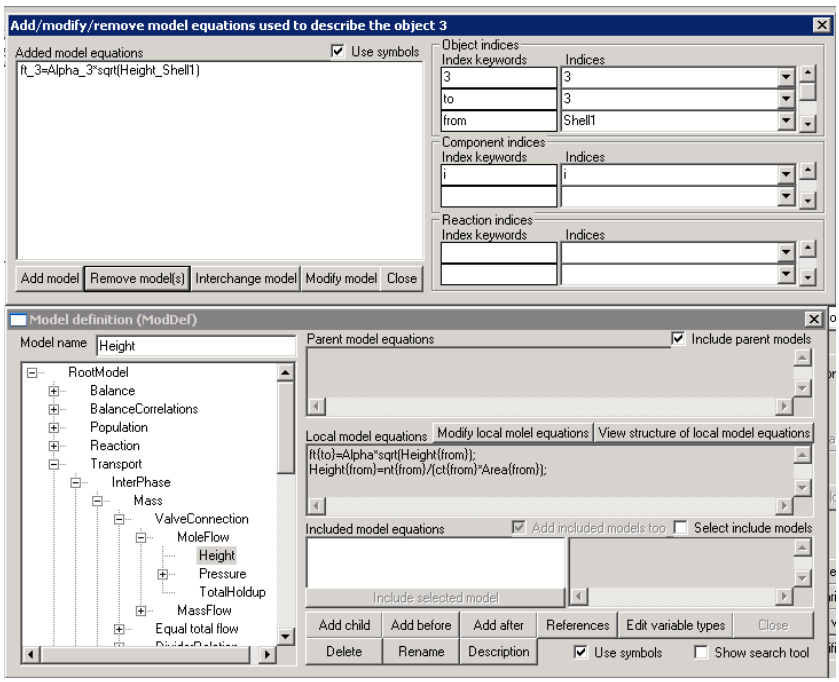

Figure 19: Addition of level-flow equation.

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.

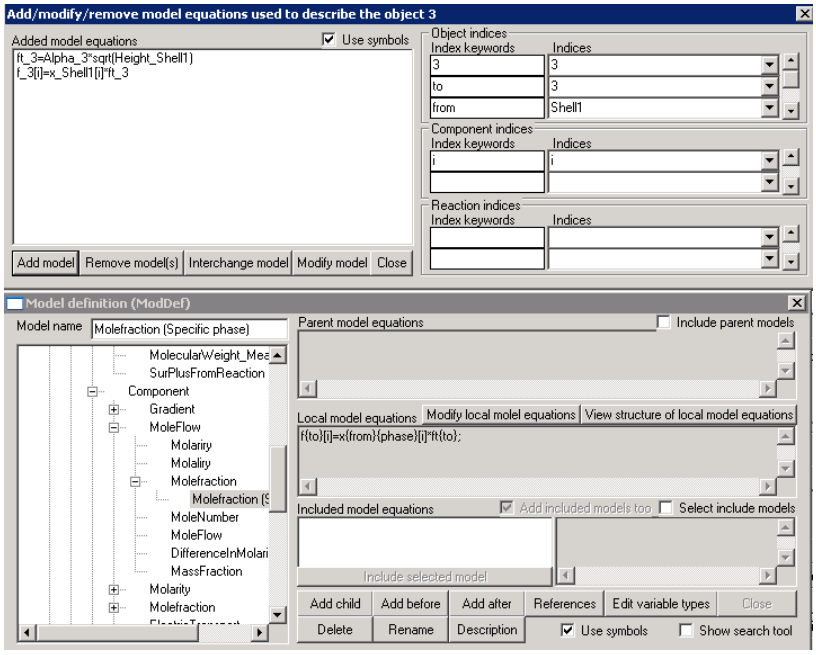

Figure 20: Addition of component flow equation.

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

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

Step3: Addition and deletion of “closure equations” – 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

$nt\_Shell1 = sum\_i(n\_ Shell1_i)$ A3

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

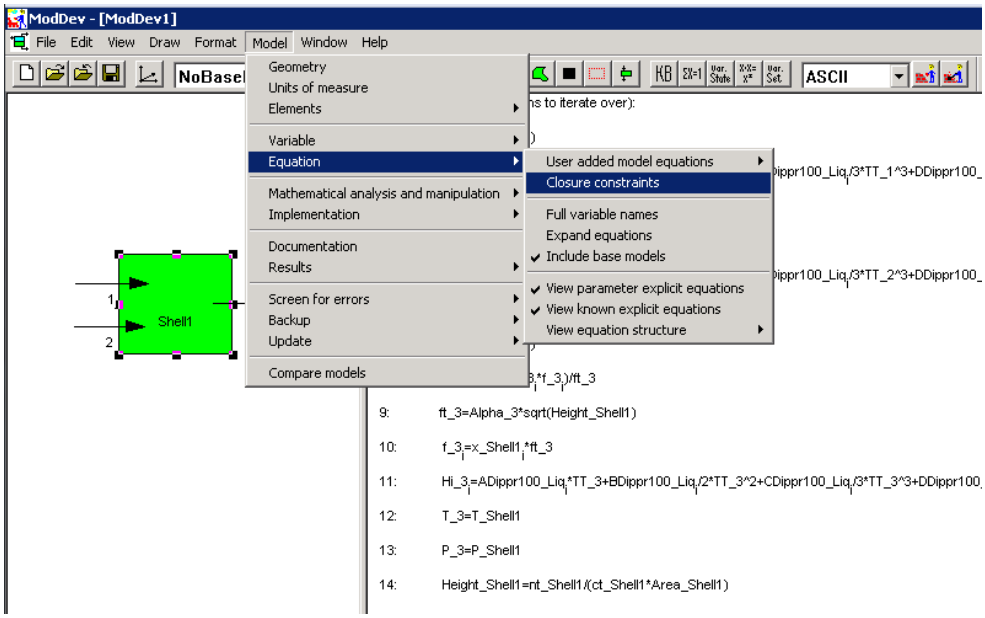

Figure 21: Selection of “closure equations” from tool-bar.

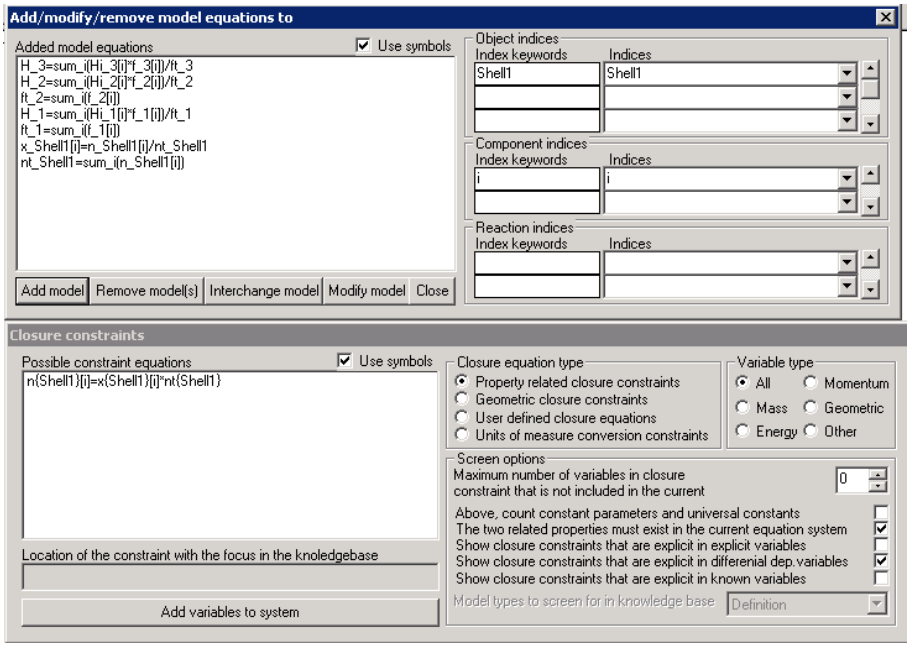

Figure 22: Addition and removal of closure equations.

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.

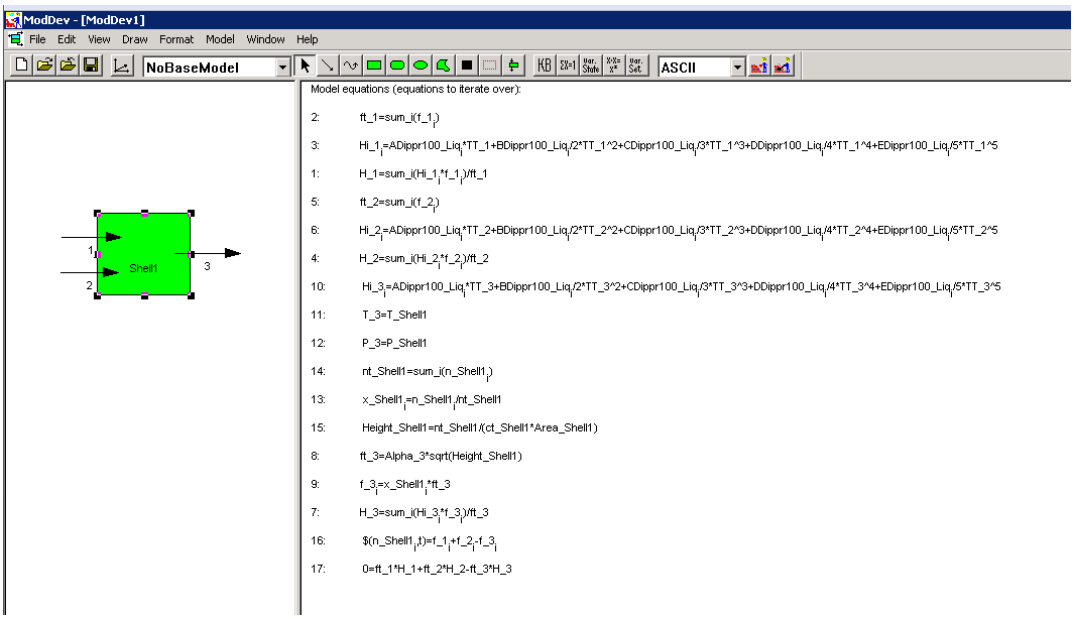

Figure 23: Dynamic model for a tank mixer with negligible energy holdup.

Step4: Save the model – 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.

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

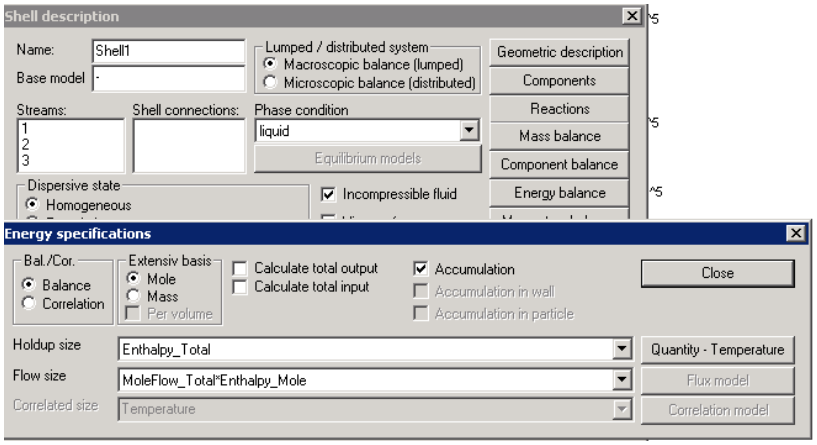

Figure 24: Energy specification for shell.

Step2: Relate the stream 3 enthalpy to the tank liquid enthalpy – 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.

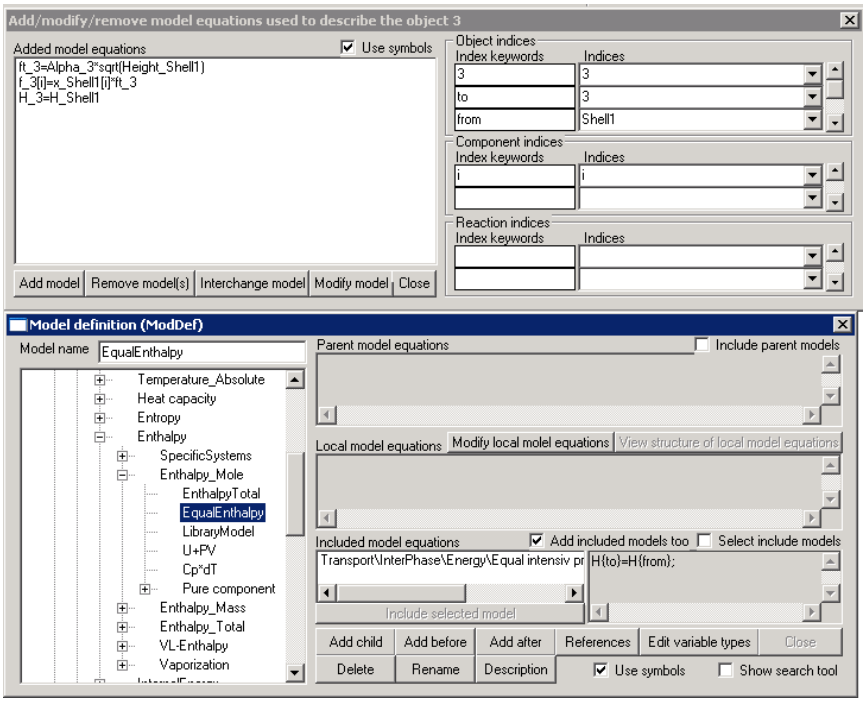

Figure 25: Addition of equation relating stream and shell enthalpies.

Step3: Addition and removal of closure equations – 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.

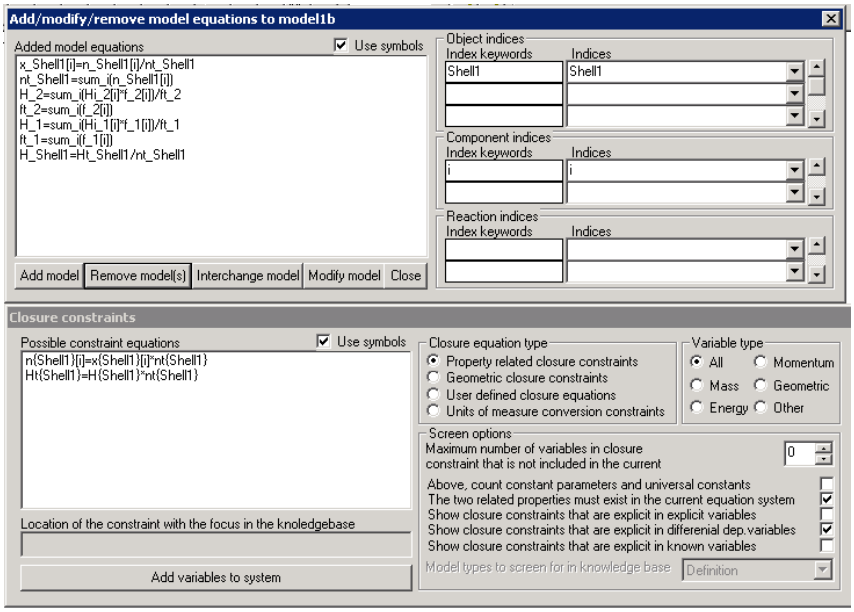

Figure 26: Addition and removal of closure equations.

H_Shell1 = Ht_Shell1/ nt_Shell1 A4

H_3 = sum_i(f_3[i]*Hi_3[i]) A5

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.

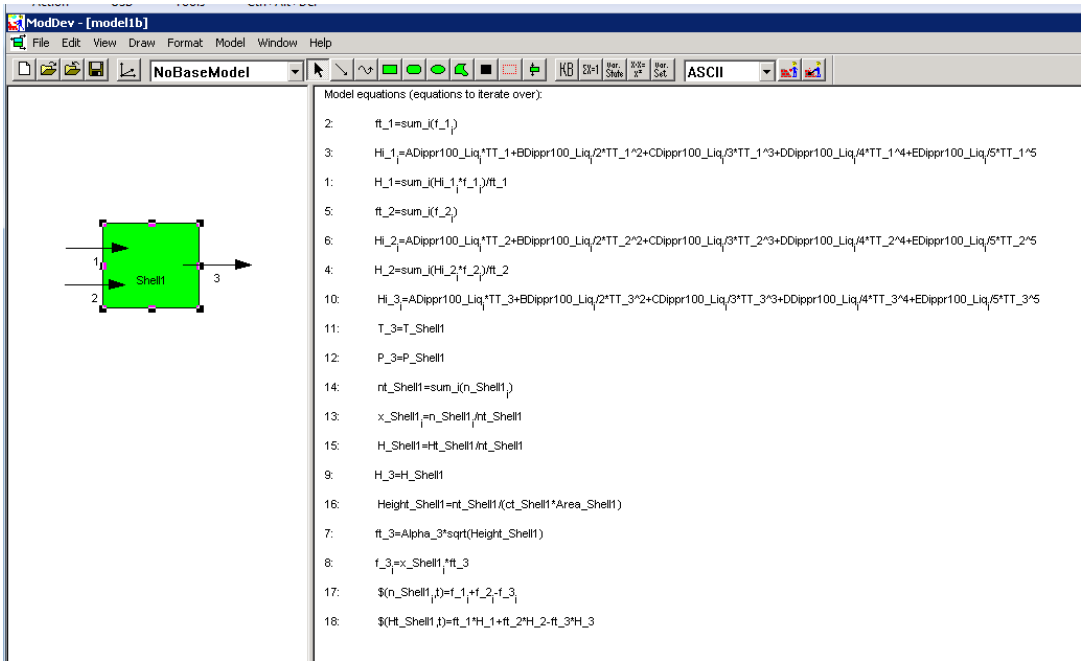

Figure 27: Dynamic tank mixer model with mass & energy holdup.

Step3: Save the model – 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.

Step1: Add the reaction term – 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.

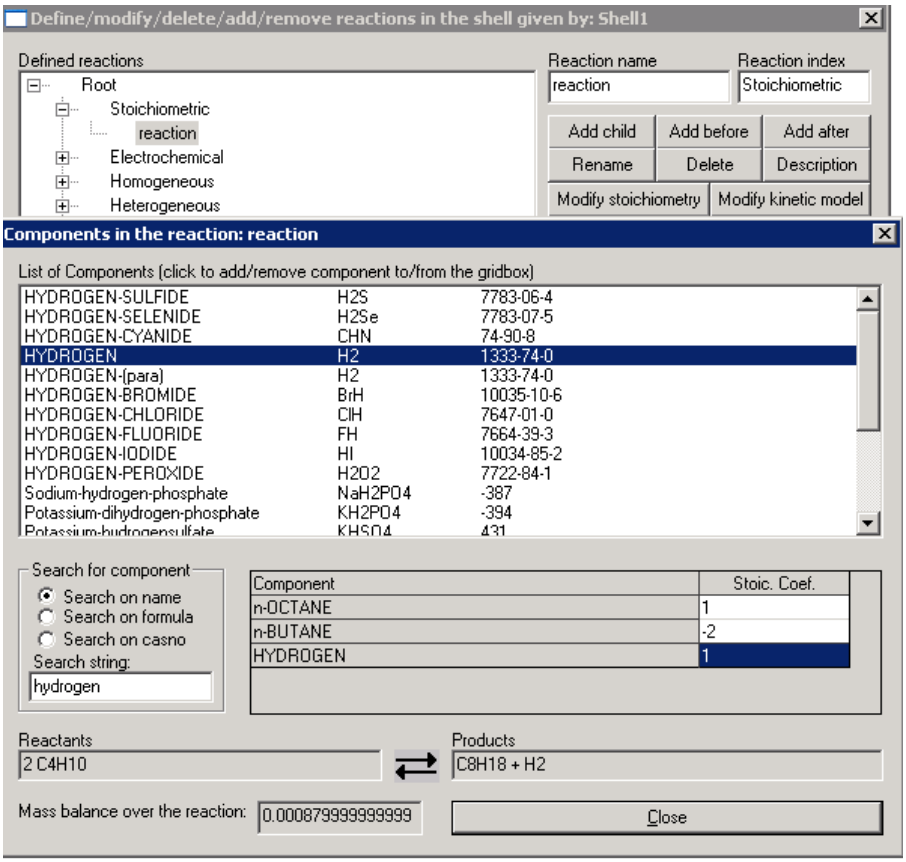

Figure 28: Reaction definition

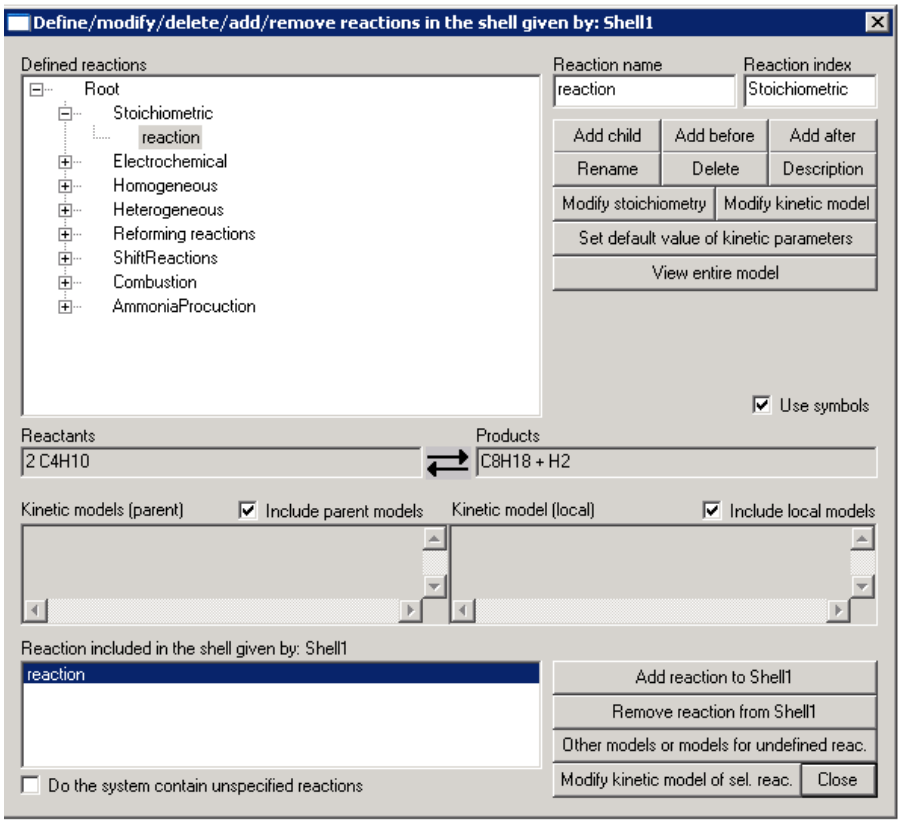

Figure 29: Adding reaction to the current system.

Step2: Define equation for degree of reaction - 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" -> "DegreeOfReaction" -> "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.

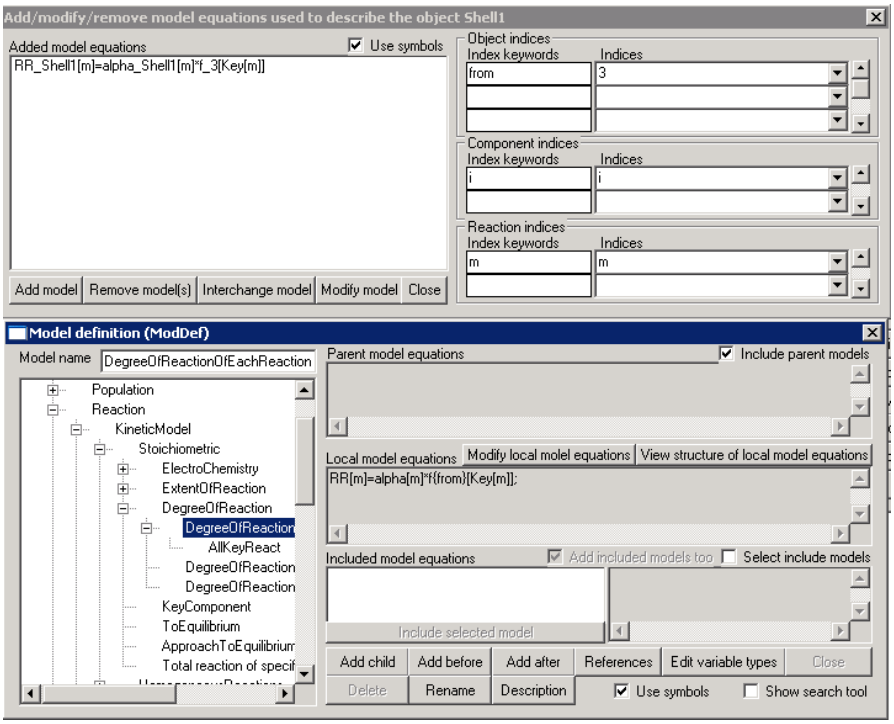

Figure 30: Defintion of degree of reaction.

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

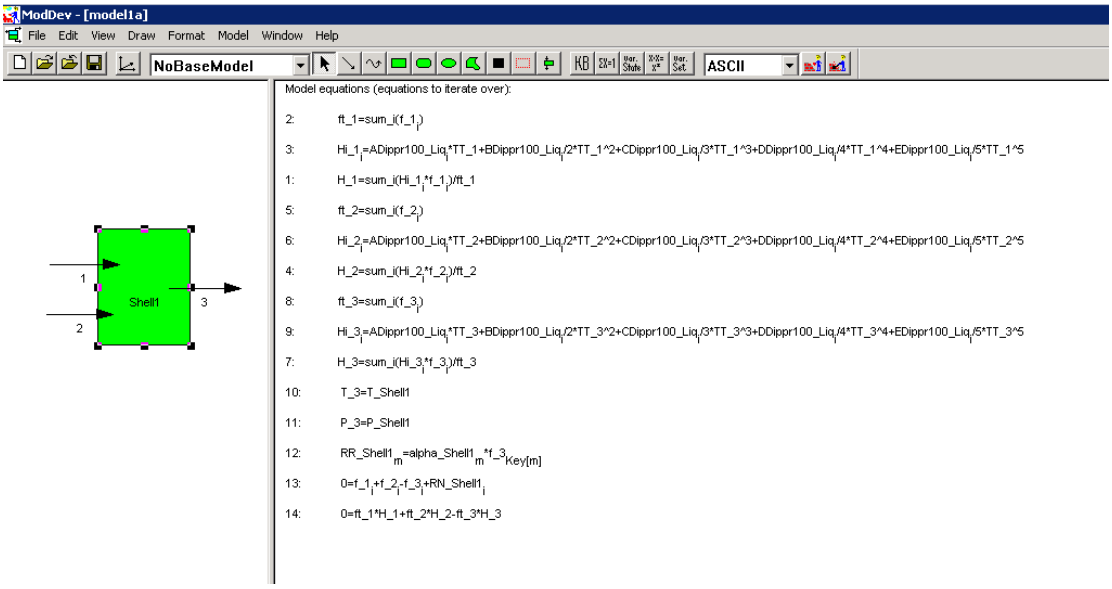

Figure 31: Steady state tank-reactor model

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.

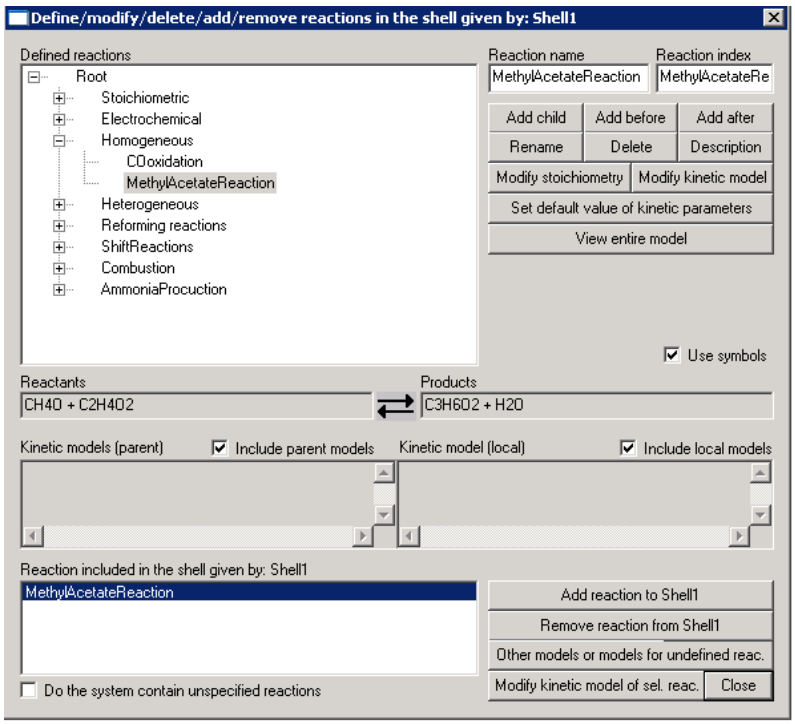

Figure 32: Selection of MethylAcetate Reaction.

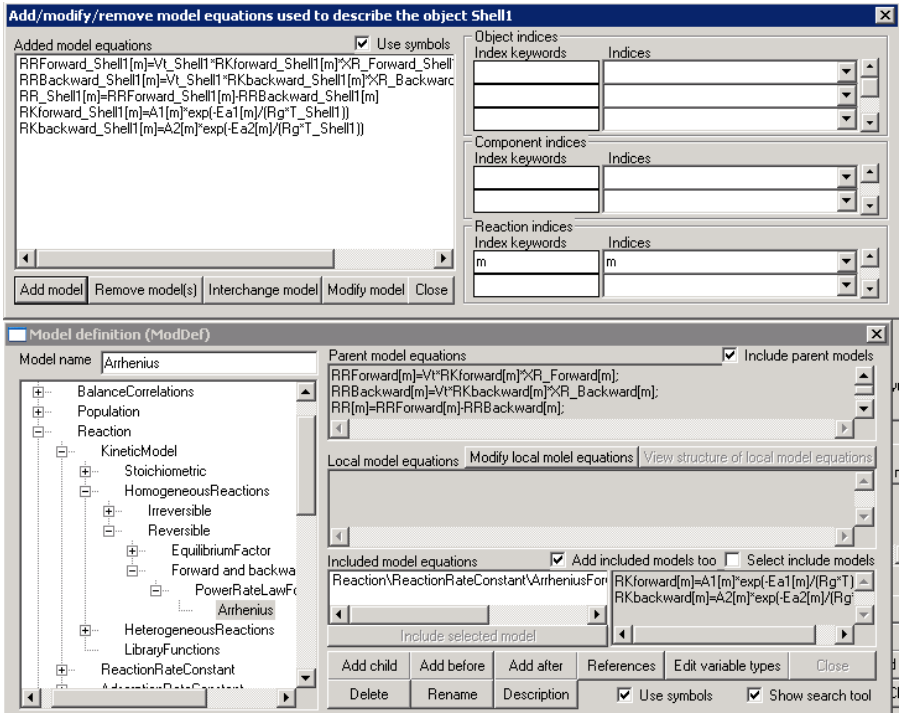

Figure 33: Kinetic model definition through the “model definition” tool.

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.

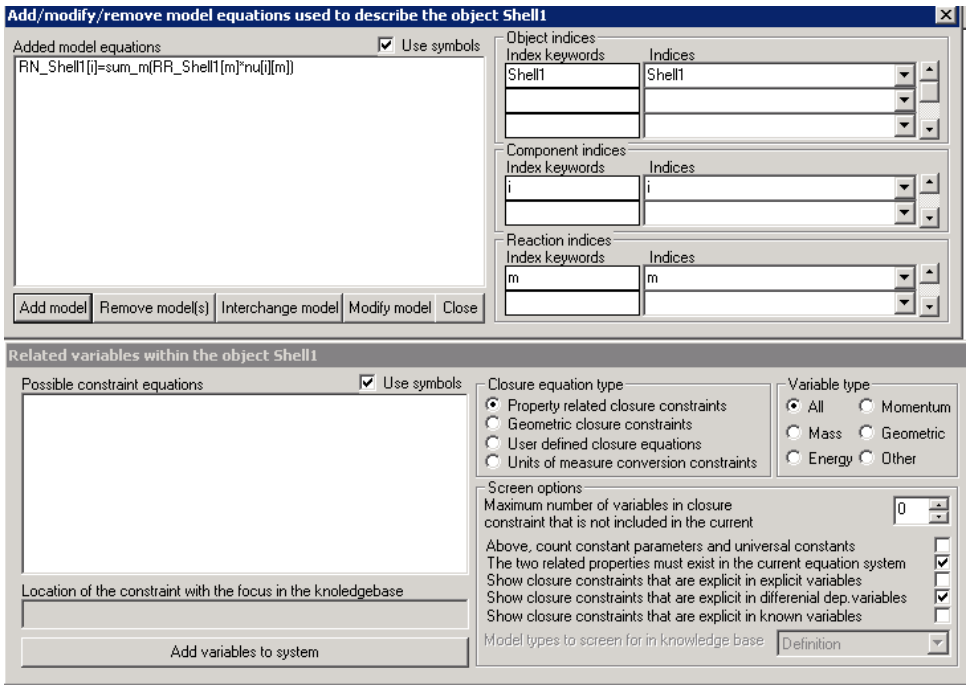

Figure 34: Adding of closure equations.

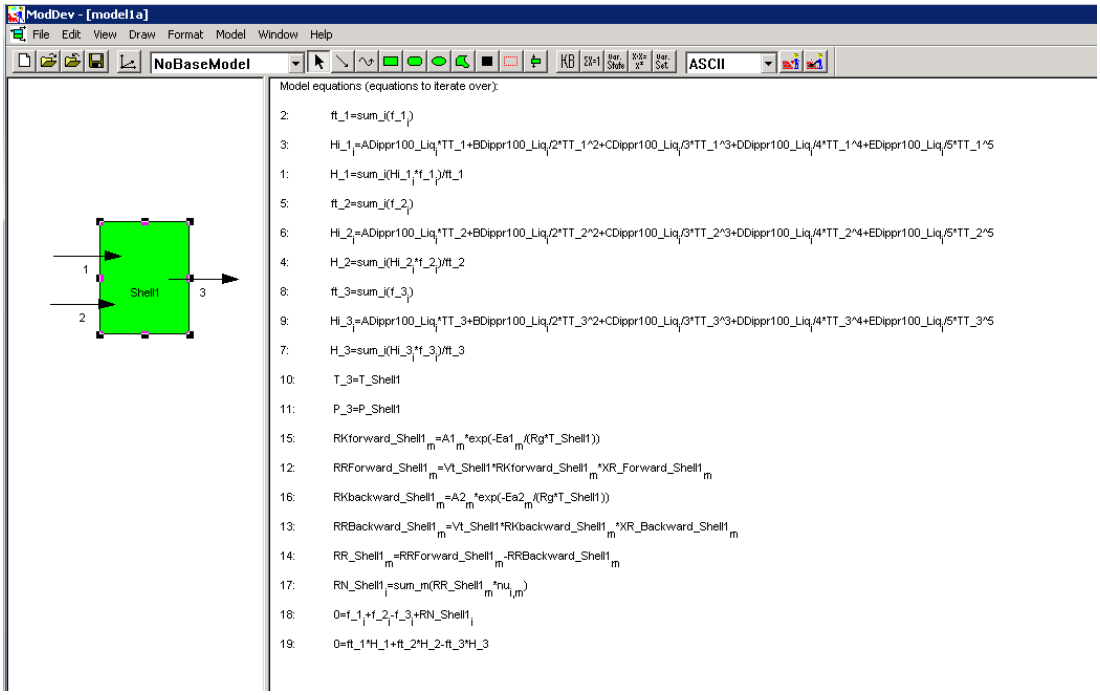

Figure 35: CSTR model with reaction kinetics.

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.