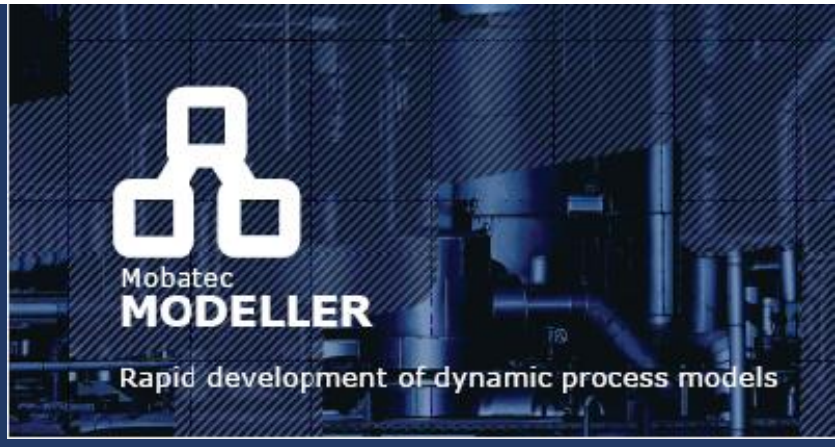
Mobatec
model-based technology



Mobatec Modeller

INTRODUCTION COURSE

Model Developer II

Advanced Equation-Based Modelling

Mobatec Modeller Intro Course – Model developer II

1 Modelling and Simulation of Continuous Stirred Tank Reactor

1.1 Objectives

By the end of this exercise, you will know:

- How to define global parameters.
- How to model discontinuities.
- How to define and add reactions in Mobatec Modeller.
- How to make variables plots.
- How to add & use a button object.

1.2 Model description

We want to model a dynamic operation of Continuous Stirred Tank Reactor (CSTR).

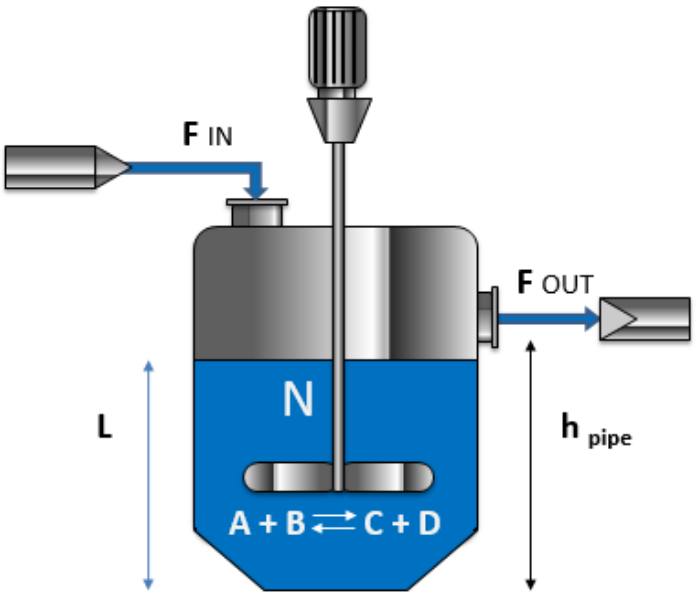


Figure 1 Continuous Stirred Tank Reactor

The tank has a single inlet at the top and single outlet at the side wall of the reactor. The geometry of the tank and the inlet flow will be provided as model inputs. The outlet flowrate is an overflow, it is dependent on the liquid level in the tank and will occur only when $L > h_p$.

The liquid inlet consists of the Formic Acid & Methanol. Formic Acid and Methanol will take part in non-catalysed esterification/hydrolysis reaction in the liquid phase according to:

$$HCOOH + CH_3\text{-}OH \xleftrightarrow{k_1,k_2} HCOO\text{-}CH_3 + H_2O$$, Methyl-Formate formation.

1.3 Assumptions

- The tank is well-stirred (ideally mixed) & operation of the tank is isothermal.
- Cross-section area is constant along the height of the reactor.
- All components are in liquid phase.
- Both esterification (direct) and hydrolysis (reverse) reactions are taking place.

1.4 Model Equations

Continuous Stirred Tank Reactor model equations

(Equations implementation will be explained in "Things to do" section of the exercise)

Mole balance (system equation – automatically generated)

- $\mathrm{d}\frac{\mathrm{n_i}}{\mathrm{dt}} = Fin_i - Fout_i + \sum_{j=REAC} \nu_{ij} \cdot r_j$, *i ϵ COMP*

Reaction equations (reaction equation)

- $r_j = k_j \cdot e^{\left(\frac{-Ea_j}{R \cdot T}\right)} \cdot \prod_{i \in COMP} \cdot Xn_i^{a_{ij}} \cdot V$, *j ϵ R1,R2*

Buffer cross-section area (system equation)

- $\mathrm{A} = \pi \cdot \frac{D^2}{4}$

Total molar holdup (system equation)

- $Nt = \sum (n_i)$

Volume (system equation)

- $Nt = \sum (rho_i \cdot Xn_i) \cdot V$

Liquid level (system equation)

- $V = A \cdot L$

Species molar fraction (system equation)

- $n_i = Nt \cdot Xn_i$

Species molar concentration (system equation)

- $n_i = V \cdot C_i$

Liquid lines equations

Inlet molar flowrate (mass connection equation)

- $\mathrm{Fin} = \alpha \cdot Fn$

Inlet component molar flowrate (mass connection equation)

- $\mathrm{Fn_i} = Fin \cdot {}_{(or)} Xn_i$

Outlet molar overflow (discontinuity) (mass connection equation)

$$\mathrm{Fout} = \begin{cases} \beta \cdot \left({}_{or} L - h_p\right) & \text{, if origin } L > h_p \\ 0 & \text{, if origin } L \le h_p \end{cases}$$

Outlet component molar flowrate (mass connection equation)

- $\mathrm{Fn_i} = Fout \cdot {}_{(or)} Xn_i$

1.5 Parameters

Symbol	Description	Model object	Units
D	**Diameter**	System	[m]
ρ_i	**Molar c. liquid density**	System	[mol/ m^3]
Fn	**Inlet molar flow**	In. Connection	[mol/s]
α	**Inl. line valve position**	In. Connection	[%]
Xn_i	**Species molar fraction**	System	[%]
β	**Outlet flowrate coeff.**	Out. Connection	[mol/s/m]
h_p	**Pipe height**	Out. Connection	[m]
k	**Reaction rate const.**	System	[mol/s/m^3]
Ea	**Activation energy**	System/React.	[J/mol]
T	**System temperature**	System/React.	[K]
R	**Gas constant**	Global	[J/mol/K]

Table 1 Model parameters

1.6 Variables

Symbol	Description	*Model Object*	Units
A	**Horizontal cross-section area**	System	[m^2]
Nt	**Amount of the liquid contained**	System	[mol]
L	**Liquid level**	System	[m]
C_i	**Species molar concentration**	System	[mol/m^3]
n_i	**Species moles number**	System	[mol]
Xn_i	**Species molar fraction**	System	[%]
V	**Volume**	System	[m^3]
r_j	**Reaction rate**	System	[mol/s]
Fin	**Inlet molar flow**	In. Connection	[mol/s]
Fn_i	**In. com. molar flow**	In. Connection	[mol/s]
Fout	**Outlet molar flow**	O. Connection	[mol/s]
Fn_i	**Out com. molar flow**	O. Connection	[mol/s]

Table 2 Model variables

1.7 Things to do

1. Use "Buffer Tank" model as a starting point

Open saved working "Buffer Tank" model from the previous exercise. Go to *File/Save Model as* ("") and save your model with a different name, use "CSTR". Choose appropriate location for your model.

2. CSTR model physical topology

As you have already noticed, the CSTR model (Figure 1) is topology the same as the buffer tank model. That is one of the reasons why we are going to use a buffer tank model as a starting point for the CSTR model. Change the "Ex_Buffer_Tank" icon of the system with the "Ex_CSTR" icon as well as the name of the system. Now, reposition the outlet liquid line mass connection and the sink system so that they appear as in Figure 2 below.

In order to choose the exact spot where the connection line will "touch" the system icon, select the line, do right click and select "**Set Graphical Connection Offsets**" (shortcut "**g**"). The white spots on the icons are the available connecting spots as it is shown in Figure 2 below. Click on the chosen spot, press "esc", and the connection will be graphically relocated.

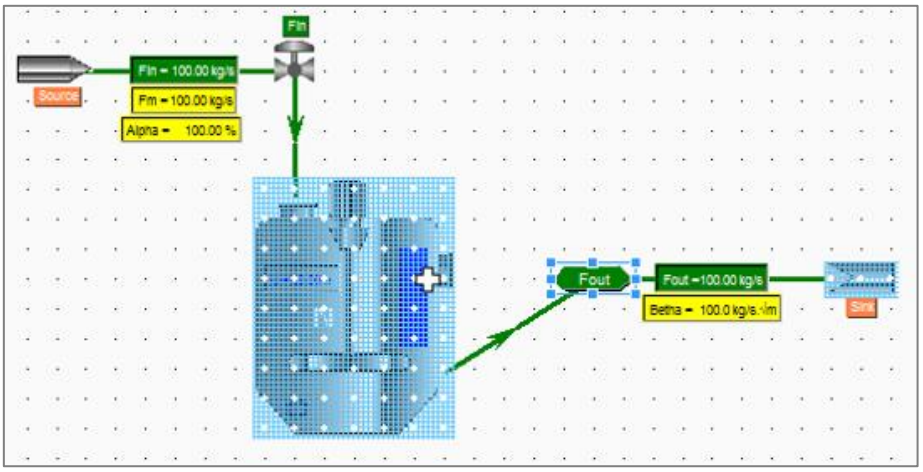


Figure 2 Graphically adjusting streamlines connecting points

As it was mentioned before, in MM you can choose to use either **mole** or **mass** based balances calculation for the capacity systems. In this model our input parameter is in molar mass units (**mol/s**) so molar based balance calculation should be used. Select the "CSTR" capacity system go to *Properties Browser/Selected Object/System/Equations* click *Equation Sorting* button and under "Equation Class" drop-down menu choose "**System (mole based balances)**". Do so for the other two systems in the model (source & sink).

3. Adding Species to your model

You need to define which species will be present in your model. Add CH_4O (Methanol), CH_2O_2 (Formic acid), $C_2H_4O_2$ (Methyl-Formate) and H_2O (Water). Inject CH_4O & CH_2O_2 to liquid source battery limit, $C_2H_4O_2$ & H_2O species will be created (injected) in the reaction that will be defined in the steps that follow so no need to inject them. MM will automatically add those species to the system where the reaction is defined (CSTR system).

4. Writing & Adding equations of CSTR model

Compare the present buffer tank model equations with the given CSTR model equations in paragraph **Model Equations**. Add new equations on the same way as in previous exercise. Some equations are very similar, so you can choose to just edit them. Open the **main editor** by clicking on "" icon (shortcut "d"). Select ***Equations* tab**, then select the appropriate equation from the list and click "**Edit**" button. Make desired changes and click "OK" to save the changed equation. The equation should change automatically in the model (in every "place" where it is used), if this does not happen go to *Propert Browser/Advanced/Tools* and click **"Update Variables & Equations"** button. You can also use "Edit Copy" button, to make a new equation (which must have different name) using the selected equation as a base, or you can choose "Remove" button to remove (delete) selected equation.

FYI: Sometimes, you may create certain equations and later decided not to use them in the model. These equations will still be visible (exist) in the equations tab (under equations database) of the main editor. If you want to "see", only the equations that are used in the model press "**Remove Unused Variables and Equations**" button (Main Editor/Equations tab). This will delete all unused equations. Be careful not to use this action before you add all the created equations to all your model parts, because this step is irreversible.

Below MM model equations definition is given, the **Pivot** variable is the variable that is solved from the used equation. The equation doesn't have to be written in explicit form in order to be solved for the pivot as Mobatec Modeler has implicit solver.

Model equations MM definition given by the model parts that should hold them

*Inlet **mass connection** equations (MM syntax):*

Equation name:	Eq'n Pivot	Function:
Inlet_molar_flowrate	`Fin:`	`Fin = Alpha * Fn`
Inlet_comp_molar_flowrate	`Fn[]:`	`Fn[] = Fin * or.Xn[]`

*CSTR **system** equations (MM syntax):*

Equation name:	Eq'n Pivot	Function:
Area	`A:`	`A = D^2 * PI() / 4`
Total_molar_holdup	`Nt:`	`Nt = SUM(n[])`
Volume	`V:`	`Nt = V * SUM(rho[]*Xn[])`
Liquid_level_CSTR	`L:`	`V = A * L`
Species_molar_fraction	`Xn:`	`n[]=Xn[] * Nt`
Species_molar_concentration	`C[]:`	`n[]= C[] * V`

*Outlet **mass connection** equations (MM syntax):*

Equation name:	Eq'n Pivot	Function:

Outlet_molar_overflow	`Fout:`	`IF or.L >= hp THEN`
		`Fout = Beta * (or.L - hp)`
		`ELSE`
		`Fout = 0`
		`END`

Outlet_comp_molar_flowrate	`Fn[]:`	`Fn[] = Fout*or.Xn[]`

Very often it is necessary to introduce conditional statements in the form of boolean expressions into the model definition. Boolean expression can be nested to any number of levels, where multiple IF/END blocks are introduced with same rules. IF/then/Else/End can be written with upper or lower case, or first letter CAP.

To learn all on **Boolean expression syntax** in MM read **Syntax – Intrinsic functions** part in **Chapter 8.** To learn all on **modelling discontinuities** read **Chapter 9.** in Mobatec Modeller handbook for beginning and advanced users.

5. Declaring variable dimensions

After you have entered all CSTR model equations you need to declare the dimensions of the used variables. Do this on the same way as in previous exercise. The variable dimensions are presented in the Table 3 below.

Name	Description	Unit Category	Eng. Unit	Bounds
D	**Diameter**	Length	[m]	[0 – 100]
ρ_i	**Molar liquid density**	Molar Density	[mol/ m^3]	[0 – 10E6]
Fn	**User specified inlet molar flow**	Molar M. Flow	[mol/s]	[0 – 1000]
α	**Valve position**	Fraction	[-]	[0 – 1]
Xn_i	**Species molar fraction**	Fraction	[-]	[0 – 1]
β	**Outlet flowrate coefficient**	-	[mol/s/m]	[0 – 100]
h_p	**Pipe height**	Length	[m]	[0 – 50]
k	**Reaction rate const.**	-	mol/s/m^3	[0 – 1E308]
Ea	**Activation energy**	-	J/mol	[0 – 1E308]
T	**System temperature**	Temperature	K	[0 – 2000]
A	**Cross-section area**	Area	[m^2]	[0 – 100]
Nt	**Total molar holdup**	Molar Mass	[mol]	[0 – 1E308]
L	**Liquid level**	Length	[m]	[0 – 100]
C_i	**Species molar concentration**	Molar Density	[mol/m^3]	[0 – 1E308]
n_i	**Species moles number**	Molar Mass	[mol]	[0 – 1E308]
V	**Volume**	Volume	[m^3]	[0 – 100]
r_j	**Reaction rate**	Molar M. Flow	[mol/s]	[0 – 1E308]
Fn_i	**Comp. molar flow**	Molar M. Flow	[mol/s]	[0 – 1000]
Fin	**Inlet molar flow**	Molar M. Flow	[mol/s]	[0 – 1000]
Fout	**Outlet molar flow**	Molar M. Flow	[mol/s]	[0 – 1000]
R	**Gas constant**	-	J/mol/K	[8.31-8.31]

Table 3 Variable dimension declarations

Go to *Properties Browser/Advanced/Tools* and click **"Update Variables & Equations"** button to make sure that all variables get their dimensions in the model. **Variables k1,k2,Ea1,Ea2 ,R & T will be declared after the reaction equations are added, variable n_i abd r_j are predefine variables** *(Properties Browser/Preferences/Pre-defined Variables)***.**

6. Defining & adding Reactions

STEP 1 - Creating the reactions in the Reaction Database

Go to the main editor tab (shortcut "d"). Select the "Reactions" tab and press "New reaction" button. In this model an equilibrium reaction is taking place. There are two possible choices that you can make. First is to define a "Two Way Reaction" by checking the checkbox next to this definition in the Reactions tab of the main editor, and the second is to make two separate one-way reactions. You will make this decision based on the reaction kinetics available.

If there is an equilibrium kinetic (mathematical) formulation than you can check "Two Way Reaction" check-box ("<==>" sign will appear in the reaction notation) and define the equilibrium kinetic reaction rate in the reaction equations. In this case two separate one-way reaction kinetic formulations are available, so **you should create two one-way reactions**, **r01: direct – esterification & r02: reverse – hydrolysis reaction.**

Select the species, set the stoichiometric coefficient (- “reactants”/+”products”) to make the correct reaction (you will make two opposite reactions). Under “Notation” the reaction will appear. Press “OK” to create the reaction (Figure 3). Create both reactions.

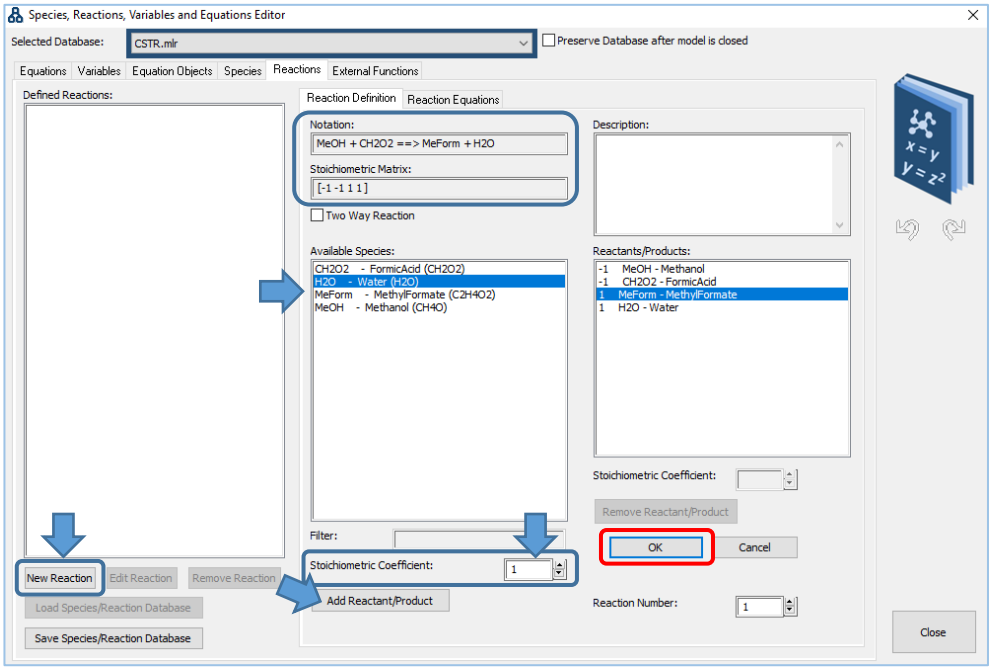


Figure 3 Creating esterification one-way reaction

STEP 2 - Injecting reactions to a specific capacity system

Select CSTR capacity system, and go to *Properties Browser/Selected Object/Systems/ Reactions/* ***Define Reactions*** tab. Click on “**Set Injected Reactions**” button. New tab will open, here you can select the reaction(s) from available **plant reactions** (defined in previous step) and click “**Add**” to inject the reaction(s). Add both reactions to your CSTR system. Now you have defined added reactions in the system, and the product species will automatically become present in that system.

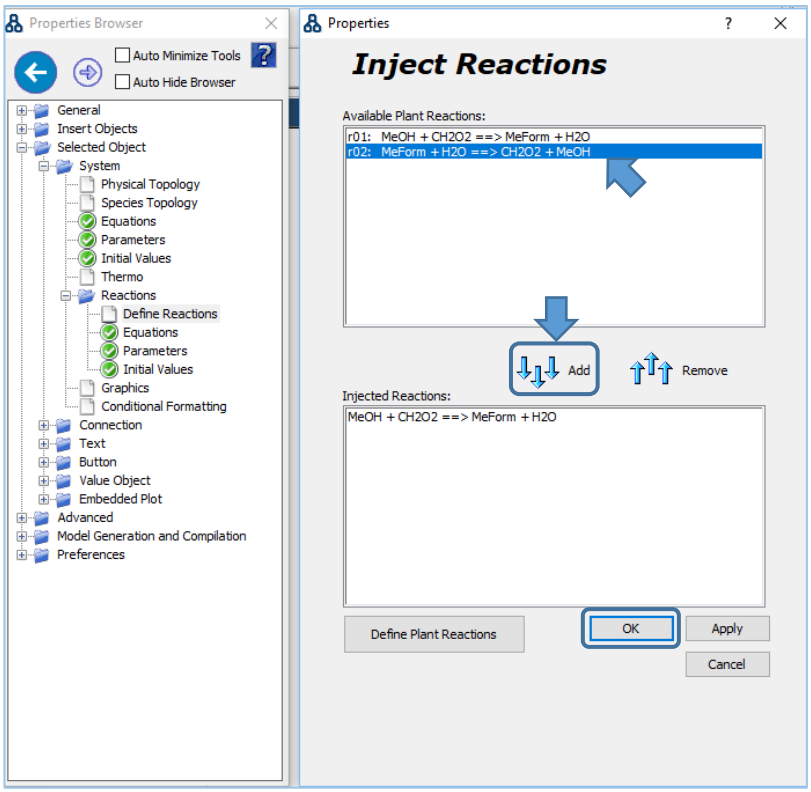


Figure 4 Injecting reactions to specific system from defined Plant Reactions

7. Defining global parameters

In Mobatec Modeller you can set global parameters. Those parameters are usually some known constants like *g*-gravity or *R*-gas constant, T_{amb}-ambient temperature. (glob.g, glob.R & glob.Tamb)

In order to define a global parameter, use a "glob." prefix when writing the parameter in the equation. In this model a global parameter can be the "Gas Constant - R", so when "writing" the reacting equations instead of typing "R" type "glob.R".

To set the global parameter value, go to *Properties Browser/General/Global Parameters, Variables & Equations/Global Parameters.* Here you will find listed all the parameters that you defined as global when you made the equations. There, you should enter the value for each global parameter.

In Mobatec Modeller, there are 3 syntax imbedded universal constants that you can use in equations without having to define them or give them values anywhere. Those are "PI" number (3.141592..), gravity constant "g" (9.81 m/s^2) and gas constant "R" (8.314 J /mol/K). To use them in equations write: **PI()**, **g()** and **R() – they are not case sensitive.**

8. Creating and Adding Reaction equations

Reactions have their own equations and therefore their own Equations, Parameters & Initial Values tabs. The reactions kinetics equations are created and **added to each defined reaction separately. Adding reactions to a specific system will make the reaction product species be present in that system automatically**.

When creating the reaction equation check the "**Reaction**" check box under the "**Equation Class**", this will make that these equations are only available to be used when adding reaction equations. Below the kinetics expressions definitions for both reactions are given:

Reaction kinetics equations (MM syntax):

Equation name:

Esterification_reaction_rate & Hydrolysis_reaction_rate

Function:

```
r = k * exp(-Ea / (glob.R * sys.T)) * sys.Xn[1] * sys.Xn[2] * sys.V
```

Equation Class:

Reaction

Note: Please declare variables k1,k2,Ea1,Ea2,ri ,R & T defined in reaction equation according to Table 3 before continuing.

Both esterification and hydrolysis reaction will use the same reaction rate expression (equation). The difference will be only between the values of "*k, Ea*" parameters assigned, and the reference species assigned to [1] & [2] referent numbers for each reaction.

Go to Properties Browser/Selected Object/System**/Reactions/Equations tab, select "r01" esterification reaction in the top of the tab and click on "Define Equations" button**. Follow the rest of the steps as illustrated in Figure 5. Do the same for the "r02" - hydrolysis reaction.

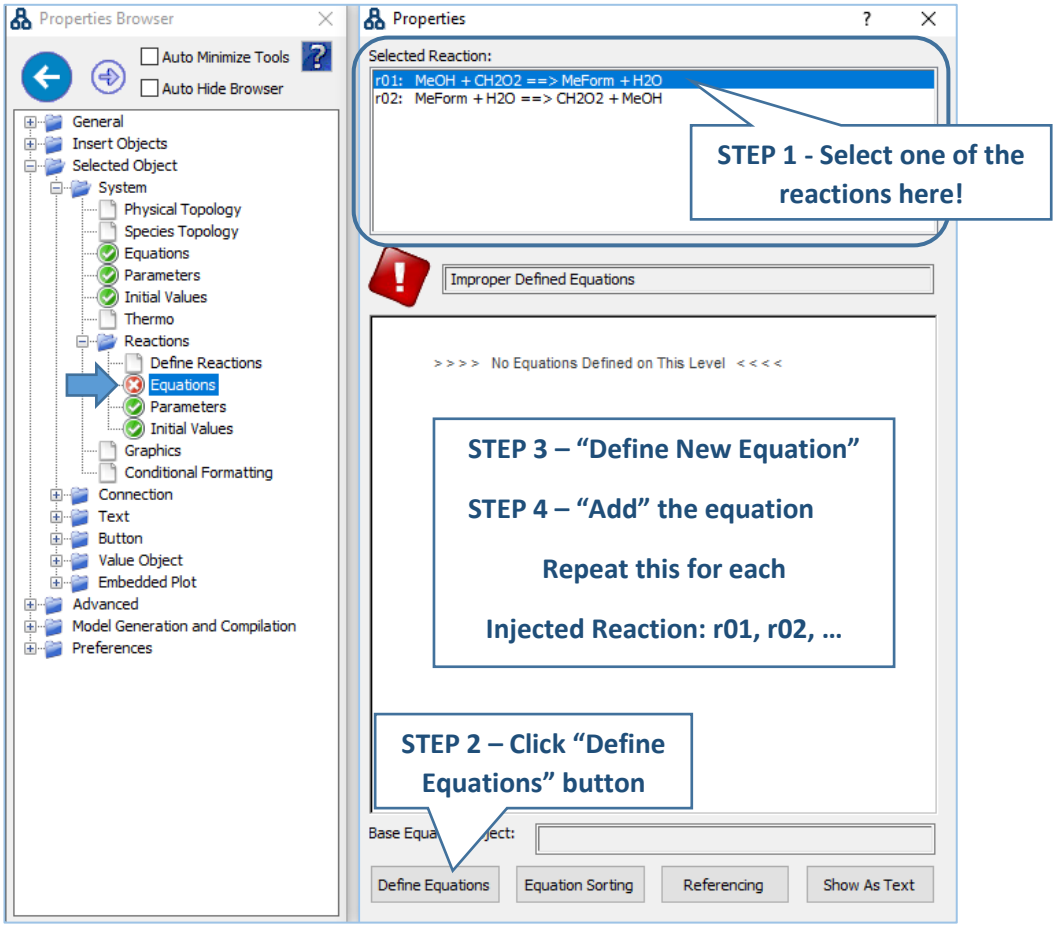


Figure 5 Adding reaction equations to the Injected Reactions

Note: "r" – is predefined variable in MM and it is used for reaction rate [mol/s]. It is perfectly OK to use variable "r = …" in both reaction kinetics equations, as these equations will be added to a different (corresponding) reactions and therefore will be unique (only "r") variable in the selected reaction equations (kinetics).

Prefix "**sys.**" is used before some variables in the kinetic expressions, **"sys.Xn[]"- species molar fraction, "sys.V"- volume** and **"sys.T" -temperature**. Prefix "**sys.**" is used to "call" variable values being calculated (variables – Xn[] & V) or given (parameters -T) from the system where the reaction is defined.

Species Referencing in reaction equations

Xn "[**1**]" & Xn "[**2**]" are **species reference numbers** which are used to declare which species are used in which expression, i.e. "1"- Methanol & "2"- Formic Acid are used in first, while in the second reaction "1" will be referenced as Methyl-Formate, while "2" will be referenced as Water. So, the same reference numbers can be assigned to different species in different reactions.

Set the referent species numbers for each reaction as they are defined in the equations (i.e. [1], [2]). To set species referent numbers for the esterification reaction, select reaction **r01**, and click on "**Referencing**" button, new tab will appear, set the species referent numbers by selecting the species and the number and pressing "**Set Reference Species**" button (Figure 6 next page). Set the referent species numbers of second reaction as well in the same way.

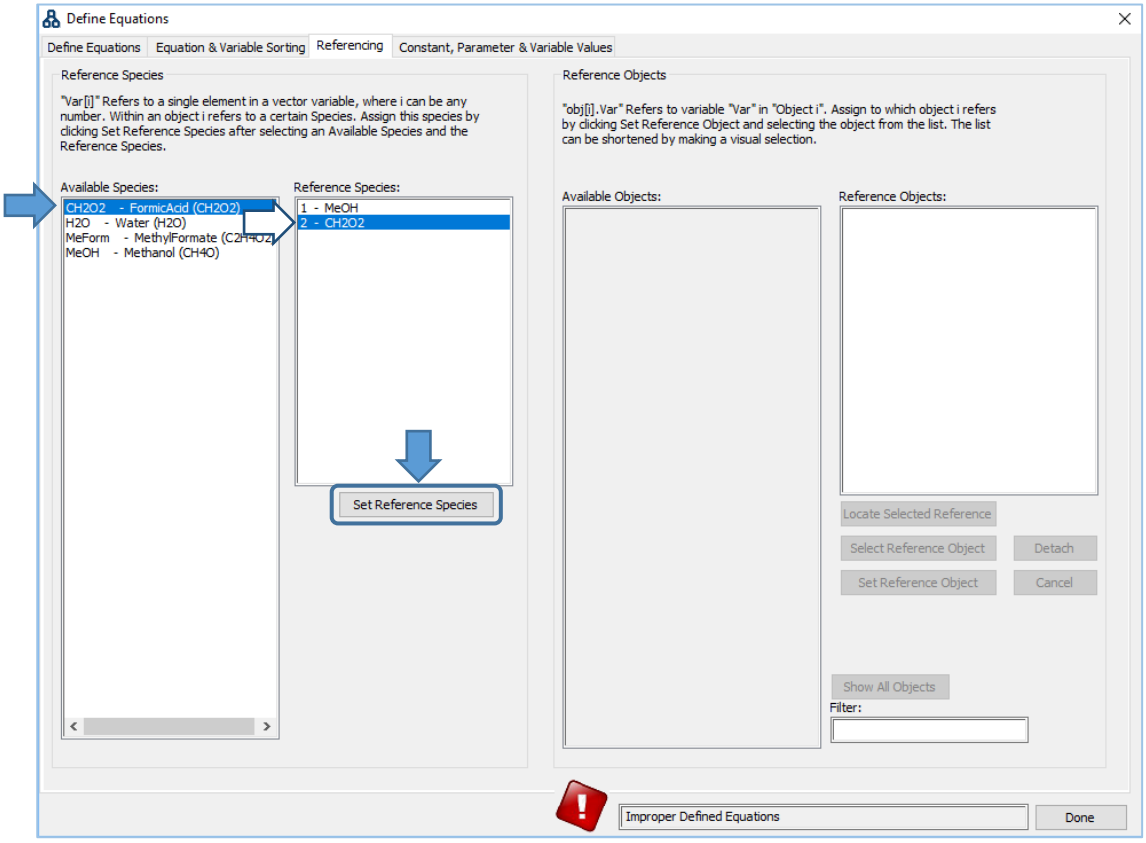


Figure 6 Referencing the species for direct (esterification) reaction

9. Sorting the model equations

Presented CSTR reactor model is Isothermal model, no energy balance is considered as system has constant temperature. As temperature is constant it must be specified as a parameter. The reaction rates expressions are containing Temperature variable "**T**" with "**sys.**" prefix in front. This means that this variable value will be taken from the system, so when sorting the system equations variable "**T**" will appear because it is used in the reaction equations with "**sys.**" prefix. Variable "T" should be selected as a parameter and given the value.

Use "**Equation & Variable Sorting**" (*Equation Sorting button located in Equations tab*) tab to sort the equations. Sort model objects equations using information provided on the model parameters. Do this for the Source battery limit system, capacity CSTR system, inlet and outlet mass connection and for the reaction equations in the CSTR system.

10. Initial conditions

Insert given parameters values to the inlet and outlet connections, CSTR system and CSTR reactions according to Table 4 in **Appendix 1**. Do that by selecting the desired system/connection then go to the *Properties Browser/Selected Object/ System or Connection/Parameters* and in the "Constants & Parameters Values" tab enter the value under the "Value" column for each parameter defined for the selected object.

Model object that needs extra inputs for initialization (initial variables values calculation) is the "CSTR" system as it is a capacity system that can store mass & energy. Initialize CSTR system on the same way as in the previous exercise using provided initial inputs:

At the start of simulation the liquid level in the tank is 2m.

Methanol molar fraction: Xn[CH4O] = 0.67 ; Formic Acid molar faction : Xn[CH2O2] = 0.33 .

There is no Methyl-Formate nor Water present, Xn[C2H4O2] = Xn[H2O] = 0.

11. Display variable values

Make value displays for Fin, Fn_"Species" variables and Fn and Alpha parameters of inlet connection. Value and filled rectangle displays of L variable of CSTR system. Fout and Fn_"Speciesname" variables an Beta parameter of the outlet connection. Your model should look similar as presented in Figure 7. Feel free to add displays for other variables as well.

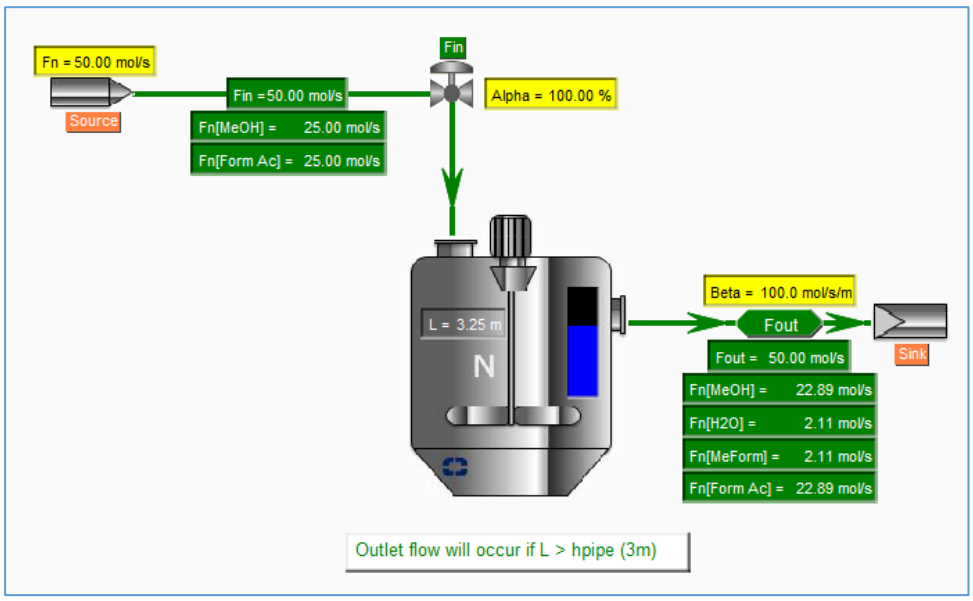


Figure 7 CSTR model

12. Running a Dynamic Simulation

To Compile the Model press the *"Compile Model and Switch to Simulation Environment"* icon in the toolbar " " (shortcut - F12), or go to *Properties Browser/General/Basic Commands* and press *"Compile Model and Switch to Simulation Environment"* button. When your Model is compiled you will get a message from Mobatec Modeller that compilation was successful!

Set a "Fix Step Size" simulation of "1" (sec) step. Click the ***"Start Calculation"*** button " Start Calculations " and run a dynamic simulation of the model. If there are no errors your model should be running the simulation and you are able to follow the *"Simulation time"* in seconds on the Basic Commands tab, or at the left bottom corner of the screen.

Monitoring variables values

You can monitor all variables and monitor & change all parameter values of any model object by selecting the object, doing the right click and choosing "Show Variable Table" or "Show Parameters Table", or just select object and press numbers from1-5 for variable tables, or numbers from 6-9 & 0 for parameter tables.

13. Plotting the variables

We want to perform a "dynamic plotting" of the species molar concentration (mol/m^3) for the first 3600 seconds of reactor operation. Compile the model again, or just use rewind button " Rewind Simulation „

First a plot model object needs to be added to the working surface. While in modelling environment go to Insert Objects/Objects and choose "Embedded Plot", click anywhere on the working surface to add embedded plot. Select added plot (adjustable size) and in the properties tab set desired plot configuration number ("1-50").

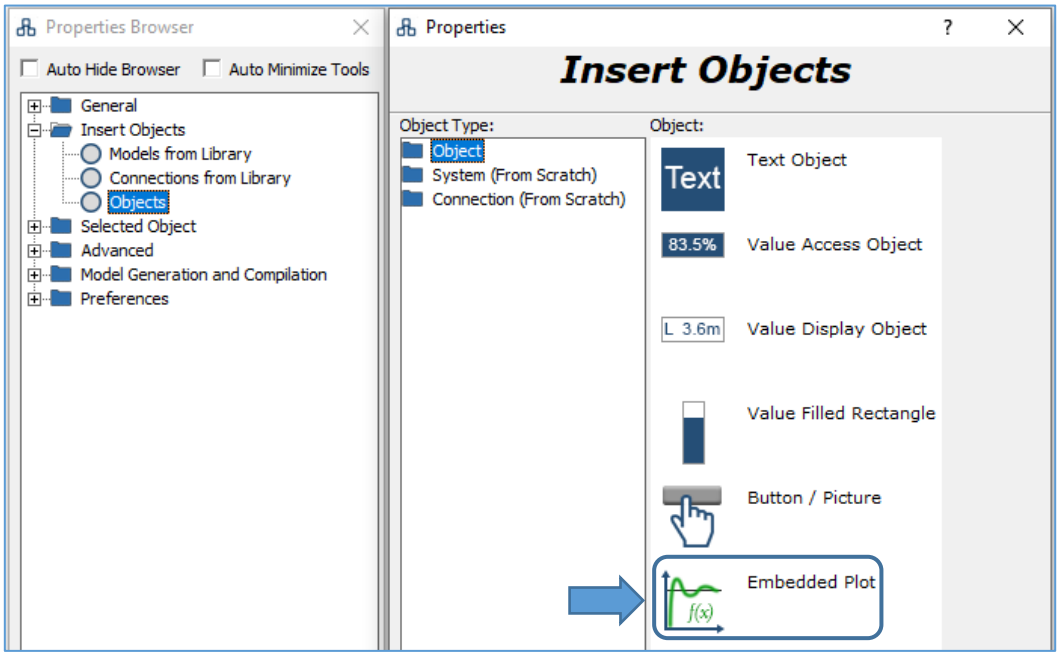


Figure 8 Embedded Plot model object - insert

Go to simulation environment, open CSTR system variable table, make selection of species concentration variables: "**C_CH2O2_CSTR**, **C_CH2O_CSTR**, **C_MeForm_CSTR** & **C_MeOH_CSTR**", do right-mouse click and select "**Add Selected Variables to Current Plot**".

Then go to *Properties Browser/General/Plotting* tab, in the "Plot Title" box type the plot name, i.e. "*CSTR C[i] Profile*". Within "**Plot Variables**" sub-tab you can set the line style and the colour of each variable. Select desired variable chose desired settings and press "Change Plot variable" button (Figure 9 n.p.).

Go to "**Plot Properties**" sub-tab and select "Normal Time Plot" plot type, you can also chose Horizontal or Vertical Profile Plot type, for plotting distributed profiles. Within this sub-tab you can select various plot properties like plot inner, outer and grid colour. Chose to show variables legend on the plot surface by using the check-box (variable alias will be used for the legend list). Set plot recording resolution for all plots (by default) or per selected plot individually by checking the check-box next to "Use This Resolution [sec]". Whatever option is chosen this means that plot data will be recorded with set resolution which can effectively be equal or lower than the current integration time step size. In other word there cannot be smaller time step within the plotting than what it is in the actual calculation. You can also "Show Time Table" or "Export Time Table" in ".csv" format (Figure 9 n.p.).

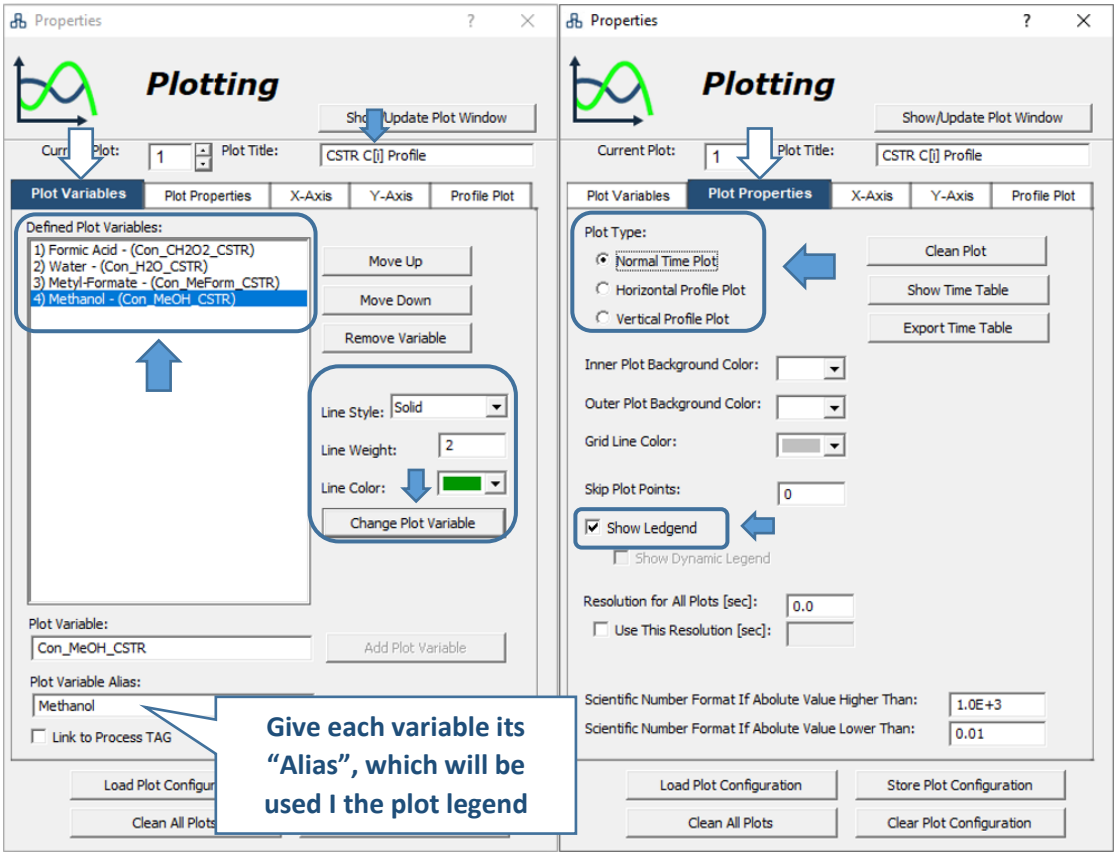


Figure 9 Plotting – "Profile Variables" & "Plot Properties" tabs

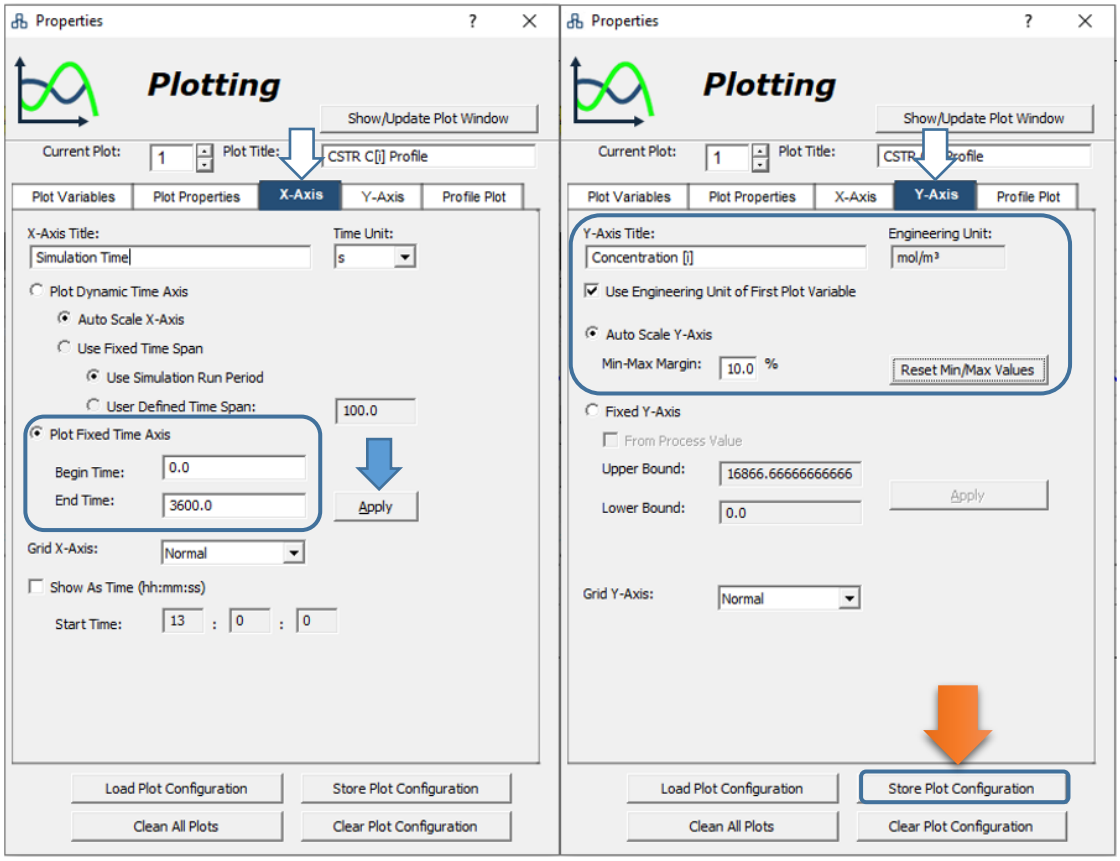


Figure 10 Plotting – "X-Axis" & "Y-Axis" tabs

Go to "**X-axis**" sub-tab and choose "Plot Fixed Time Axis" option (the lower one). Set beginning and end time to "0 & 3600" seconds and press apply button (you can also choose different time units as well). With dynamic time axis option you can choose between "auto-scaled" and "fixed" time span. Auto-scaled X-axis option will show entire simulation while fixed time span option can show automatically chosen span or user defined time span on x-axis. Within this tab you can also shoos grid density and chose to show time in "hh:mm:ss" if needed and the start of counting (Figure 10 p.p.).

Now go to "**Y-Axis**" sub-tab and type "Concentration [i]" in the Y-axis title box. Check the check-box next to "Use Engineering Unit of First Plot Variable" and the eng. unit box should be populated with correct unit automatically. This unit will also show next to Y-axis title on the plot. If not checked you can input desired units yourself, just make sure to type it in a way that software will recognize it. Choose to auto scale the Y-axis with 10% min/max margin (Figure 10 p.p.).

Within the "**Profile Plot**" sub-tab, you can se the profile-axis title (usually "segment number #", etc.) and once the simulation is performed (or at any point) you can use the scroll bar to move along the integration step number and check the simulation time at chosen step in a box below.

When you are done with setting the plot properties as described save your plot configuration by clicking on "Store Plot Configuration" (bottom right corner). To autoload plot configuration when compiling the model go to (while in SIM environment): General/Settings, your plot file name should appear within the "Plot Configuration" box, then click "Attach Current Simulation Settings to Focused Model" button and save the model afterwards.

Start the simulation and watch the live plot emerging dynamically with the time (Figure 11):

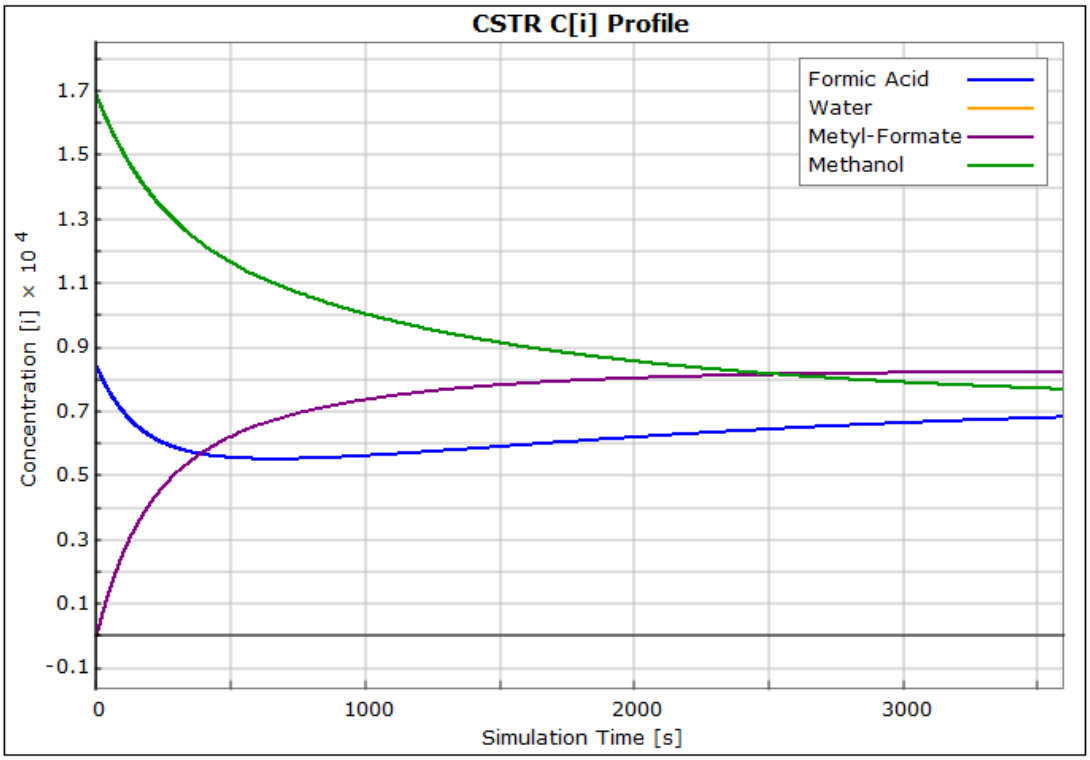


Figure 11 CSTR 3600s (1h) of operation dynamic plot

You could also choose a steady state simulation type and set the number of steps to be 3600, with fix time step of 1 second, and click on "**Perform a Simulation Run**". In this case model would calculate in the background (showing the calculation progress in % in the bottom right corner of the screen) and would stop the calculations after 3600 seconds, and your plot would just appear.

It is also possible to obtain floating (separate) plot window (Figure 12), to do that go to Plotting tab and click on "**Show/Update Plot Window**" button and the plot will appear, use the active corner points to resize the plot to desired dimension. This option is suitable when having large models, then you are able to check any plot without having to go back to the view where the embedded plot is which makes it very handy.

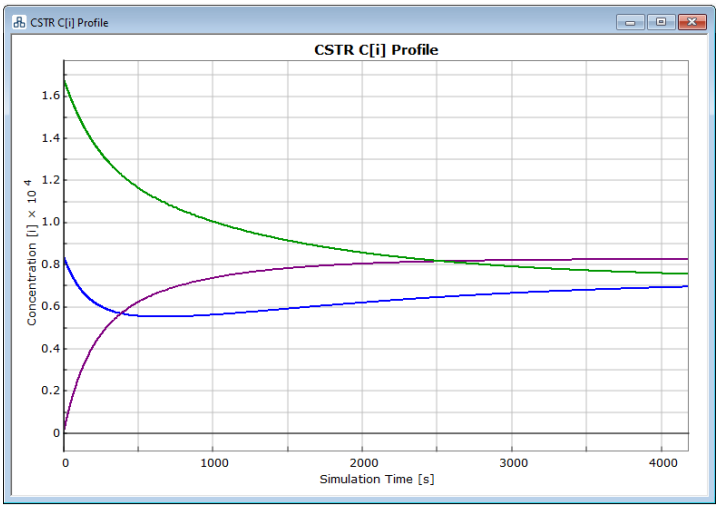


Figure 12 Floating dynamic plot

14. Adding a button model element & making alarm indicator

Button model element contains a predefined routine. You can make use of this element to make ON/OFF valve switches, alarm indicators and much more. Let us replace "Alpha" value object display with an Open/Closed (binary) function button. Go to *Properties Browser/Insert Objects/Objects* select "Button" (Figure 13) and click anywhere on the work surface to add a button object. The default button object will appear on your working area "BUTTON". We want to use the button to switch the "Alpha" parameter value between "1" & "0" i.e. to close and open the inlet valve.

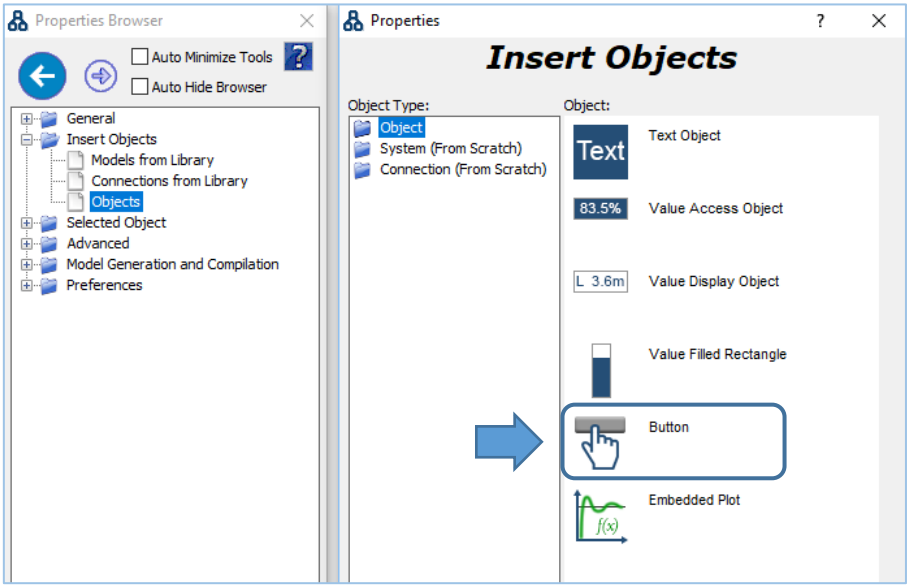


Figure 13 Inserting Button model object

Select the button, in the properties tab make statements according to Figure 14 below.

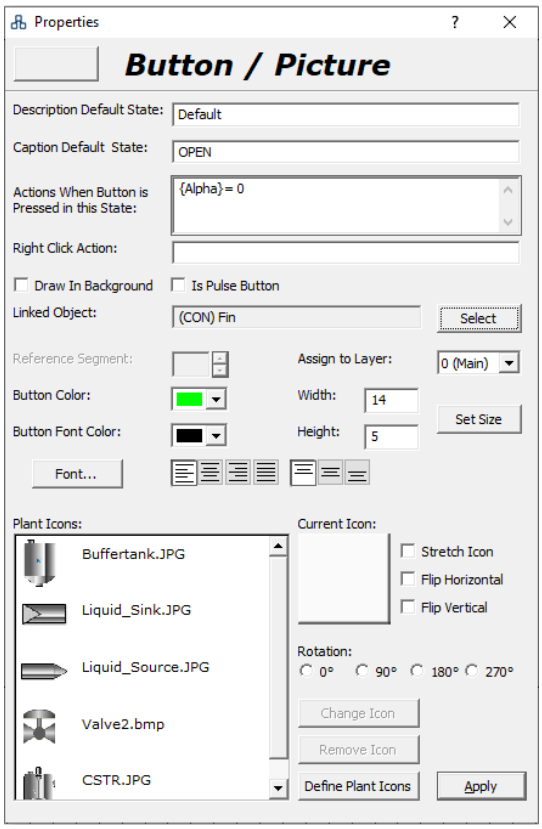


Figure 14 Button Open-function definition

As the valve is open in this state, meaning that Alpha > 0 (green colour is used), the action when pressing the button will change to: Alpha = 0.

Brackets "{}", "{Alpha}>0" are used to link the variable name to the linked model object. You can also use the entire variable simulation name (full variable path) instead e.g.: "Alpha_Fin" without the"{}" brackets. Press "Apply" when done.

To define button alternative action (closing condition) select "*Conditional Formatting*" tab just below the properties tab in the browser, there the closing condition will be defined. Make statements according to Figure 15 below.

As the valve is closed in this state, meaning that we have a condition "{Alpha} == 0" (red button colour used for closed valve), the action when pressing the button will now be: "{Alpha} = 1". In conditional statements the conditional expressions syntax must be used, i.e. equal sign is written as "==" not "=" as in action statements.

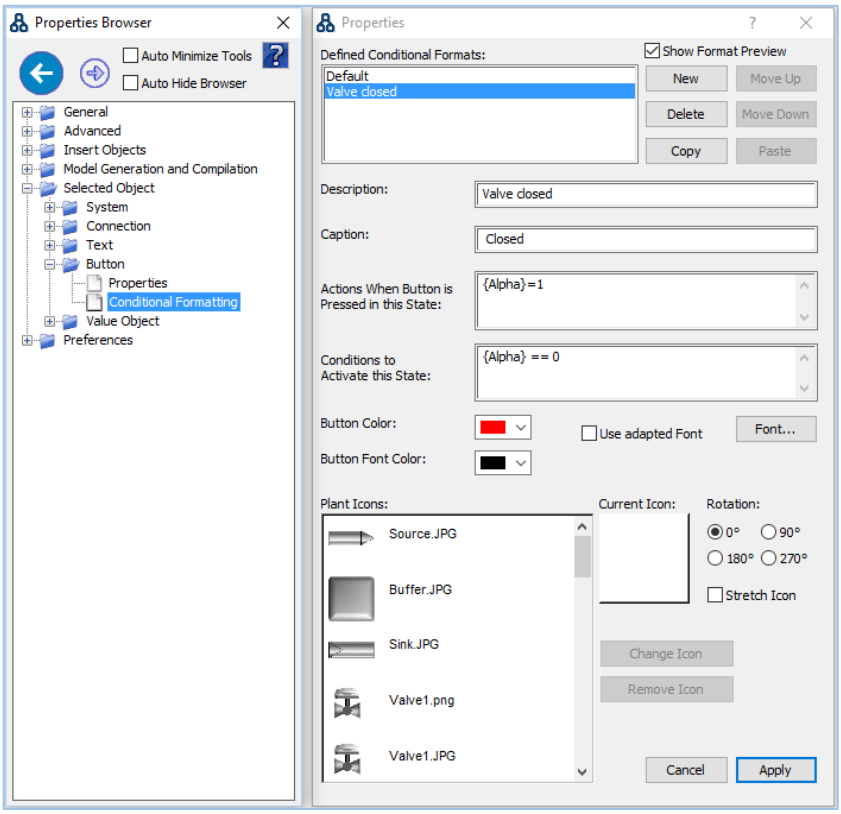


Figure 15 Conditional Formatting Close-function definition

Making Alarm indicator

Button object is also used to make an alarm indicator. To store (use) the alarm equation, we will use the information system just to divide the physical (CSTR) and "processed" equations. Go to *Properties Browser/Insert Object/Objects/System from Scratch* (SHIFT+s) and choose *"Information"* system. Click on the working surface to insert the info system and rename the system into "LA_high". Now connect the CSTR system with the information system using information connection from the scratch (SHIFT+c & choose information connection), "CSTR" as origin, "LA_high" as target. It should look similar as presented in Figure 16 below.

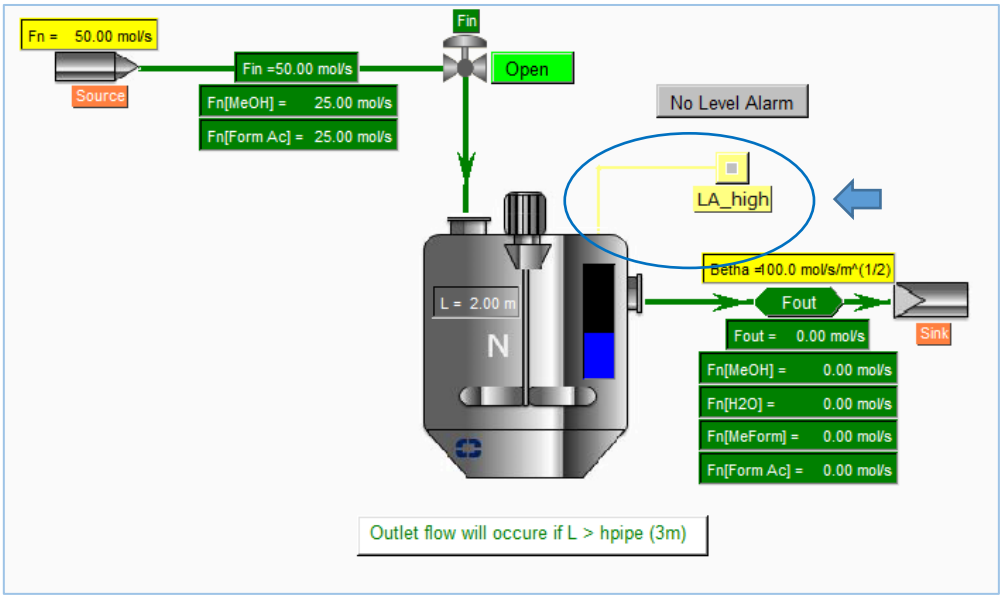


Figure 16 CSTR with Open/Close button switch & High level Alarm Indicator

Create & add equations to the info connection and the info system according to the list below:

Alarm Indicator equations (MM syntax):

Equation name:

```
Alarm
```

Function:

```
IF L > Lmax THEN
   Alarm = 1
ELSE
   Alarm = 0
END
```

Equation Class:

System *add to info system*

Equation name:

Liquid_level_info

Function:

```
or.L = tar.L
```

Equation Class:

Information connection *add to info connection*

Info connection will send the liquid level “L” variable value of CSTR system to the LA_high information system and the variable that will appear in that system will have the same name and will be used in the “Alarm” equation. In the info system sort “Lmax” as parameter and give it the value “**4”** [m].

Now it is the time to add an indicator of alarm state. Use the same way as in previous step to add a button object which will now ser as an indicator. Link this button to the “LA_high” info system object. The default caption is “No Level Alarm” and no conditions should be defined here (Figure 17).

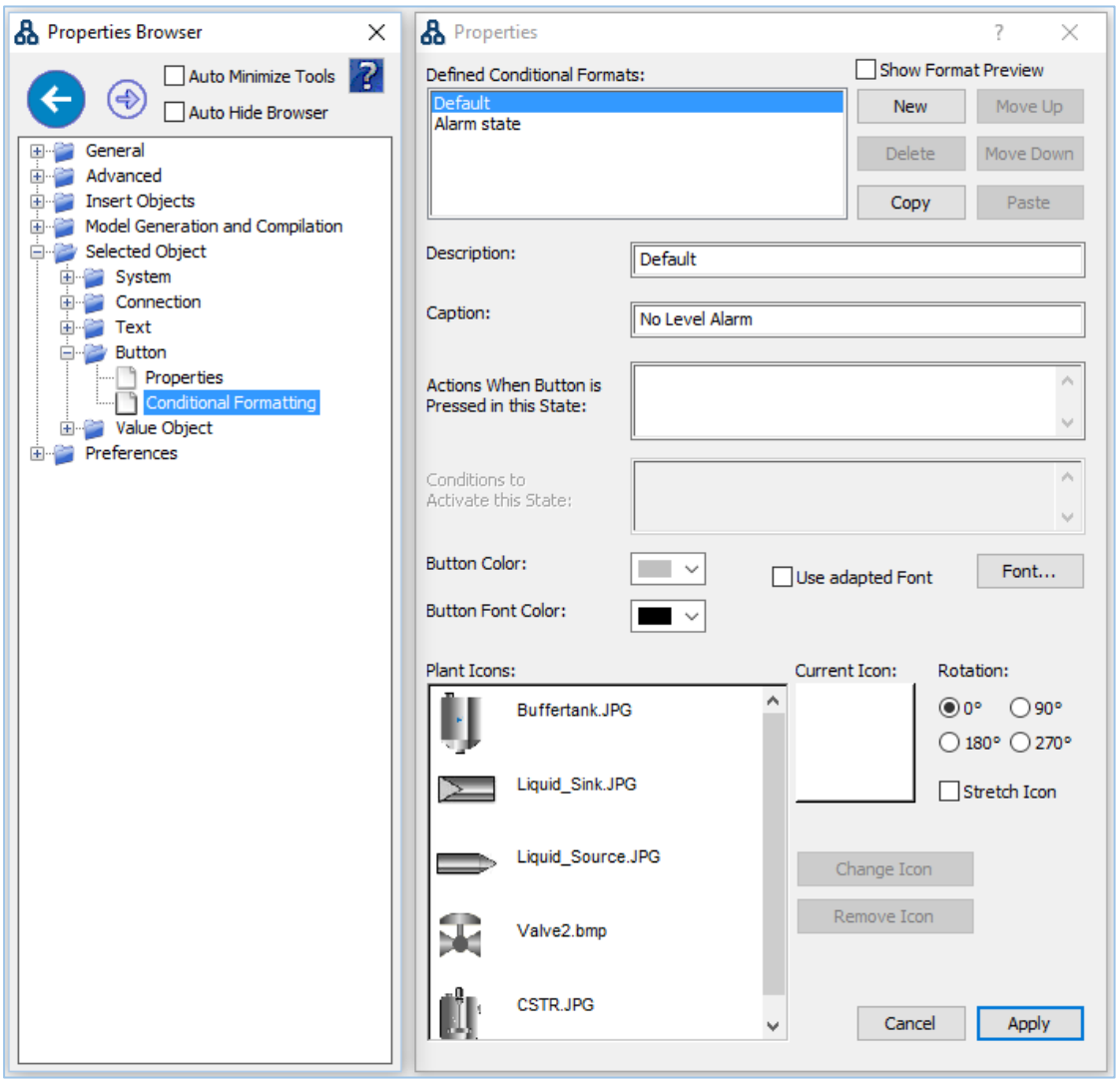


Figure 17 Alarm Indicator button “No Alarm” state definition

Then define the Alarm state, do as presented on the Figure 18 on the next page.

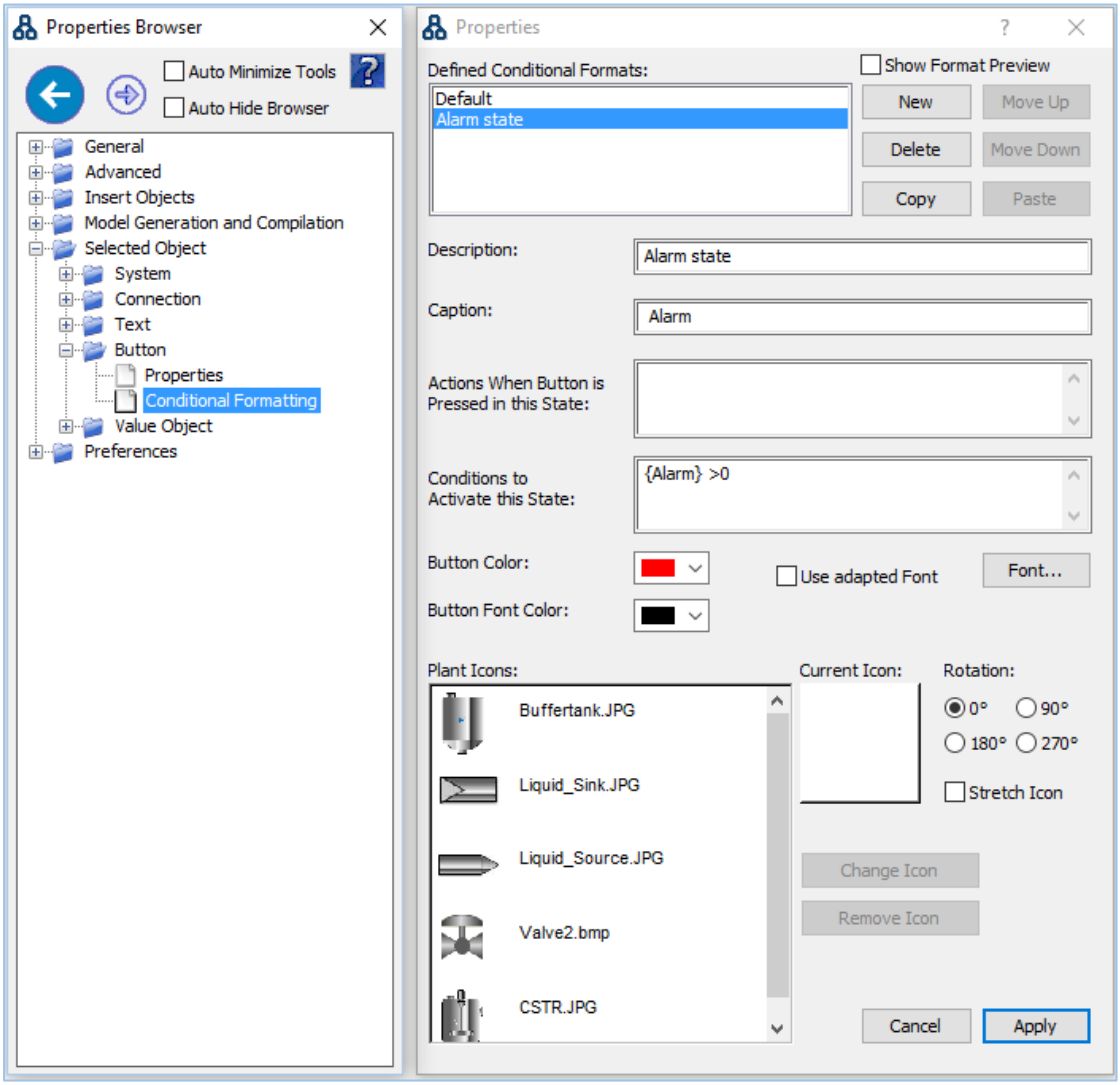


Figure 18 Alarm Indicator button definition

Once you are making and defining the alar, compile your model such that those changes take effect in the simulation environment (since we added physical systems and equations to it).

Run the model, open the inlet valve and close the outlet valve by setting “Beta” parameter of the outlet connection to “0”. The level will rise in the CSTR, and when L > Lmax (defined as parameter in the info. system) “Level Alarm” caption will appear, and the button colour will turn red indication an alarm state. Opening the outlet connection, the level in the CSTR system will drop and the alarm indication will turn off when condition L < Lmax is met.

Make sure to link the “alarm button” to the corresponding object (“LA_high”) from the button properties tab.

1.8 Questions:

Question1:

What is the final conversion of Formic Acid?

After what time the reactor enters the "Steady State" operation?

Plot the "*Fn_MeOH_Fout*" variable for the first 3600 seconds, at which time the outlet flow occurs and what is the Methanol max molar outlet flowrate?

Question 2:

How many CSTR's connected in series (cascade) is needed to achieve conversion of Formic Acid greater than 80%?

Question 3:

What should be the reactor(s) temperature to achieve conversion of Formic Acid greater than 80% after only two CSTR's in series?

What should be the reactor temperature to achieve conversion of Formic Acid greater than 80% using only one CSTR reactor?

Appendix 1

1. Model parameter values

Symbol	Description	Model Object	Value	Units
D	**Diameter**	CSTR sys.	**1.0**	**[m]**
ρ[CH4O]	**Molar liquid density**	CSTR sys.	**24.7E3**	**[mol/ m^3]**
ρ[CH2O2]	**Molar liquid density**	CSTR sys.	**26.5E3**	**[mol/ m^3]**
ρ[C2H4O2]	**Molar liquid density**	CSTR sys.	**16.32E3**	**[mol/ m^3]**
ρ[H2O]	**Molar liquid density**	CSTR sys.	**55.5E3**	**[mol/ m^3]**
Fn	**Inlet molar flow**	In. Conn.	**50**	**[mol/s]**
α	**In. line valve position**	In. Conn.	**100**	**[%]**
Xn[CH4O]	**Species molar fraction**	In. Conn.	**50**	**[%]**
Xn[CH2O2]	**Species molar fraction**	In. Conn.	**50**	**[%]**
β	**Outlet flowrate coeff.**	Out. Conn.	**100**	**[mol/s/m]**
h_p	**Pipe height**	Out. Conn.	**3.0**	**[m]**
k(r01)	**Reaction rate const.**	CSTR/Reactions	**6.61E12**	**mol/s/m^3**
k(r02)	**Reaction rate const.**	CSTR/Reactions	**8.0E12**	**mol/s/m^3**
Ea(r01)	**Activation energy**	CSTR/Reactions	**62500**	**J/mol**
Ea(r02)	**Activation energy**	CSTR/Reactions	**77300**	**J/mol**
T	**System temperature**	CSTR/Reactions	**40**	**[C]**
R	**Gas constant**	Glob. Parameter	**8.315**	**J/mol/K**

Table 4 CSTR model parameters