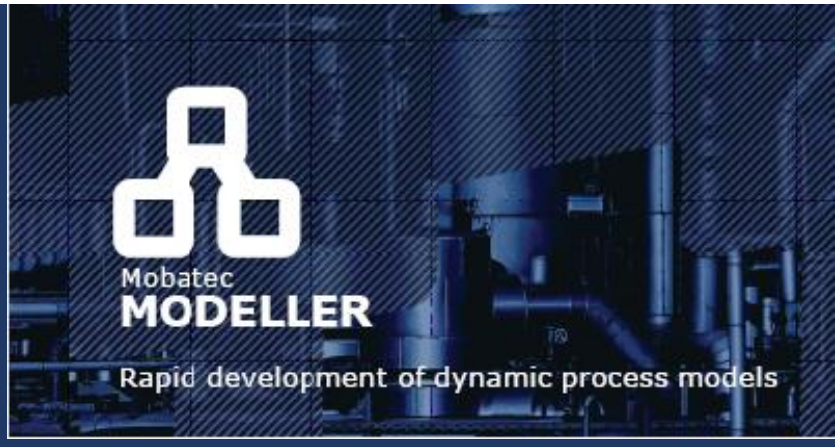
Mobatec
model-based technology



Mobatec Modeller

INTRODUCTION COURSE

Model Developer III

Advanced Equation-Based Modelling

Mobatec Modeller Intro Course – Model developer III

1 Modelling and Simulation of Non-Isothermal Continuous Stirred Tank Reactor with Cooling Jacket

1.1 Objectives

By the end of this exercise, you will know:

- How to generate Energy Balance in Mobatec Modeller.
- How to use special functions & Thermodynamic database in Mobatec Modeller.
- How to group systems and make a multi-level hierarchical models.
- How to connect variables in hierarchical models.
- How to import current simulation state (variable values) as initial conditions.

1.2 Model description

We want to model a dynamic operation of Non-Isothermal Continuous Stirred Tank Reactor with Jacket (CSTRwJ).

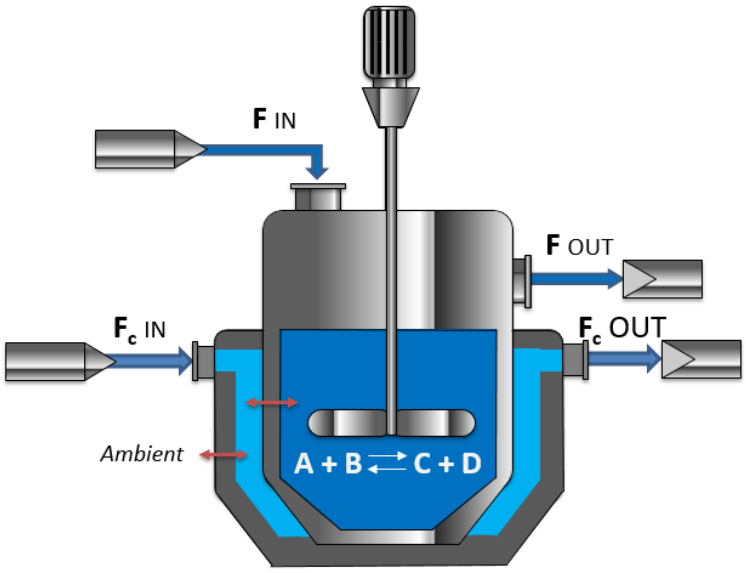


Figure 1 Non-Isothermal Continuous Stirred Tank Reactor with Jacket

This CSTR model is similar to previous exercise CSTR model, but some new equations are added, and some existing equations modified (replaced). Advective heat flows of the inlet and outlet mass connections will be defined and the energy balance of the CSTR will be obtained. A water jacket (capacity system) is added to the CSTR to control the reactor temperature (which will be calculated, instead of being set as constant as in previous exercise). CSTR & Jacket walls capacity systems will be added as well as the ambient battery limit system. Advective heat flows of the inlet and outlet jacket mass connections will be defined and the jacket energy balance will be obtained as well. Heat (transfer) connections will be added between the systems.

The CSTR model (Ex. 4.) will be used as a starting point for this exercise. In the following chapters parameters, variables & equations will be presented with respect to previous exercise (Intro - IV).

1.3 New Model Equations

Continuous Stirred Tank Reactor system equations

Energy balance

- $\frac{dH}{dt} = HF_{Fin} - HF_{Fout} + Q$ ← NEW (will generate automatically)

Temperature *(from molar enthalpy eq.) (system equation)*

- $Hn = @THERMO.ENTH(P, T, Xn[])$ ← NEW (to be added)

Molar Enthalpy *(from system energy holdup eq.) (system equation)*

- $H = Hn \cdot Nt$ ← NEW (to be added)

Molar Volume *(system equation)*

- $Vn = @THERMO.SPECV(P, T, Xn[])$ ← NEW (to be added)

Liquid Volume *(system equation; replace the existing Ex. 4. equation "V=Nt/SUM(rho[]*Xn[]",with:)*

- $V = Vn \cdot Nt$ ← NEW (replacing existing)

Water Jacket system equations

Mass balance *(system equation – generated automatically)*

- $\mathrm{d}\frac{\mathrm{n_i}}{\mathrm{dt}} = Fn_{i\,Fwin} - Fn_{i\,Fwout}$

Energy balance *(system equation – generated automatically)*

- $\frac{dH}{dt} = HF_{Fwin} - HF_{Fwout} + \sum Q$

Temperature *(from molar enthalpy equation) (system equation)*

- $Hn = @THERMO.ENTH(P, T, Xn[])$

Molar Enthalpy *(from system energy holdup eq.) (system equation)*

- $H = Hn \cdot Nt$

Total molar holdup *(system equation)*

- $Nt = \sum(n_i)$

Liquid Volume *(system equation)*

- $Nt = rho_{H2O} \cdot V$

Liquid level *(system equation)*

- $V = A \cdot L$

CSTR & Jacket - Source battery limit systems

Molar Enthalpy *(system equation)*

- $Hn = @THERMO.ENTH(P, T, Xn[])$ ← NEW (to be added)

Wall systems

Temperature *(energy holdup equation) (system equation)*

- $H = m \cdot Cp_m \cdot T$

Ambient battery limit equation

Ambient temperature *(system equation)*

- $T =_{(glob)} T_{ambient}$

Mass connections (CSTR & Jacket)

Inlet component molar flowrate *(mass connection equation - replace the existing equation)*

- $Fn_i = Fin \cdot_{or} Xn_i$ (already existing in CSTR inlet conn.)

Mass connections heat flow equation (CSTR & Jacket)

Inlet & Outlet connection heat flow *(mass connection equation)*

- $HF = \sum (Fn_i \cdot_{or} Hn)$ ← NEW (to be added)

Heat connections equations

Heat flow *(heat connection equation)*

- $Q = A \cdot U \cdot ({}_{or}T - {}_{tar}T)$

1.4 New Parameters

Symbol	Description	Model object	Units
T_{in}	**Inlet temperature**	Sources BL	[K]
P	**Pressure**	Jacket & CSTR	[Pa]
Cpm	**Metal heat cap.**	Jacket & CSTR Wall	[J/kg/K]
m	**Metal mass**	Jacket & CSTR Wall	[kg]
A	**Jacket cross-section a.**	Jacket	[m^2]
rho_{H2O}	**Molar density**	Jacket (spec.)	[mol/ m^3]
$T_{ambient}$	**Ambient temperature**	global	[K]
U	**Overall heat tr. c.**	Heat Connections	[$W/m^2/K$]
A	**Heat transfer area**	Heat Connections	[m^2]

Table 1 New parameters

1.5 New Variables

Symbol	Description	*Model Object*	Units
H	**Enthalpy**	System	[J]
Hn	**Molar Enthalpy**	System	[J/mol]
HF	**Heat flow**	In./Out Mass Conn.	[J/s]
Q	**Heat flow**	Heat connection	[J/s]
Vn	**Molar Volume**	System	[m^3/mol]

Table 2 Model variables

1.6 Mobatec Modeller multi-level topology approach

Conventional equation based models are represented as single piece of code, where all the model equations are coded, using the software programming language. Model transparency has shown to be an issue especially with the large models and when the models are created by someone else it can be troublesome and time consuming to understand and use such models.

To overcome this, Mobatec Modeller adopted a **model decomposition methodology** – creating a composite model consisting of as many layers as needed. Instead of defining all the model phenomena (equations) stacked in one unity, user can create hierarchical multi-level models where model equations can be divided into separate groups and make one visually transparent interconnected composite model.

To illustrate this let's use colours instead of equations:



Figure 2 Colour analogy on the model transparency

All model defined parts are inter-connected:

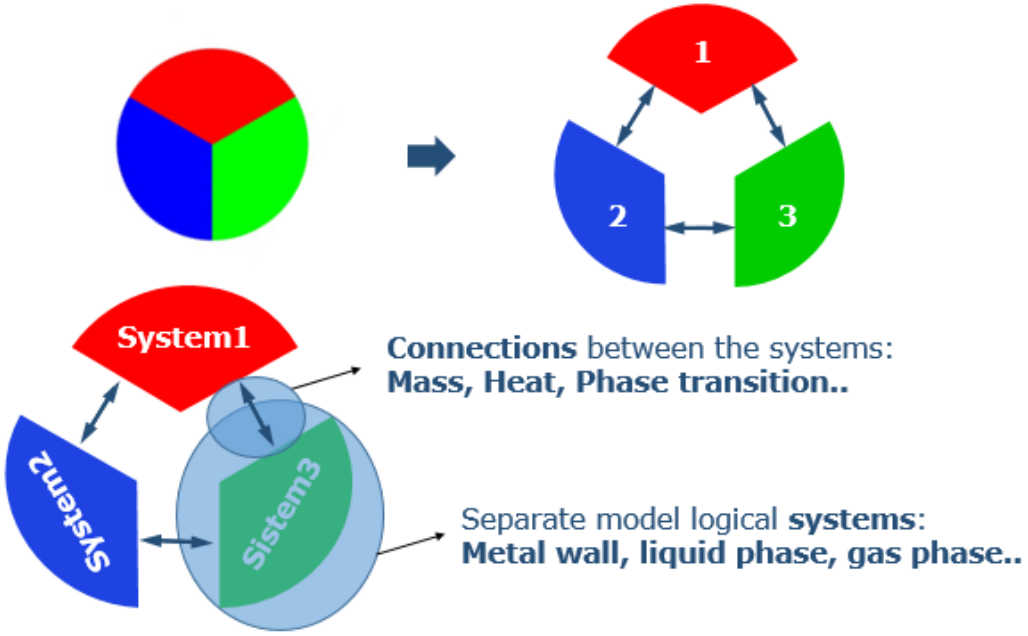


Figure 3 Systems & Connections

Let us look at some real modelling examples now:

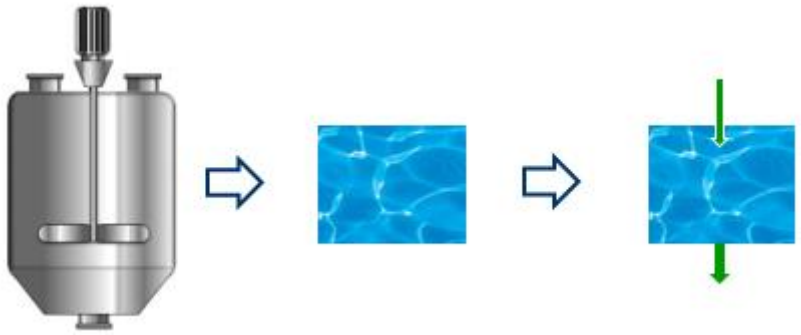


Figure 4 Continuous Stirred Tank Reactor; Single phase, Adiabatic

Model showed in Figure 4 can physically be represented as a single **Liquid phase**, since there is no heat loss (adiabatic reactor) there is no need to define the reactor wall and ambient systems. Green arrows are inlet & outlet **mass connections** (flow lines).

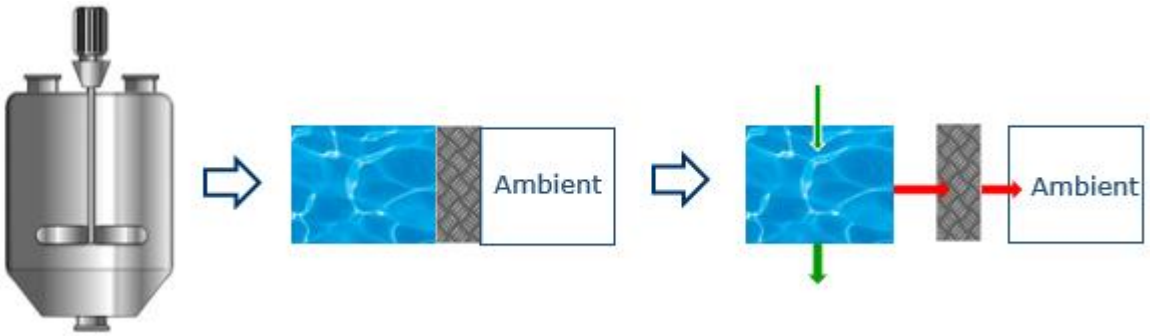


Figure 5 Continuous Stirred Tank Reactor; Single phase, Non-Adiabatic

Physical parts of model showed in Figure 5 are **Liquid phase,** reactor **Wall** and the **Ambient**, since heat is exchanged between the reactor liquid phase and the surroundings. Red arrows are the **heat connections** (heat flow) from the reacting phase to the wall, and from the wall to the ambient.

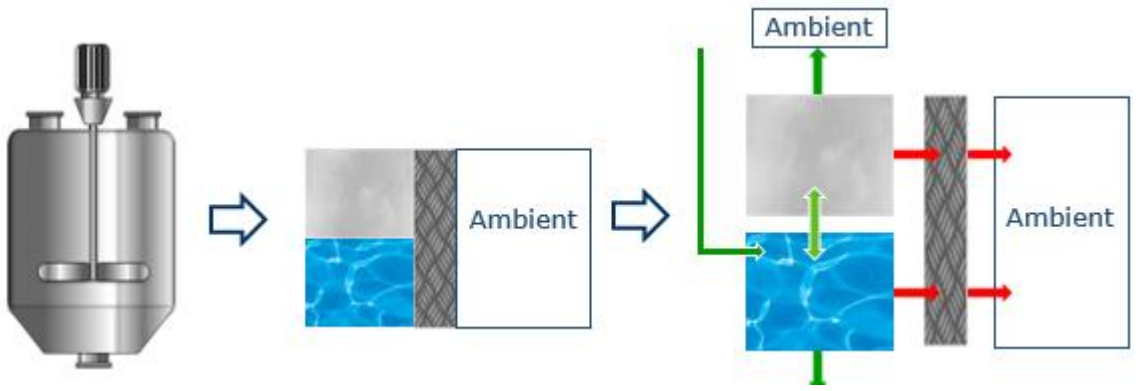


Figure 6 Continuous Stirred Tank Reactor; Two phase, Non-Adiabatic

Physical parts of model showed in Figure 6 are **Liquid phase, Gas Phase,** reactor **Wall** and the **Ambient**, since heat is exchanged between the reactor liquid & gas phase phases and the surroundings (ambient). Light green arrow is the **phase transition** (mass) **connection** between the phases.

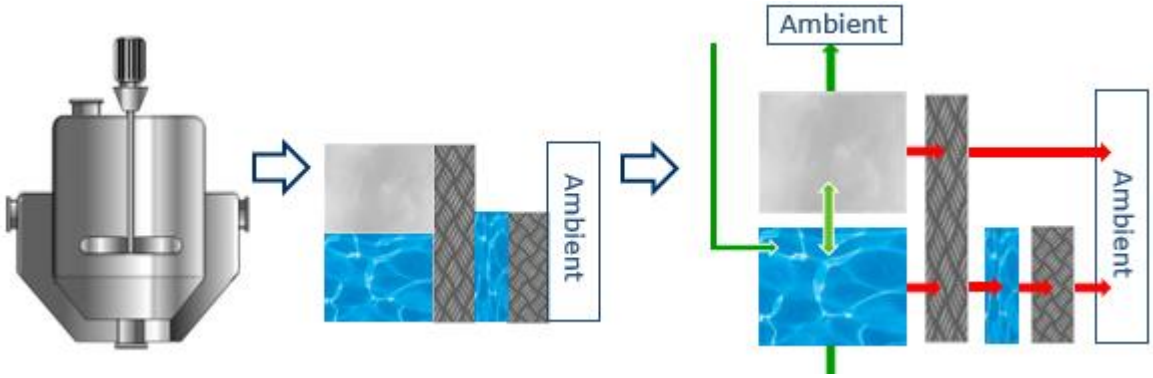


Figure 7 Continuous Stirred Tank Reactor with Cooling Jacket; Two phase

Physical parts of model showed in Figure 7 are reactor **Liquid phase & Gas Phase,** reactor **Wall**, **Jacket liquid phase, Jacket wall** and the **Ambient**.

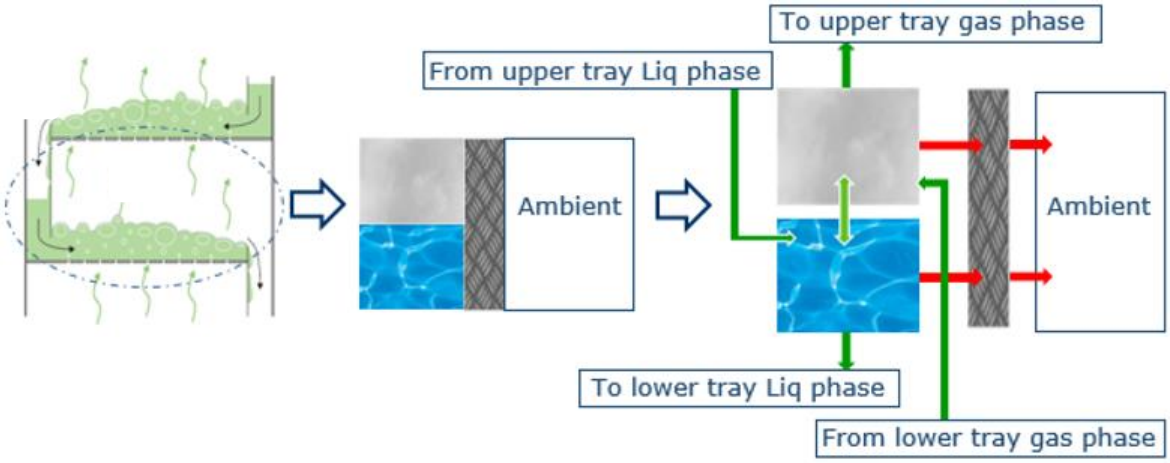


Figure 8 Distillation Column tray; Two phase, Non-adiabatic

Physical parts of model in Figure 8 are **Liquid phase, Gas Phase,** column **Wall** and the **Ambient**, since heat is exchanged between the reactor liquid & gas phase phases and the surroundings (ambient).

Each system will hold the equations defining that system. Mass connection and phase-change connection will hold equations describing the mass and accompanying convective heat flow between connected systems. Heat connections will hold the equations describing the heat flow between connected systems.

1.7 Things to do

1. Use "Isothermal CSTR" model as a starting point

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

2. CSTRwJ model physical topology

Replace the CSTR icon with "Ex_Racting_Phase" icon. Add jacket, jacket wall (representing wall around the jacket) & CSTR wall (reactor wall) capacity systems. Add water source, water sink & ambient battery limit systems. Make (unidirectional) mass connections from water source to the jacket system and from jacket to water sink battery limit.

Make heat flow connections (default colour red), by connecting the jacket system, CSTR wall and CSTR from one side and the jacket wall and ambient battery limit from the other side as presented in Figure 9. Heat connections are made the same way as mass connections, just select (SHIFT+c) “Heat” (red icon) connection. Use the same sink and source icons to change the icons of cooling water battery limits. Add icons to the Jacket, Jacket Wall, CSTR Wall & the “Ambient” system as well.

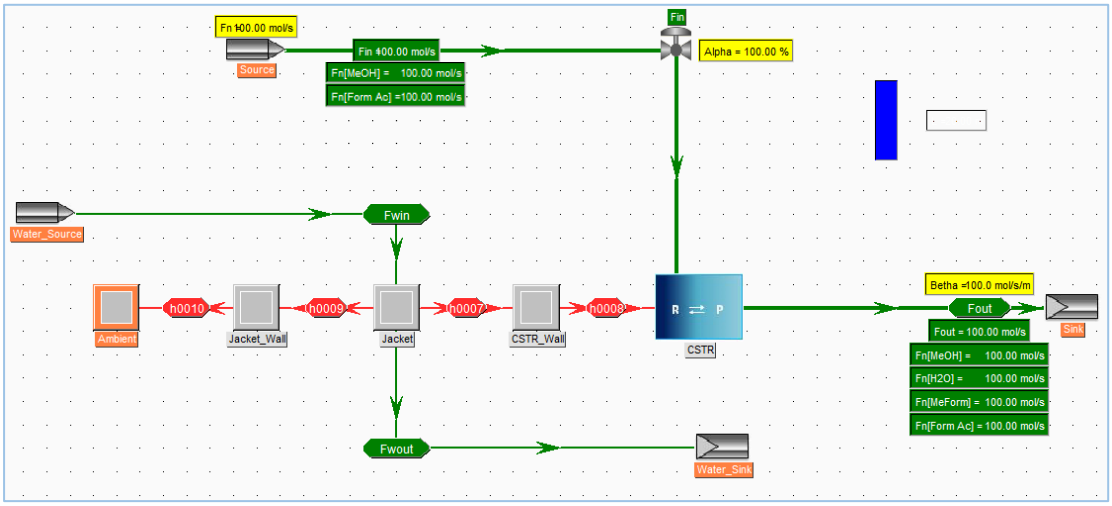


Figure 9 CSTR with Jacket model physical topology

FYI: When re-using the same icons, you can use a **shortcut**, select the system with the desired icon and press “**shift+s**” together, then select the system where you want to set the icon and press “**s**”. The same holds for the connection icons, press “**shift+c**” together and then select the connection where you want to add the same icon and press “**c**”. It is also possible to copy/paste the parts of the model. For example, you could select the reactants battery limit and the inlet connection system and copy & paste it to reuse it for the water battery limit and inlet connection. Before pasting, right mouse click and choose appropriate pasting scheme.

3. Adding Species to your model

The reactant species are already defined in the previous exercise. Inject **H_2O** species to the water battery limit.

4. Defining species parameters – “spec.*parametername*”

In Mobatec Modeller you can set a special type of parameters associated to the species in your model called “species parameters”. Those parameters can be used in multiple equations (“places”) and you need to define these parameters only once. These are like global parameters but for the species only.

These parameters are usually some known species properties like *rho[]*-molar density or *Cp[]*-molar heat capacity, etc. In order to define a species parameter use a “**spec.**” prefix when writing the parameter in the equations. In this model a jacket water density “rho_{H2O}” can be defined as species parameters, so when “writing” the equations instead of typing “rho_H2O” type “**spec.rho[1]**”. Now MM recognizes rho[1] as a species parameter and will treat this parameters as known in the “Equation Sorting” tab, while “1” is species referent number.

To add values of species associated parameters open the main editor tab (“d”) and go to “Species” tab. Select the correct species (H_2O in this case) and in the “Defined Variables” list-box the defined “rho[]” will be available. Select it and click add species parameter button, then enter the value (Figure 10). This action of course makes sense if you are about to reuse species parameters in many objects.

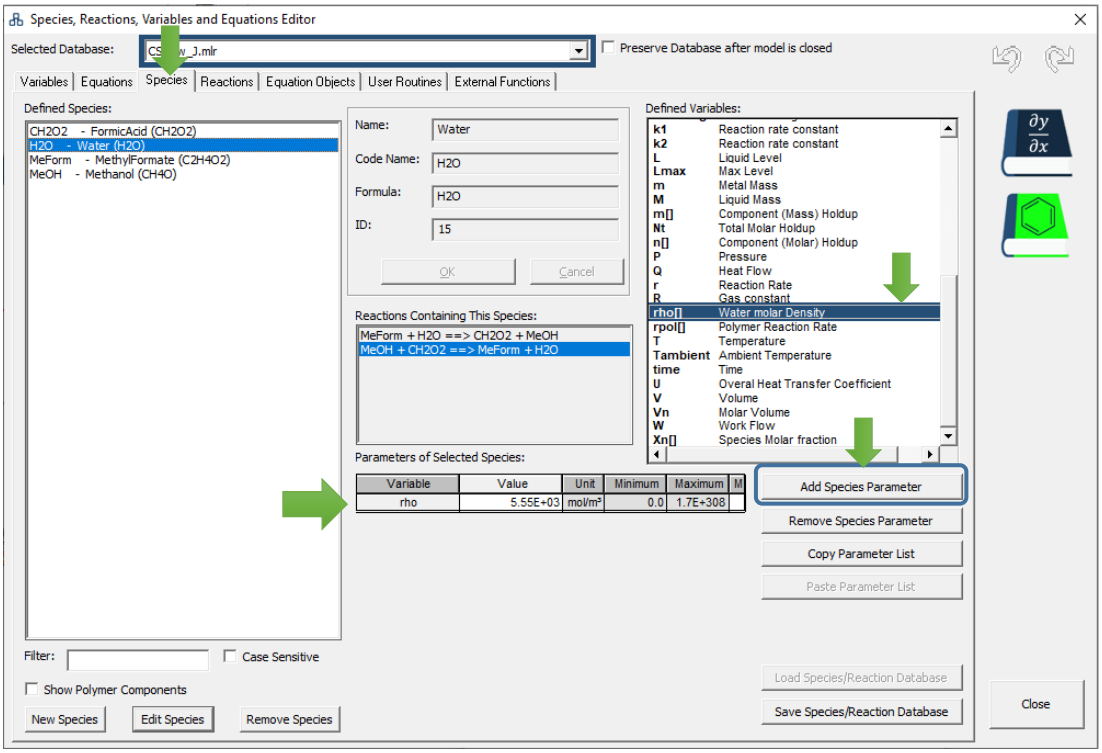


Figure 10 Adding species parameter

5. Writing & Adding the Equations of CSTRwJ model

Add all new equations to the equation model objects they belong to. When writing the mass connections equations check the "Mass Connection" under "Equation Class" in the equations tab, for the heat connections check the "Heat Connection" & for the systems check "System". This classification divides the equations into groups, e.g. when adding equations to a mass connection only the equations that you declared as "Mass Connection" will be available to be added. You could also check multiple equation class identifiers.

The inlet & outlet mass connection equations are the same for both reactor and the jacket as they are flow equations. First, add the heat flow equations to the reactor inlet and outlet connection. Now, **you can copy the equations** of reactor inlet connection and paste them to the inlet jacket connection directly. Select the reactor inlet connection, press "**shift+e**" (right click/copy equations), then select the jacket inlet connection and just press "**e**" (right click/paste equations). Check if you pasted the equations successfully. Do the same for the outlet jacket connection.

FYI: Some equations that you need for the "Jacket" system already exist in the model, like "total molar holdup" & "liquid level", equation, so you do not have to create these equations again, just reuse them. **The same-name variables & parameters can be used in the different model objects**, as they belong to a different system there will be "**no confusion**", and **you can re-use the same equations in as many equation objects as you need**.

After you have added the heat flow equations (**HF =** …) to the streams the **energy balance will be automatically generated**. Heat transfer (**Q**=…) through the heat connection will also be a part of the generated heat balance.

To learn all on **Composite-multilevel models** & **Energy Balance generation** read **Chapter 11.** in Mobatec Modeller handbook for beginning and advanced users.

Use the list below to create and add (or just edit) the equations to specific model objects.

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

***CSTR & Jacket** inlet **mass connection(s)** 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[]`
Inlet_heat_flow	`HF:`	`HF = SUM(Fn[]*or.Hn)`

***CSTR & Jacket** outlet **mass connection**(s) 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[]`
Outlet_heat_flow	`HF:`	`HF = SUM(Fn[]*or.Hn)`

***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[])`
Liquid_level_CSTR	`L:`	`V = L * A`
Species_molar_fraction	`Xn[]:`	`n[]= Xn[] * Nt`
Species_molar_concentration	`C[]:`	`n[]= C[] * V`
Energy_holdup	`Hn:`	`H = Hn * Nt`
Molar_Enthalpy	`T:`	`Hn = @THERMO.ENTH(P,T,Xn[])`
Molar_Volume	`Vn:`	`Vn = @THERMO.SPECV(P,T,Xn[])`
Liquid_Volume	`V:`	`V = Vn * Nt`

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

Equation name:	Eq'n Pivot:	Function:
Total_molar_holdup	`Nt:`	`Nt = SUM(n[])`
Molar_Enthalpy	`T:`	`Hn = @THERMO.ENTH(P,T,Xn[])`
Energy_holdup	`Hn:`	`H= Hn * Nt`
J_Volume	`V:`	`Nt = V * spec.rho[1]`
Liquid_level	`L:`	`V = L * A`

***CSTR & Jacket - Source systems** equation (MM syntax):*

Equation name:	Eq'n Pivot	Function:
Molar Enthalpy	`Hn:`	`Hn=@THERMO.ENTH(P,T,Xn[])`

***Wall system(s)** equations (MM syntax):*

Equation name:	Eq'n Pivot	Function:
Wall_Temperature	`T:`	`H = m * Cpm * T`

***Heat connection(s)** equations (MM syntax):*

Equation name:	Eq'n Pivot	Function:
Heat_flow	`Q:`	`Q = A * U * (or.T - tar.T)`

***Ambient system** equation (MM syntax):*

Equation name:	Eq'n Pivot	Function:
Ambient_temperature	`T:`	`T = glob.Tambient`

6. Declaring variable dimensions

After you have created and added all new CSTRwJ model equations, declare the dimensions of the new variables. Do this on the same way as in previous exercise. Only new variables dimensions are presented in the Table 3 below.(*Note: HF,Q & P are predefined variables*)

Name	Description	Eng. Unit	Unit Category	Bounds
Cpm	**Mass metal h.c.**	[J/kg/K]	Heat capacity	[0 – 10000]
m	**Metal mass**	[kg]	Mass	[0 – 1e308]
rho[]	**Molar density**	[mol/ m^3]	Molar density	[0 – 1e308]
T	**Inlet temperature**	[K]	Temperature	[0 – 3000]
$T_{ambient}$	**Ambient temperature**	[K]	Temperature	[0 – 3000]
U	**Overall heat tr. c.**	[W/m^2/K]	Heat Tr. Coeff.	[0 – 1.5e4]
H	**Enthalpy**	[J]	Energy	[-1E100 – 1e100]
Hn	**Molar Enthalpy**	[J/mol]	Specific Energy	[-1E308– 1E308]
HF	**Heat flow**	[J/s]	Power	[-1E100 – 1e100]
Q	**Heat flow**	[J/s]	Power	[-1E100 – 1E100]
Vn	**Molar volume**	[m^3/mol]	Specific Vol.	[0 – 1E308]
P	**Pressure**	[Pa]	Pressure	[0 – 1E308]

Table 3 Variable dimension declarations

7. Grouping systems & model hierarchy

Once the model parts are connected, we want to group all the reactor & jacket parts inside of one (top level) higher hierarchy system, the "CSTRwJ" system. To do this, make selection of all the reactor & jacket model parts (except sinks & sources) and then do right click and select "Group", or click on "" icon in the toolbar or just press "g". Enter the name "CSTRwJ" of the new grouped system and press "Group Systems" button. The selected systems will be grouped inside of the higher hierarchy system. Use "CSTRwJ" icon for this system, and relocate the connection "entrance" points so that your model looks similar as presented in Figure 11 on next page.

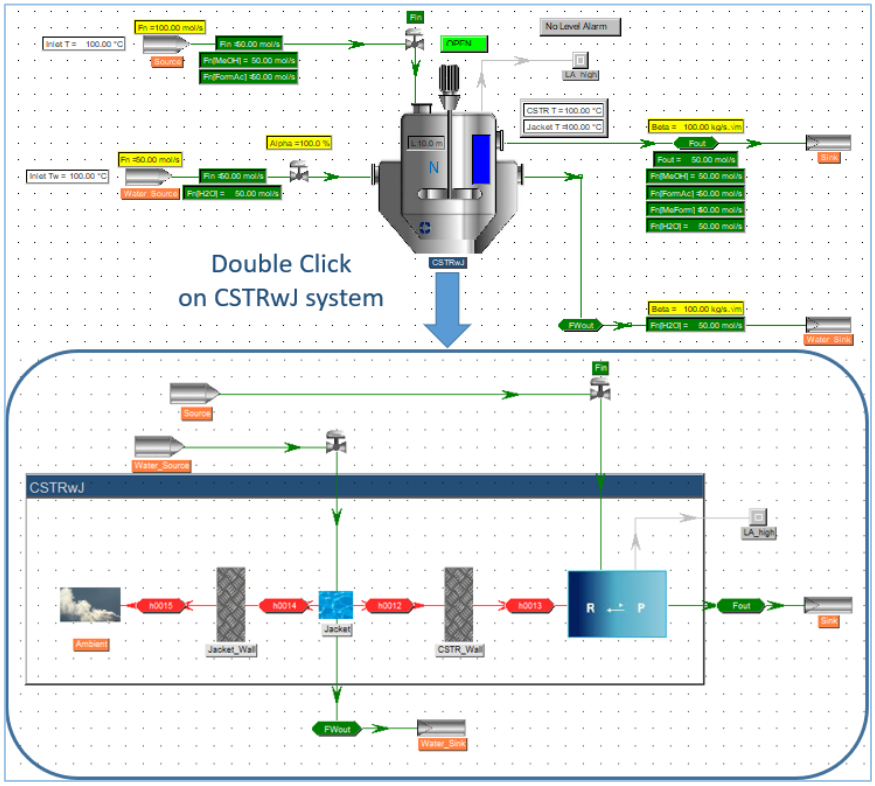


Figure 11 Multi level CSTRwJ model

When doing a double click on the parent system you will be able to "enter" the lower hierarchy systems. This is done because of two main reasons, first is to have a nice (intuitive) overview of the model topology and not to overpopulate the work space when having bigger models, the second reason is to keep the number of equations per system as low as possible and distribute the whole model equations over a different logical hierarchy levels which "communicate". This way it is much easier to use and manipulate the model.

When having a multi-level models, the lower level model can always make use of any variable which is being calculated on a higher hierarchy level model. This will be explained in the section "**Connecting "upper" & "lower" level variables"**, later.

8. Equation sorting

Sort the equations of the all systems & connections using the information provided on the model parameters (section 1.4 - page 3.).

9. Defining THERMO definitions of the phase(s)

Before the model is initialised, the thermodinamic property calculations of **Hn (molar enthalpy) & Vn (molar volume)** through MM special functions **"@THERMO"** for reacting phase should be set if the user does not want to use "Ideal" property method which is set as default. In our model we will use Ideal property method but will demonstrate how to define phase property calulations. In Mobatec Modeler you can choose a different property method calculations for: (**Species) Fugacity Coefficient**, **Specific Entalphy** & **Specific Volume**.

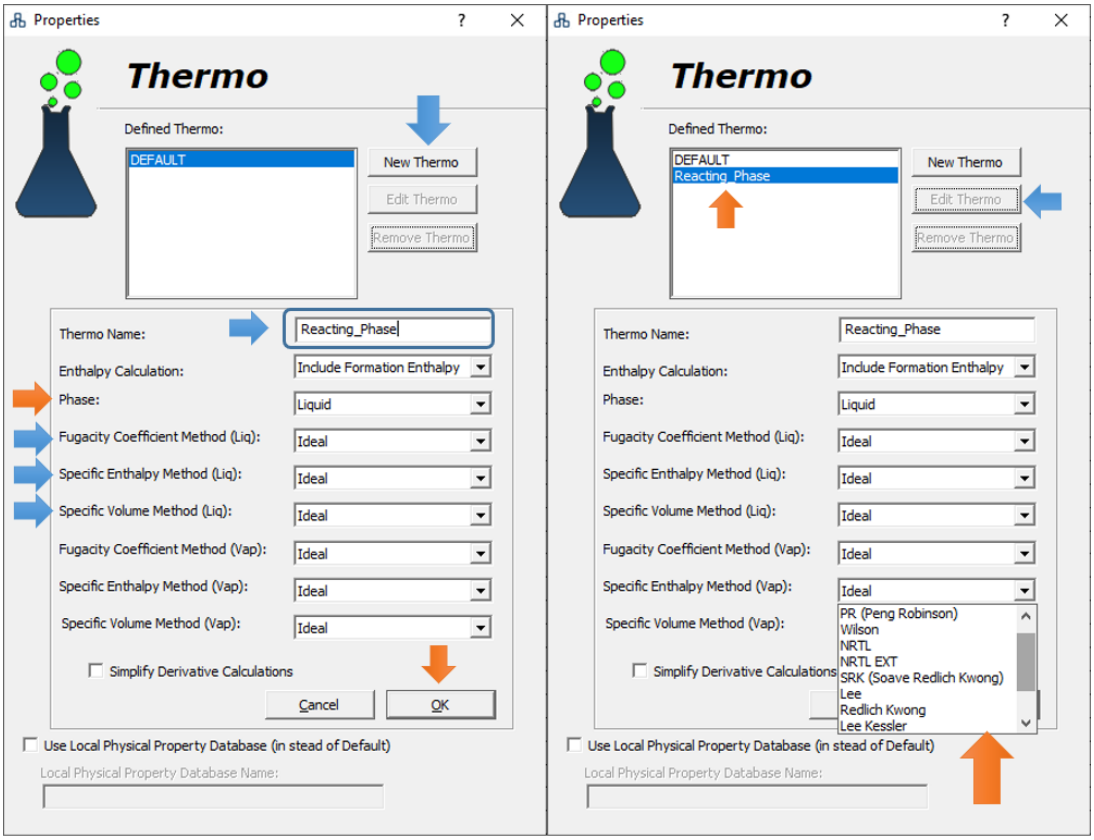


Figure 12 Thermo-Definitions

To define a phase property calculation method make no selection and go to *Properties Browser/General/Thermo Definitions* tab. Click on "New Thermo" button as shown in Figure 12, assign a name "**Reacting_Phase**" select the "Liquid" phase, as our reacting phase is liquid and leave "Ideal" EOS property method for calculations of thermodynamic parameters (Hn & Vn). Click "OK" to save your thermodynamic definition.

In order to use defined thermo definition(s), you have to "apply" created thermo definitions to your model systems. To do that select CSTR system (Racting_Phase), go to *Properties Browser/Selected Object/System/Thermo* tab and in "**Use Phase Name to Link Thermo**" box type the thermo definition name "**Reacting_Phase**" and press "Rename Phase" button as shown in Figure 13. You have now linked the thermo definition to the selected system by giving your phase the same name.

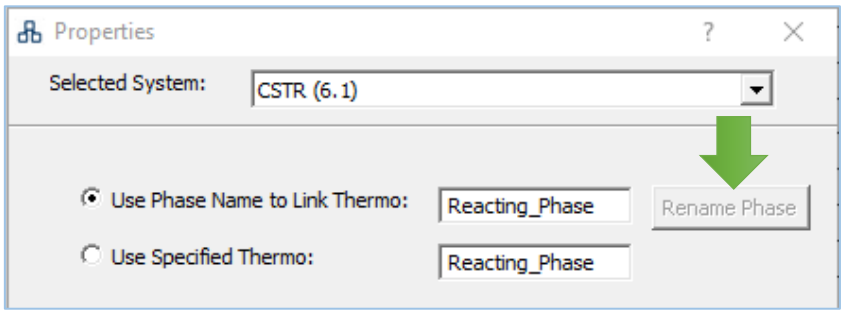


Figure 13 Linking Thermo definition to selected system

If you want to choose "**Use Specified Thermo**" then you should first type the exact name of available-listed thermo definition and select that option. Selection will not be available if wrong name/non-existing thermo definition name is typed.

10. Initial conditions

Insert given (newly defined) parameters values 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 input to be initialized (calculate initial variables values) are the "CSTR" & "Jacket" system as they are a capacity systems that can store mass & energy. Initialize the CSTR system on the same way as in the previous exercise using provided initial inputs.

Initial conditions for the CSTR system are:

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

Starting temperature is 20 °C.

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.

Initial conditions for the Jacket system are:

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

Starting temperature is 20 °C.

Initial conditions for the Jacket & CSTR wall-systems are:

At the start of simulation, the Jacket & CSTR Wall T is 20 °C.

After you have successfully initialized the model systems initialise all the connection variable values as well.

11. 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 *Property 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 "Fix Step Size" simulation of "1" (sec) time step. Click ***"Start Calculation"*** button 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.

12. Monitoring variable values

Make value displays for Fn, Fin, Fn_"Speciesname" variables of inlet connections. Fout, Fn_"Speciesname" of outlet mass connection and their Alpha & Beta parameters. Also add CSTR and Jacket systems temperature displays. Feel free to add displays for other variables.

13. Connecting "upper" & "lower" level variables – "group.*variablename*"

Till now your CSTRwJ model should be running. Stop the simulation, select the top level "CSTRwJ" model and go to its equation tab. You will see that this tab is **empty** as we still did not used this model level for any calculations. Now, we are going to define the CSTR cross-section area calculation on a top model level. Add already existing "A = D^2*PI()/4" equation

to the CSTRwJ (top level) system. Sort “D” as parameters (use the same D value) and “A” variable should be calculable.

We want to use the “A” variable now being calculated on the top model level for calculation of liquid level of the “CSTR” and the “Jacket” systems as these systems are defined to have the same cross-section area value.

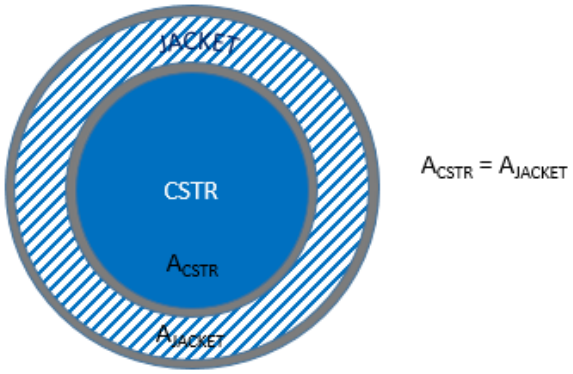


Figure 14 CSTRwJ cross-section

We can “connect” the top level calculated variables values to the lower level by adding the prefix “**group.**” before the variables e.g. “group.A”. To do this open the main editor and use “**Edit**” function selecting the liquid level calculation equation “V=A*L”. New equation should be written as “V=group.A*L”. Go to Advanced/Tools/ and click “Update Variables &Equations” button to make sure that equation have changed in the CSTR & Jacket system (check if equation did change).

Select the CSTR system go to equations and remove the cross-section area calculation equation as now the cross-section area is being calculated on the model top level (CSTRwJ). CSTR system should be well-posed now. Run the model simulation.

14. Importing current model simulation state

After a successfully model run, most probably you would like to save the simulation results, so that you can run the model next time from that preserved simulation state point. Simulation state represents the values of all model variables and parameters at certain point. To import the current simulation state, only possible when in simulation environment, use the button in the toolbar indicated in the below.

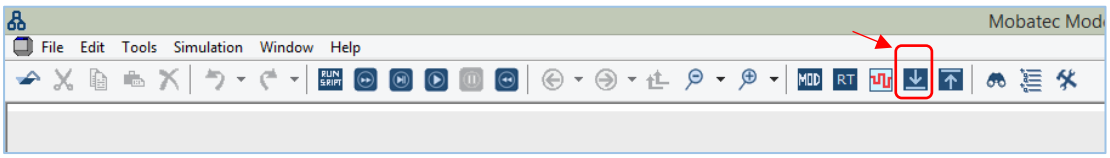


Figure 15 Import current model simulation state button

By importing the current model variables values, you will make those values the initial values of your model. For example, if you have your model reached the steady state, and you would like to save that state of the model, then you can use the import button. User can also save as many model different states as needed by using “snapshot” function; *General/Snapshots* while in Simulation environment. Type the name in the snapshot box and press “Make Snapshot” button. Afterwards you can find desired snapshots in the snapshots list and load them to the simulation by selecting a snapshot from the list and by clicking on “Load Snapshot” button.

15. Using “prop.” prefix

The “prop.” prefix (short for property), is used to call species database engine and calculate number of species properties like: Liquid density, Critical P, T, V, … etc. Search for all “prop.” properties in MM Handbook under the “**Syntax - variable prefixes**” in **Chapter 8**. We will use the molecular weight property function “prop.MW[]” (kg/mol) to calculate the reacting mass, using the equation:

$$M = SUM(prop.MW[] * n[])$$

Add this equation to the CSTR capacity system, model object.

16. Making your simulation “more dynamic”

You got familiar with Conditional Formatting tab in the previous exercise when making buttons and alarm indicators from button objects. The connection lines also have conditional formatting tab, and the system objects as well. Let’s make the model interactive, by changing the colour of the water inlet and outlet connection to blue colour when the flow is > 0 while in simulation. We can do this by setting the conditional formatting of these connections. For the water inlet connection, set the CF as presented Figure 16 below.

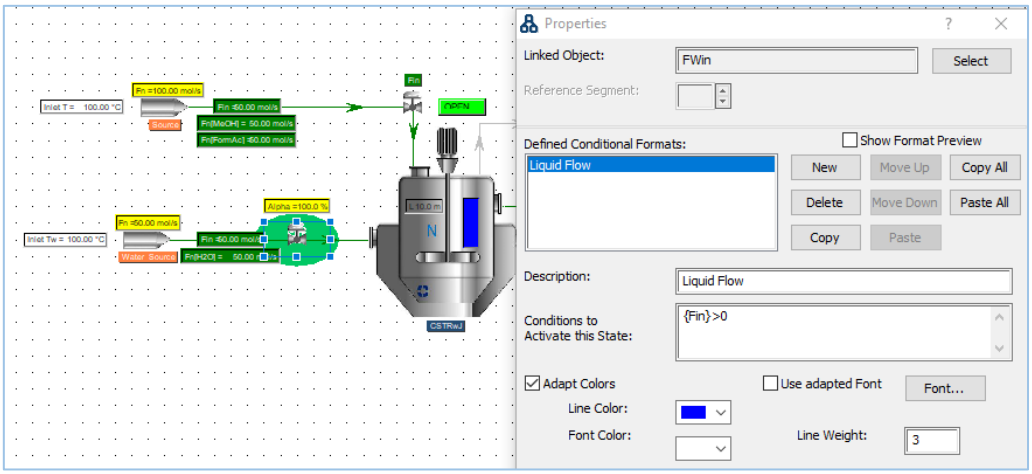


Figure 16 Line colour change – conditional formation

Do the same for the outlet connection as presented Figure 17 in below.

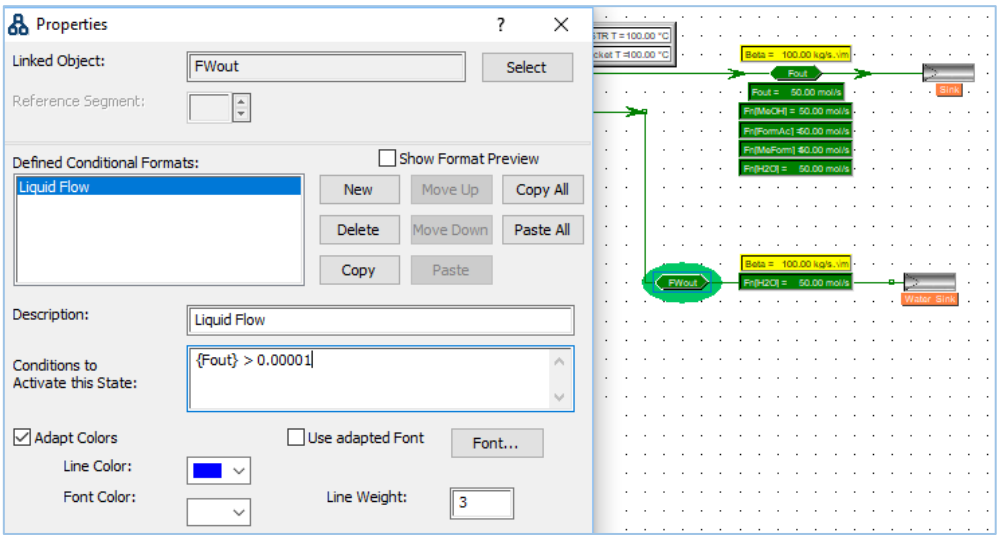


Figure 17 Line colour change – conditional formation

Brackets “{}” ➔ {Fout}>0 are used to link the variable name to the selected model object. You can also use the full variable simulation name instead ➔ Fout_Fwout > 0 without brackets. The effect we get after doing this is presented in Figure 18 below.

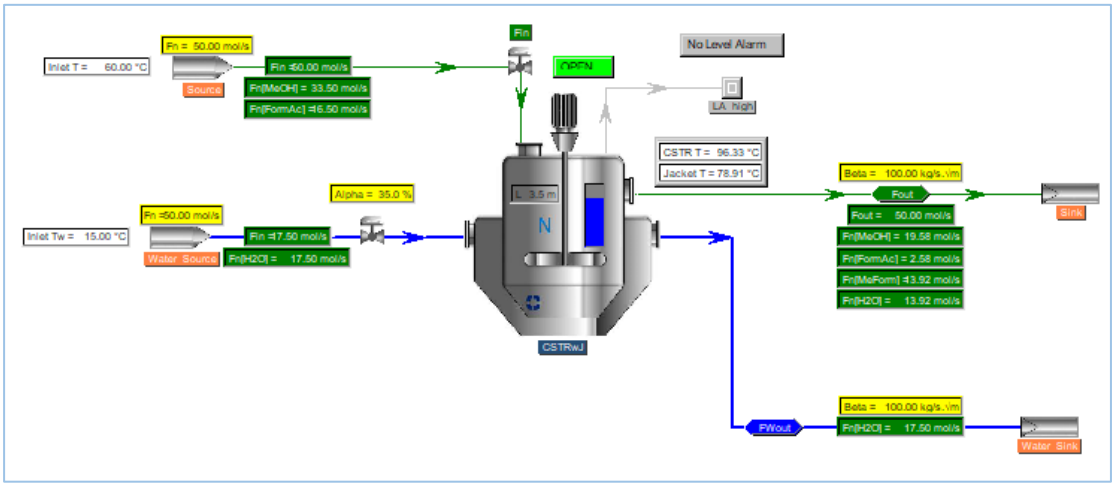


Figure 18 Cooling water lines colour change – conditional formation

Do the same formatting for the reactor inlet and outlet connections, just use different colours. Get creative with conditional formatting options of your system models. For example, you can set the CF of filled rectangle display to change colour from blue (default) to red, when the level goes over some maximal value.

1.8 Questions:

Question1:

What is the conversion of the Formic Acid and what is the CSTR steady-state temperature?

What is the combined reactions heat effect, exothermic or endothermic?

Suggestion:

- Plot the "*T_CSTR*" variable for the first 3600 seconds.
- Change heating water inlet flowrate and observe the (T) conversion effect.
- "Play" with heat connections, heat transfer "U" and heat transfer area "A" parameters and observe the (T) conversion effects.

Appendix 1

1. Model new-parameters values

Symbol	Description	Model Object	Value	Units
T_{in}	**Inlet temperature**	CSTR In. Conn.	60	[C]
Xn[CH2O2]	**Molar fraction**	CSTR In. Conn.	33	[%]
Xn[MeOH]	**Molar fraction**	CSTR In. Conn.	67	[%]
Fn(water)	**Molar flow**	Jacket. In. Conn.	50	[mol/s]
Xn[H2O]	**Molar fraction**	Jacket In. Conn.	100	[%]
T_{in}	**Inlet temperature**	Jacket In. Conn.	15	[C]
Cpm	**Mass metal h.c.**	Wall(s) System	800	[J/kg/K]
m	**Metal mass**	Wall(s) System	1000	[kg]
A	**Jacket cross-section a.**	Jacket System	0.78	[m^2]
P	**Pressure**	Jacket/CSTR sys. & In. Conn.	1.0/9.0	[bar]
rho_{H2O}	**Molar density**	"spec." param.	55.5E3	[mol/ m^3]
$T_{ambient}$	**Ambient temperature**	global	20	[C]
U	**Overall heat tr. c.**	Heat Conn.	1E3/1E3/1E3/5	[W/m^2/K]
A	**Heat transfer area**	Heat Conn.	10	[m^2]

Table 4 CSTR model parameters

2. Reaction new-parameters values

Symbol	Description	Model Object	Value	Units
k1	**Reaction rate const.**	CSTR/Reactions	1.90E9	mol/s/m^3
k2	**Reaction rate const.**	CSTR/Reactions	1.16E8	mol/s/m^3
Ea1	**Activation energy**	CSTR/Reactions	48600	J/mol
Ea2	**Activation energy**	CSTR/Reactions	56600	J/mol

Table 5 New kinetics parameters