Tutorial: Reactor and Manipulator Blocks

Question:

Ethyl acetate is produced in an esterification reaction between acetic acid and ethyl alcohol.

Acetic acid + Ethyl alcohol ↔Ethyl acetate + Water

The feed mixture, consisting of 52.5 mole% acetic acid, 45 mole% ethyl alcohol and 2.5 mole% water, enters the reactor model with a flow rate of 400 kmol/hr at 75℃ and 1.1 atm. The reactor operates at 70℃ and 1 atm. Both the reactions are first-order with respect to each of the reactants (i.e., overall second-order). For these liquid-phase reactions, the kinetic data for the Arrhenius law are given below:

Forward reaction: $\boldsymbol{k = 2.0 \times 10^{8} \frac{m^3}{kmol.s}}$ $\boldsymbol{E = 6.0 \times 10^{7}\ J/kmol}$

Reverse reaction: k = $\boldsymbol{5.0 \times 10^{7} \frac{m^3}{kmol.s}}$ **E= 6.0×10^{7} J/kmol**

[Ci] basis = Molarity

1. Perform the Aspen Plus simulation using the *NRTL thermodynamic model* for:

a) RCSTR reactor block with reactor volume of 0.15 m^3

b) RGibbs reactor block

c) RPlug reactor block with length of 2 m and diameter of 0.3 m

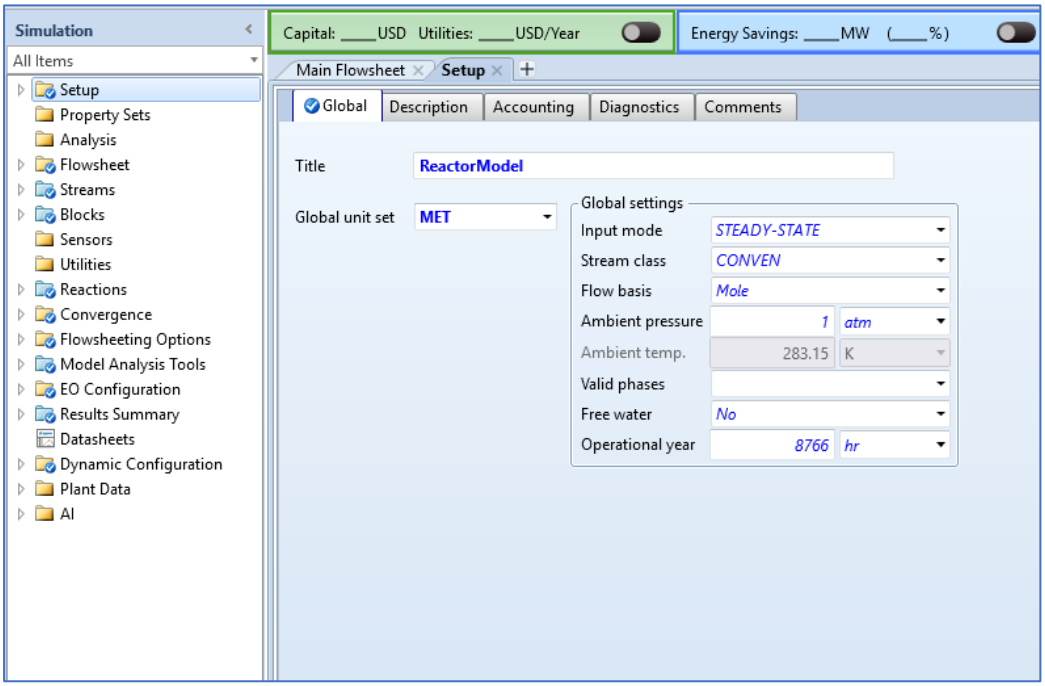
2. Which reactor types produces the most and the least amount of ethyl acetate?

3. What is the net heat duty required for RCSTR reactor block GJ/hr?

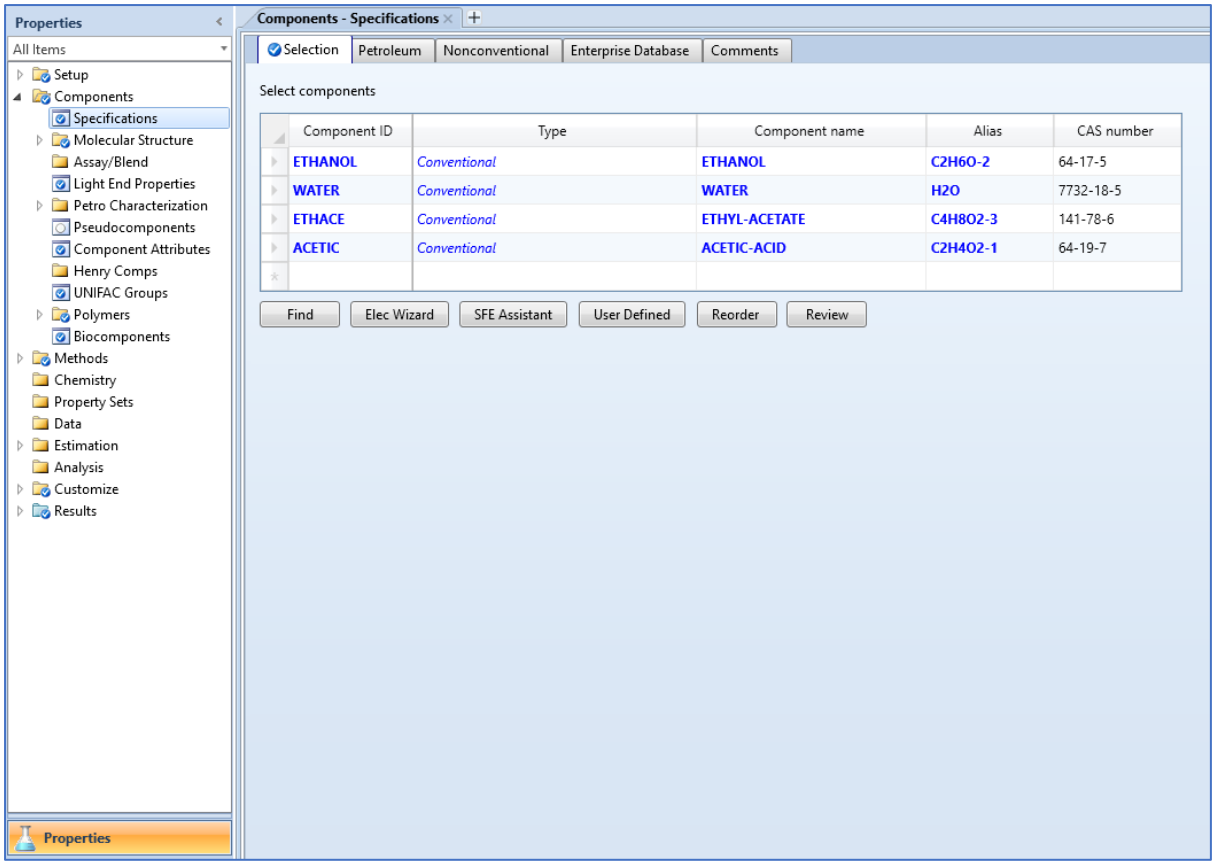
4. Plot the effect of CSTR temperature on the product component molar flows (Sensitivity Analysis).

Solution:

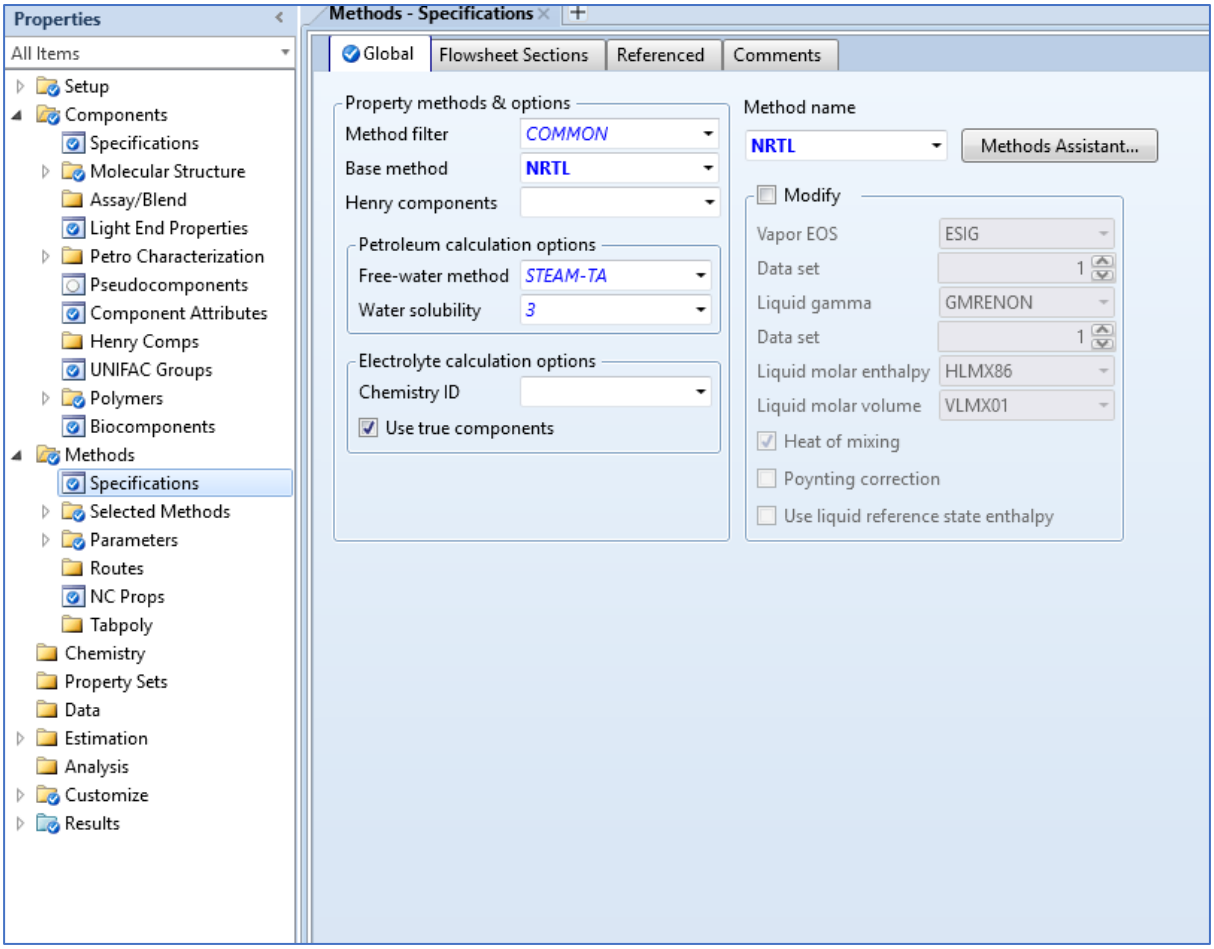
1. Start a Blank Simulation on Aspen Plus. Set the Specifications as in the image.



2. In the *Properties* environment of the *Navigation Pane*, enter the Component Specifications.


Properties
All Items
Setup
Components
Specifications
Molecular Structure
Assay/Blend
Light End Properties
Petro Characterization
Pseudocomponents
Component Attributes
Henry Comps
UNIFAC Groups
Polymers
Biocomponents
Methods
Chemistry
Property Sets
Data
Estimation
Analysis
Customize
Results
Properties
Components - Specifications
Selection
Petroleum
Nonconventional
Enterprise Database
Comments
Select components
Component ID
Type
Component name
Alias
CAS number
ETHANOL
Conventional
ETHANOL
C2H6O-2
64-17-5
WATER
Conventional
WATER
H2O
7732-18-5
ETHACE
Conventional
ETHYL-ACETATE
C4H8O2-3
141-78-6
ACETIC
Conventional
ACETIC-ACID
C2H4O2-1
64-19-7
Find
Elec Wizard
SFE Assistant
User Defined
Reorder
Review

3. In the *Methods Specifications* tab select the Thermodynamic Property Model as mentioned in the question.

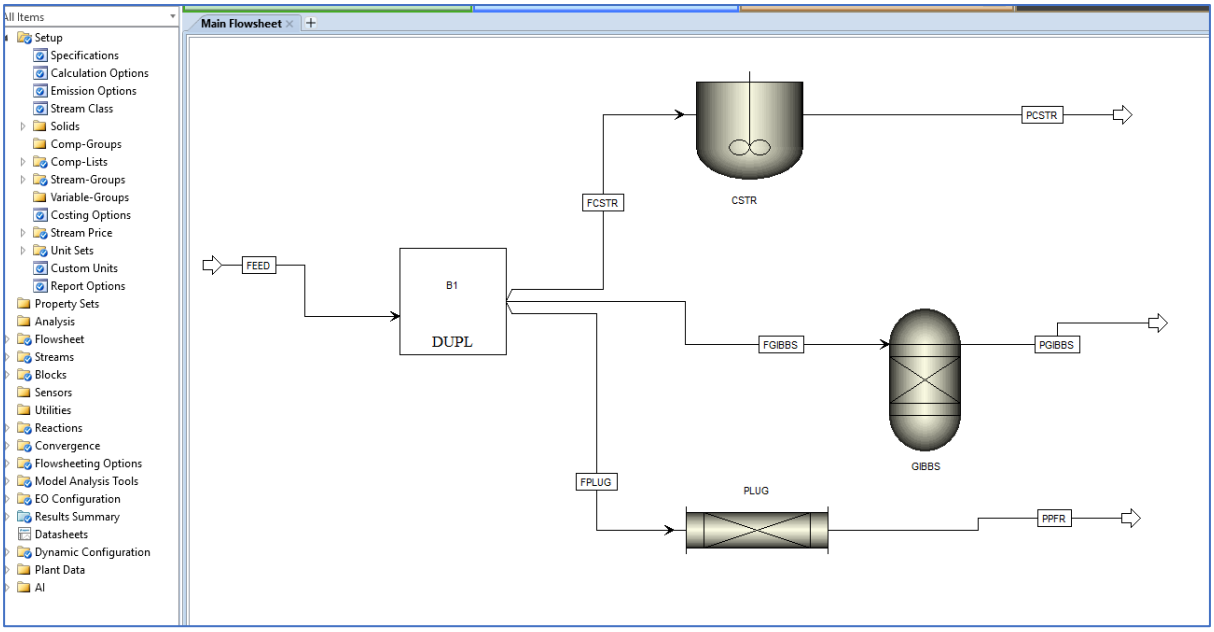


4. Click Next and run the property analysis/setup and the Control Panel should open up without any error log.
5. Now, move to the *Simulation Environment* of the Navigation Pane and set up the flowsheet using Reactor and Manipulator Blocks on the Model Palette.

   In Aspen Plus, the DUPL block, a manipulator block, is used to duplicate a stream, creating two identical streams from a single input stream. It's a tool for creating multiple paths for a stream in a flowsheet, without altering the original stream's properties.

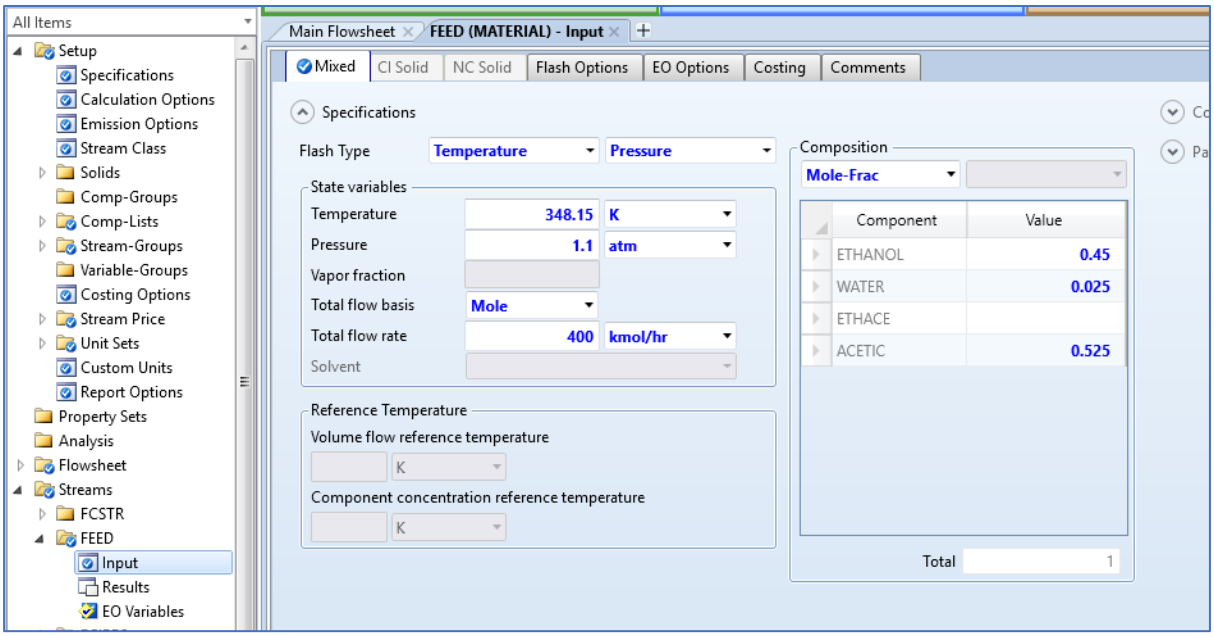
   There are many built-in reactor models, RSTOIC, RYIELD, REQUIL, RGIBBS, RPLUG, RCSTR and RBATCH, in Aspen Plus. RGIBBS block models chemical equilibrium by minimizing Gibbs free energy, while the PFR (Plug Flow Reactor) block, RPLUG, simulates a plug flow reactor, which is

a type of continuous reactor. RCSTR models a continuous stirred tank reactor (CSTR).

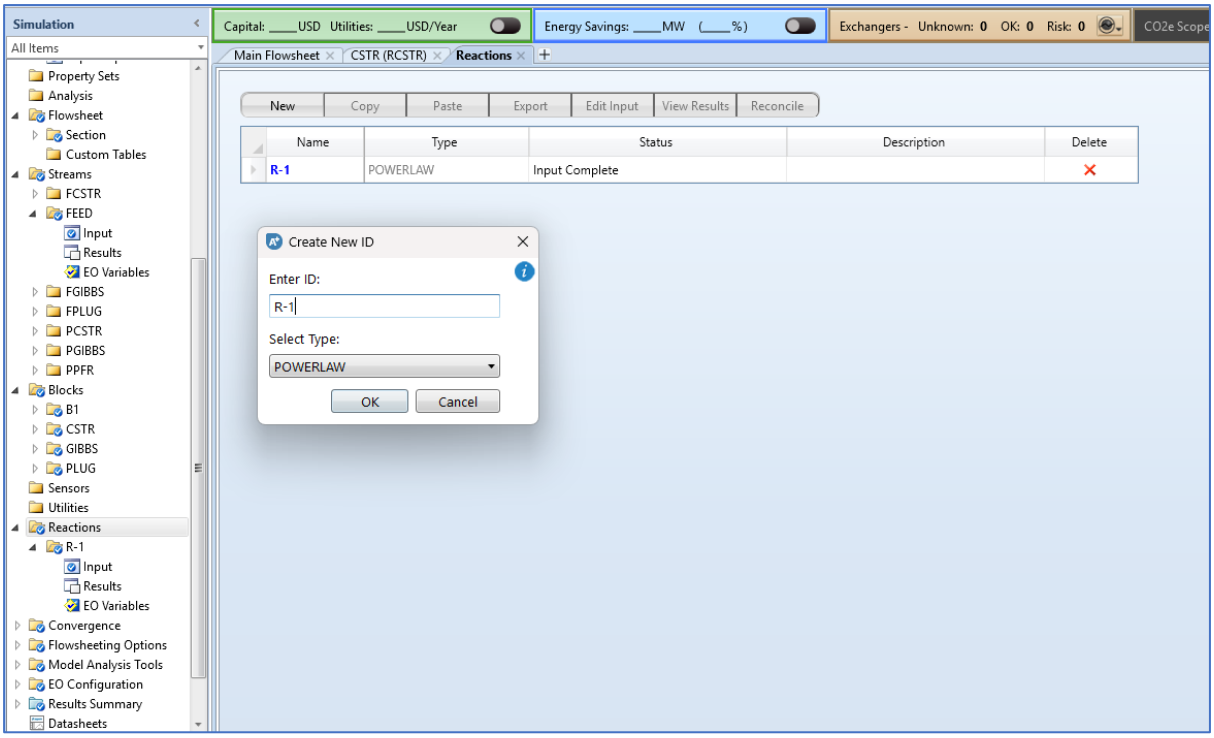


Name the streams as shown in the figure. Since a comparative study among these three reactors are being conducted, the DUPL block is used.

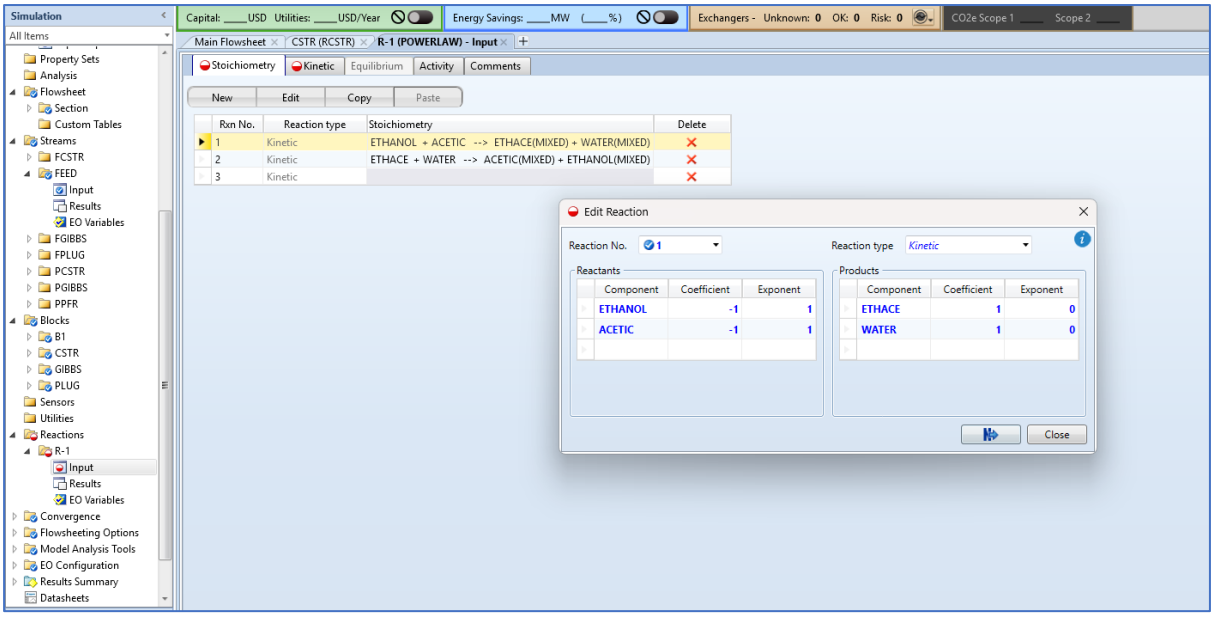
6. Click Next and add the details for Feed stream in the input tab for the stream as given in the question.



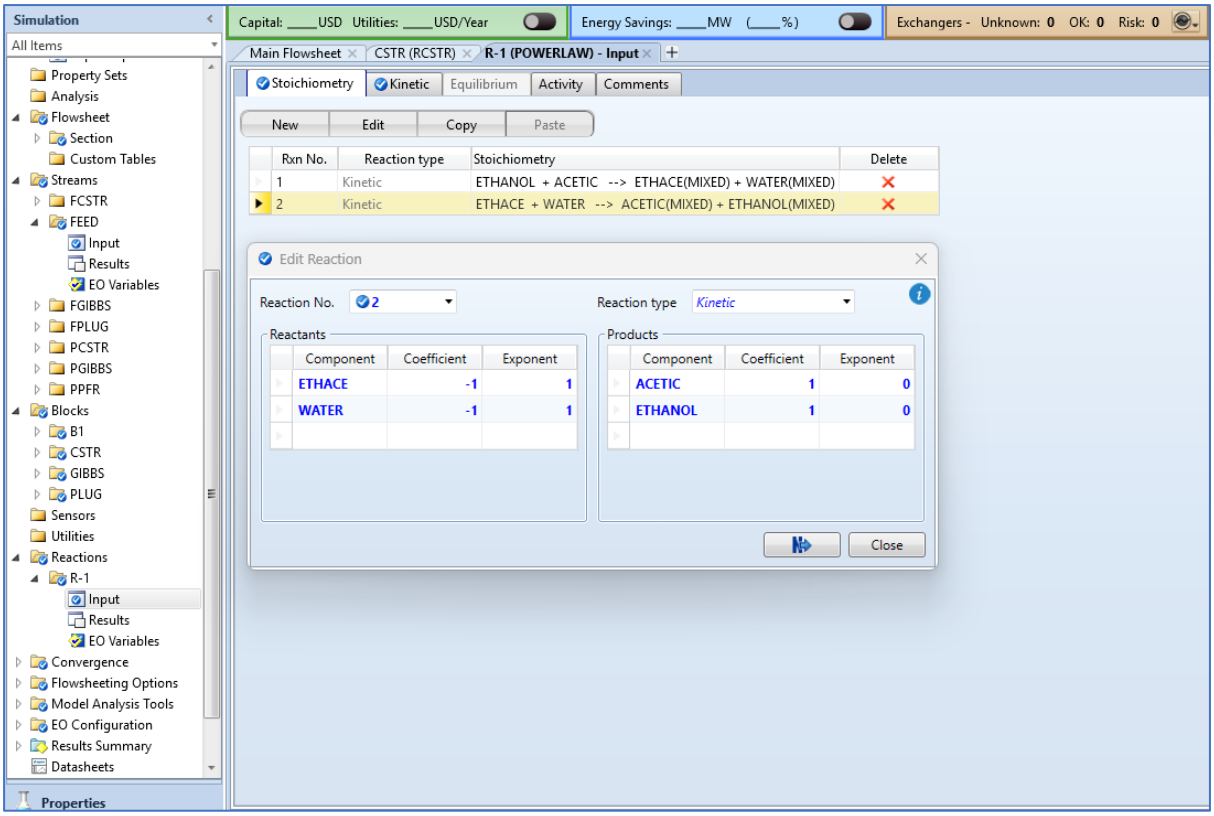
7. In the *Reactions* tab of the *Simulation Environment*, add the reaction mentioned in question. Click *New* reaction and specify *POWERLAW* type.



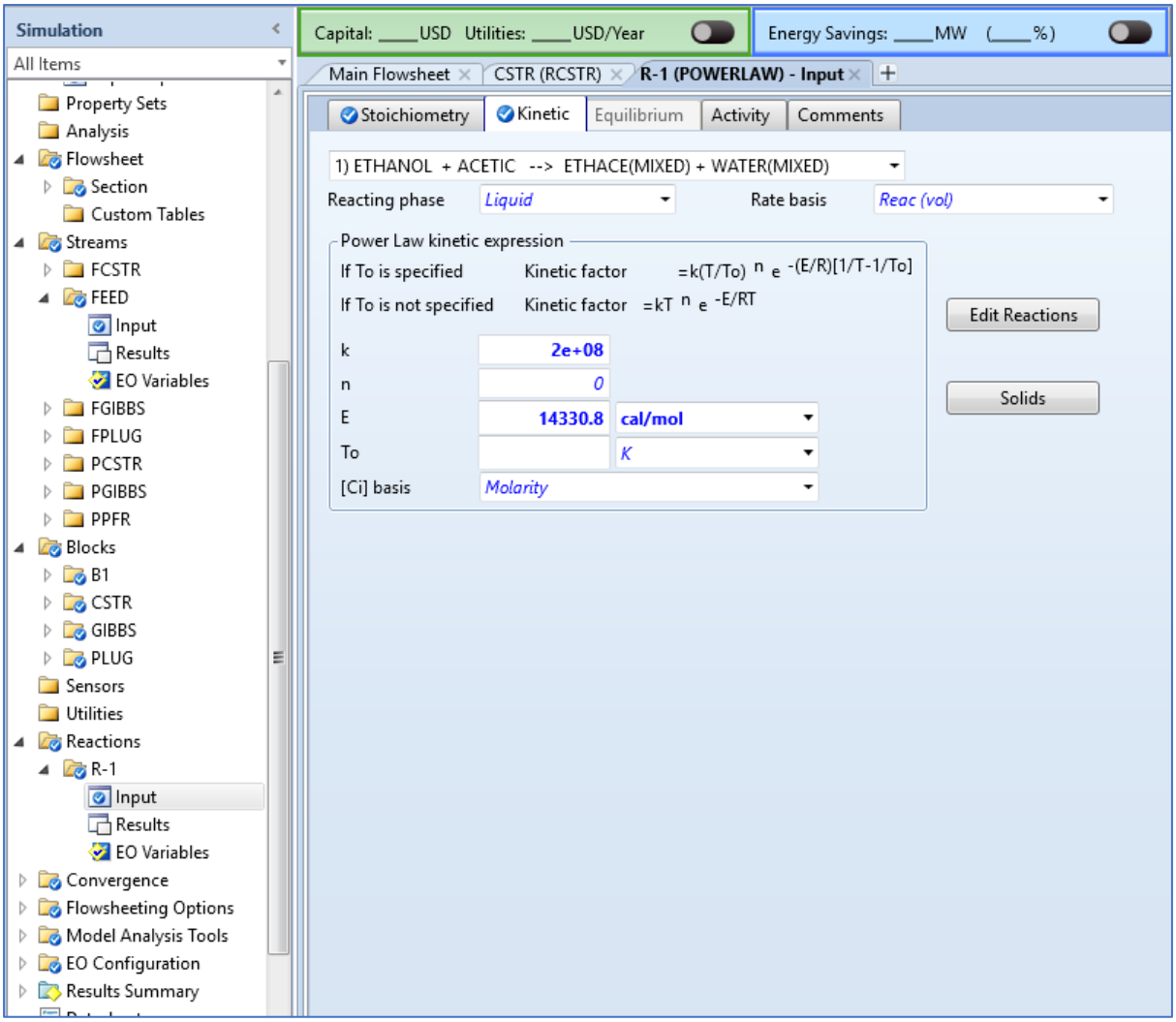
8. Edit a *New* reaction under the Stoichiometry input tab of R-1 interface. First enter details of only the forward reaction as shown in the image. For the reactant side, coefficient bears a negative sign while on the product sign the coefficient bears a positive sign. The exponents for reactants have the value 1 and the exponents of products have the value 0.

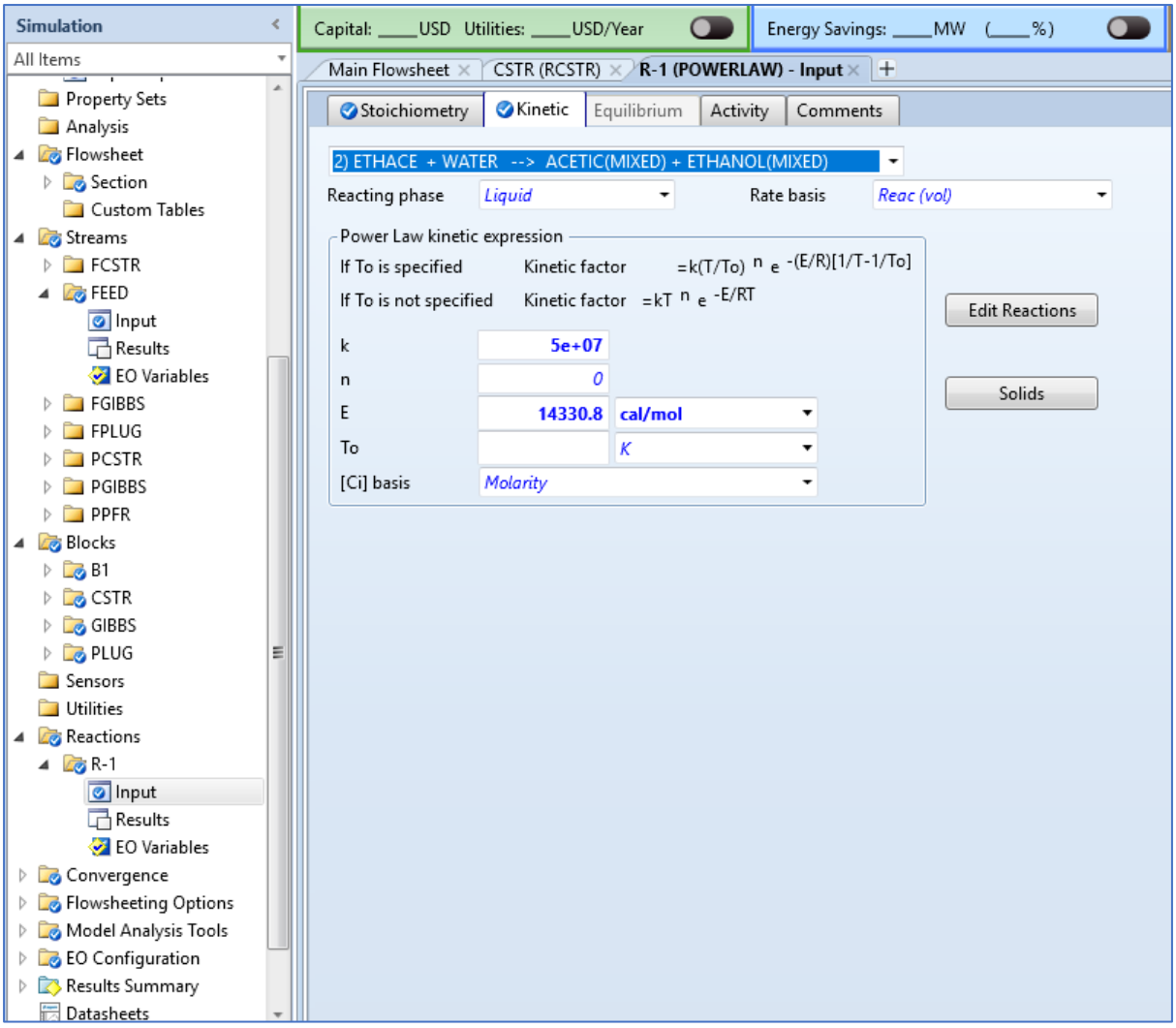


In similar fashion, enter the details of the backward reaction as well.

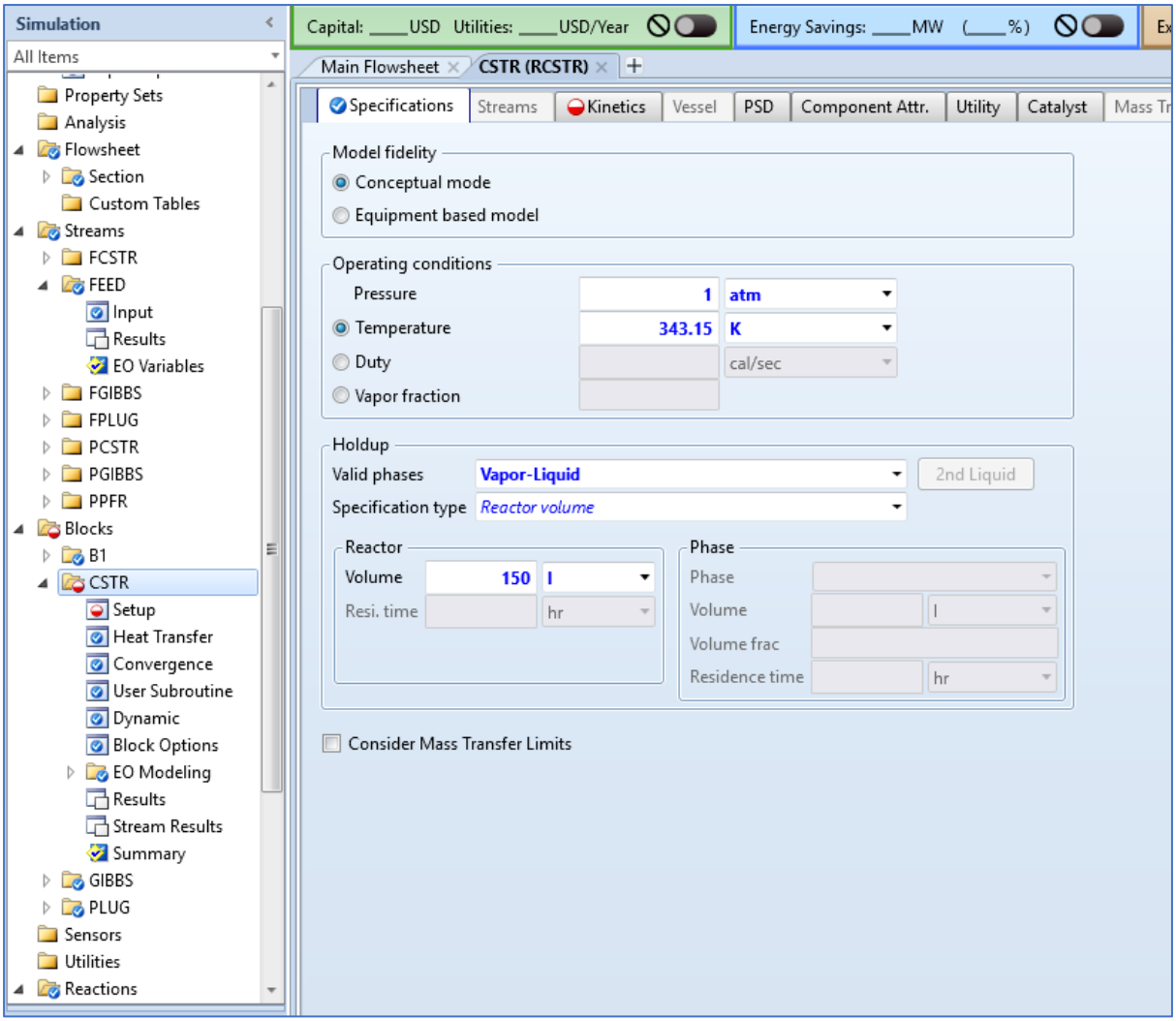


9. Set the *Kinetics* information in the R-1 input interface. Select the appropriate reactions (forward and backward) and then enter the information following power law expression. Ensure that the reaction phase is liquid.

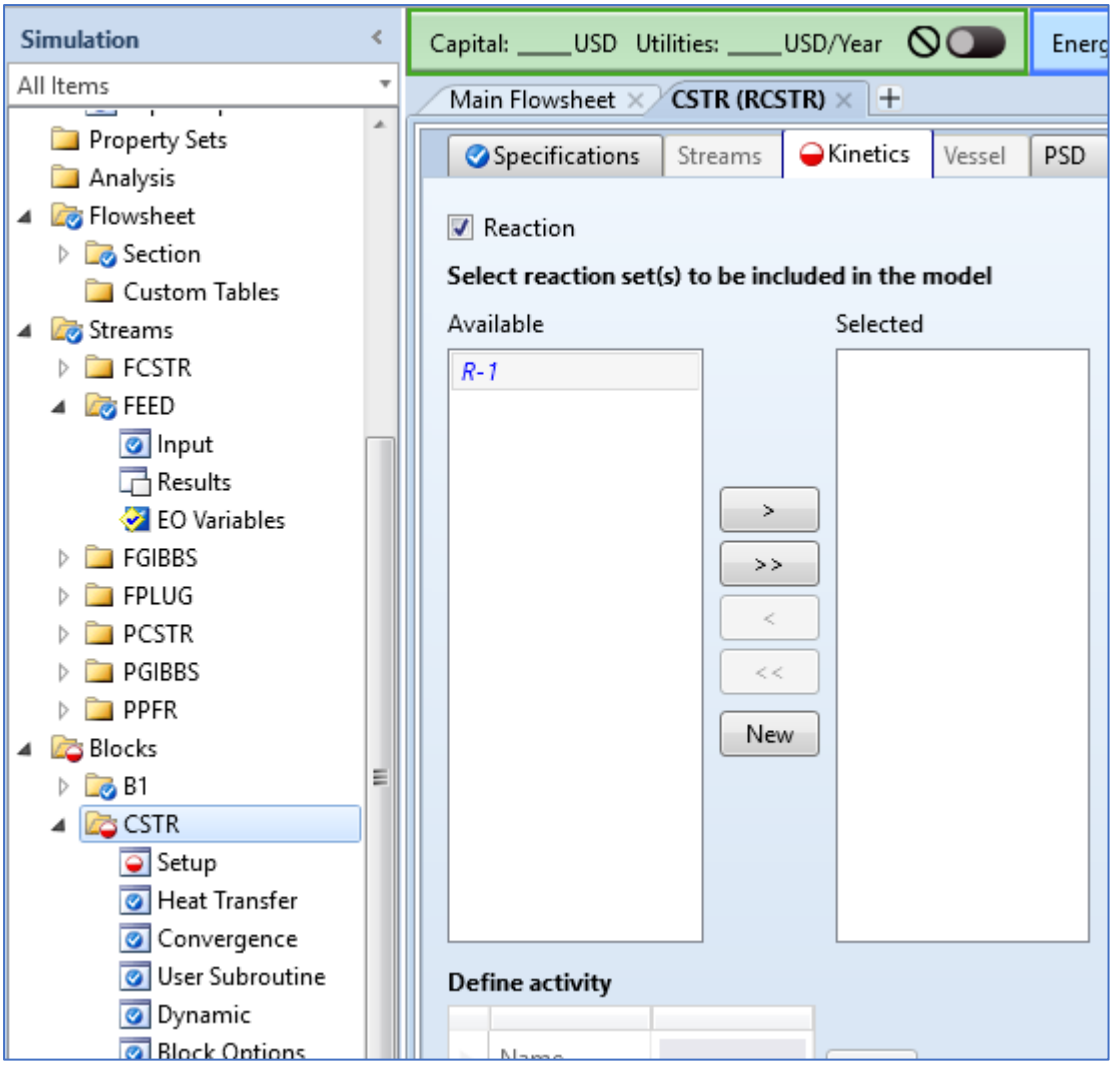

Simulation
All Items
Property Sets
Analysis
Flowsheet
Section
Custom Tables
Streams
FCSTR
FEED
Input
Results
EO Variables
FGIBBS
FPLUG
PCSTR
PGIBBS
PPFR
Blocks
B1
CSTR
GIBBS
PLUG
Sensors
Utilities
Reactions
R-1
Input
Results
EO Variables
Convergence
Flowsheeting Options
Model Analysis Tools
EO Configuration
Results Summary
Capital: ____USD Utilities: ____USD/Year
Energy Savings: ____MW (____%)
Main Flowsheet
CSTR (RCSTR)
R-1 (POWERLAW) - Input
Stoichiometry
Kinetic
Equilibrium
Activity
Comments
1) ETHANOL + ACETIC --> ETHACE(MIXED) + WATER(MIXED)
Reacting phase
Liquid
Rate basis
Reac (vol)
Power Law kinetic expression
If To is specified
Kinetic factor =k(T/To) n e -(E/R)[1/T-1/To]
If To is not specified
Kinetic factor =kT n e -E/RT
k
2e+08
n
0
E
14330.8
cal/mol
To
K
[Ci] basis
Molarity
Edit Reactions
Solids



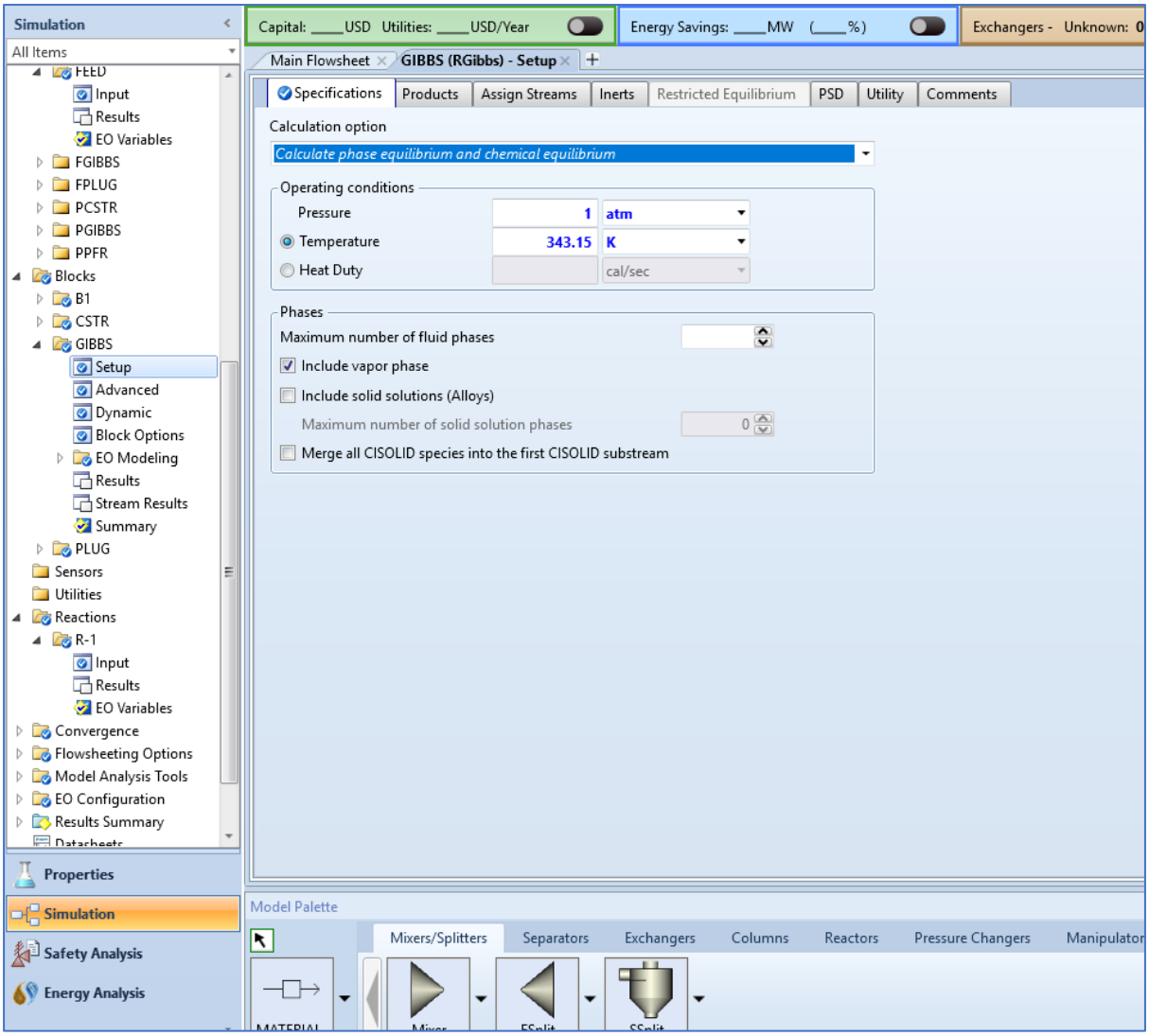
10. Now move to the CSTR block tab. First enter the specifications as mentioned in the question.



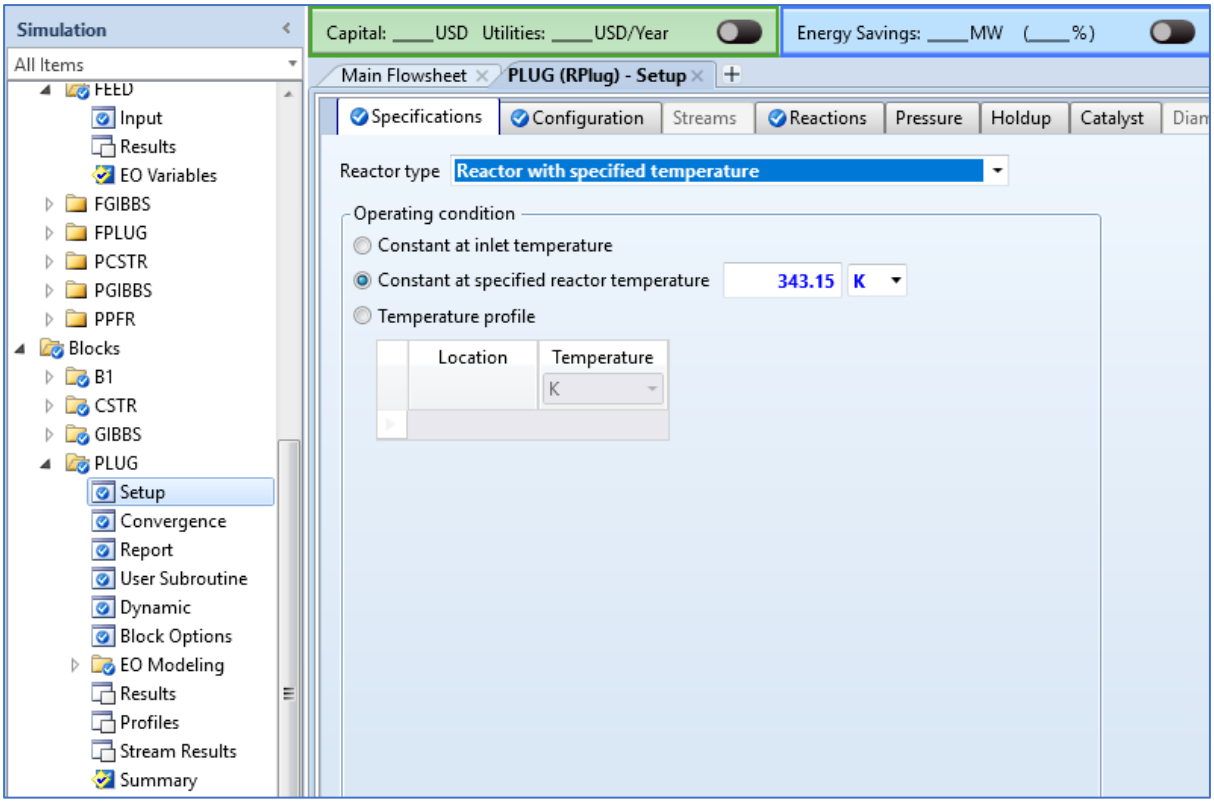
Then move to the *Kinetics* tab and select Reaction check-box. Then move the Available Reaction R-1 to the Selected Reaction box.



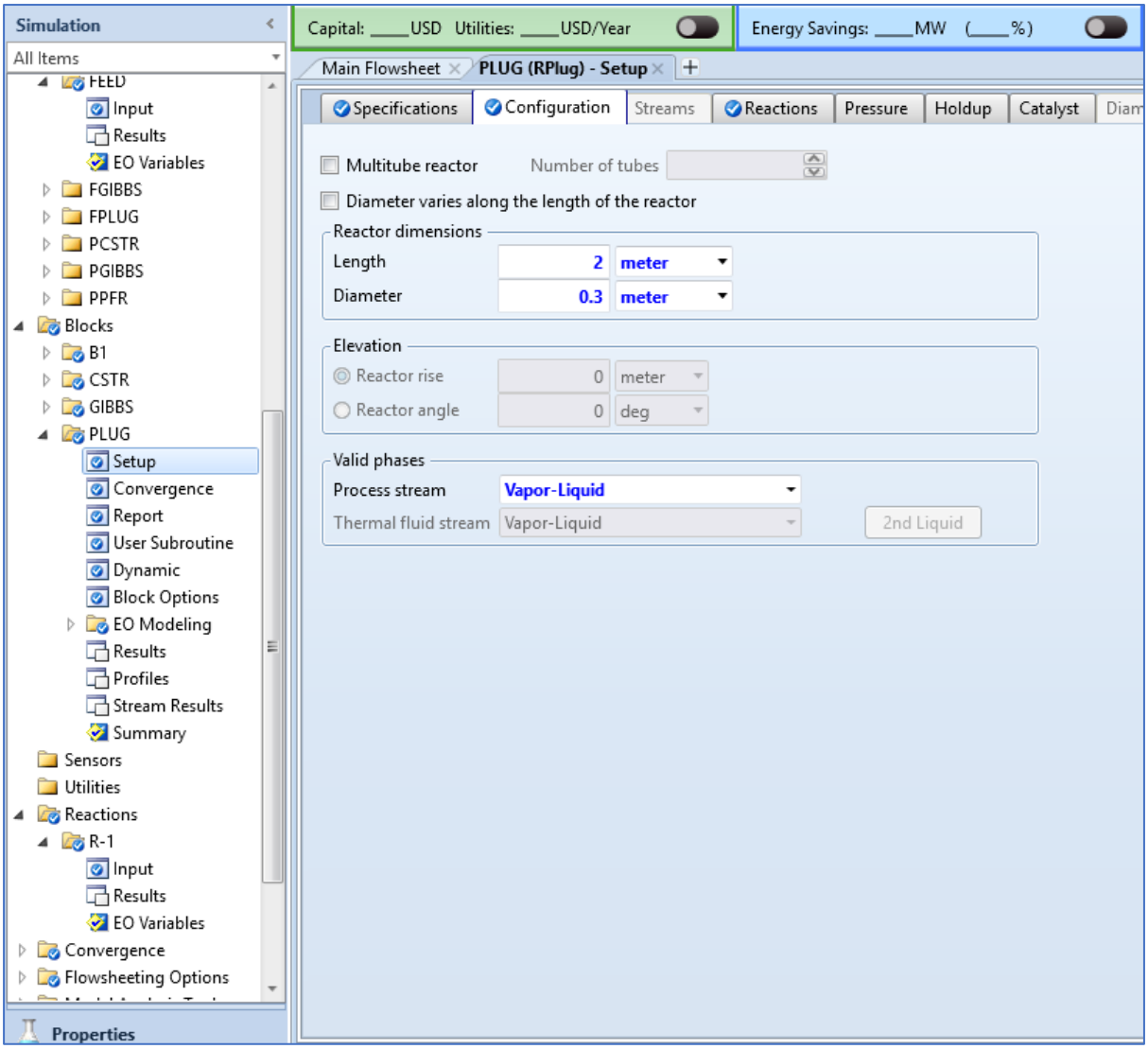
11. Move to the GIBBS block tab. Enter the specification to *Calculate phase equilibrium and chemical equilibrium* with the details given in question.



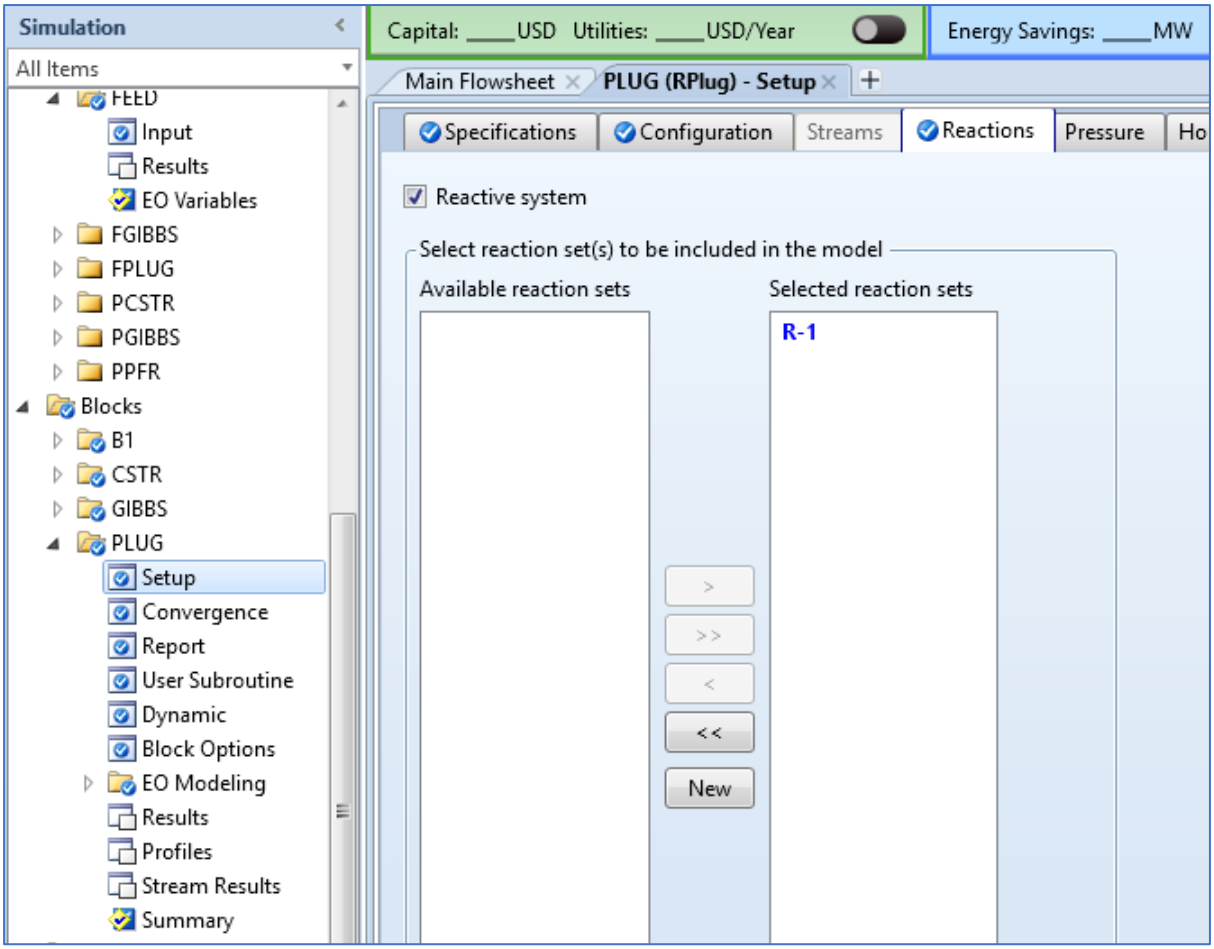
12. Proceed to PFR block and enter the Specifications input as *Reactor with Specified Temperature*



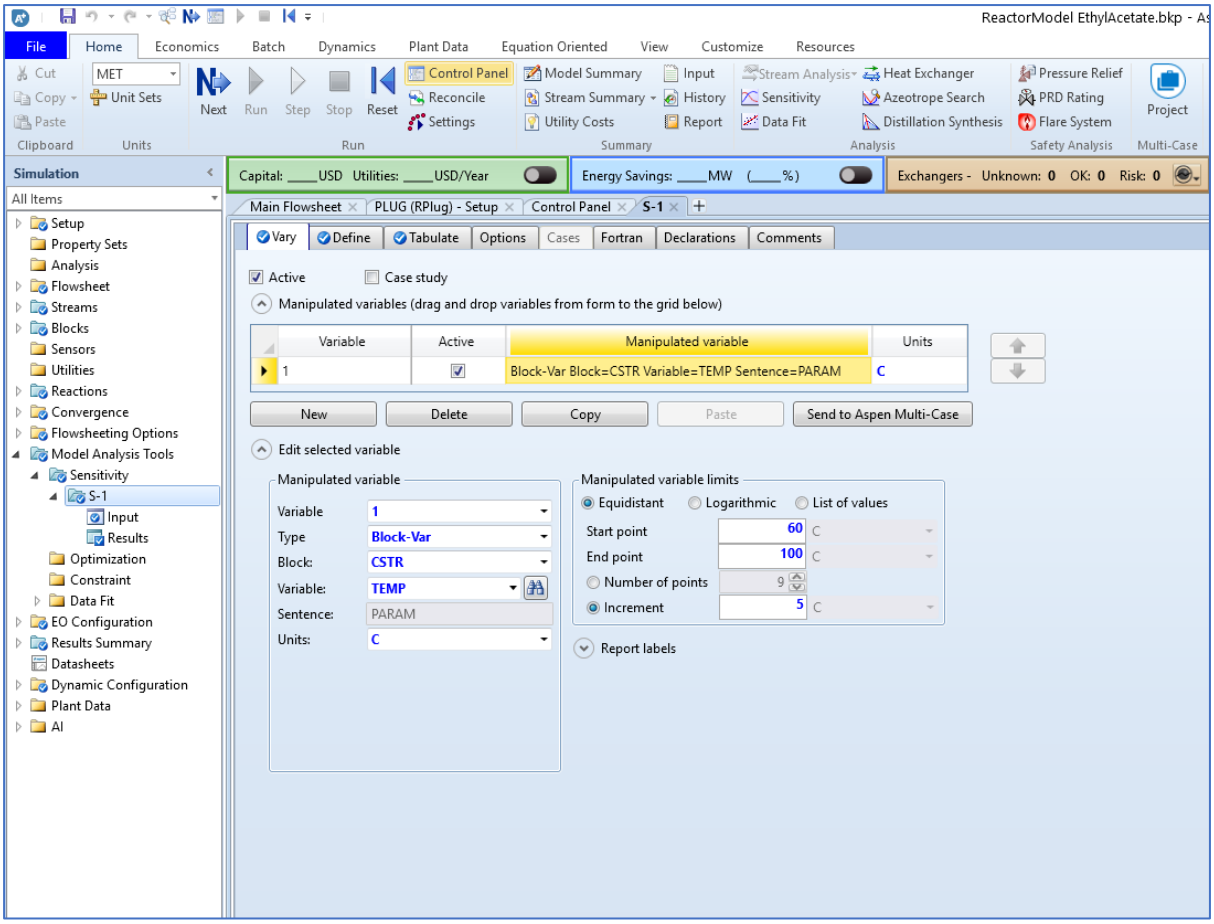
Click on *Configurations* tab and input the reactor configuration as mentioned in the question.



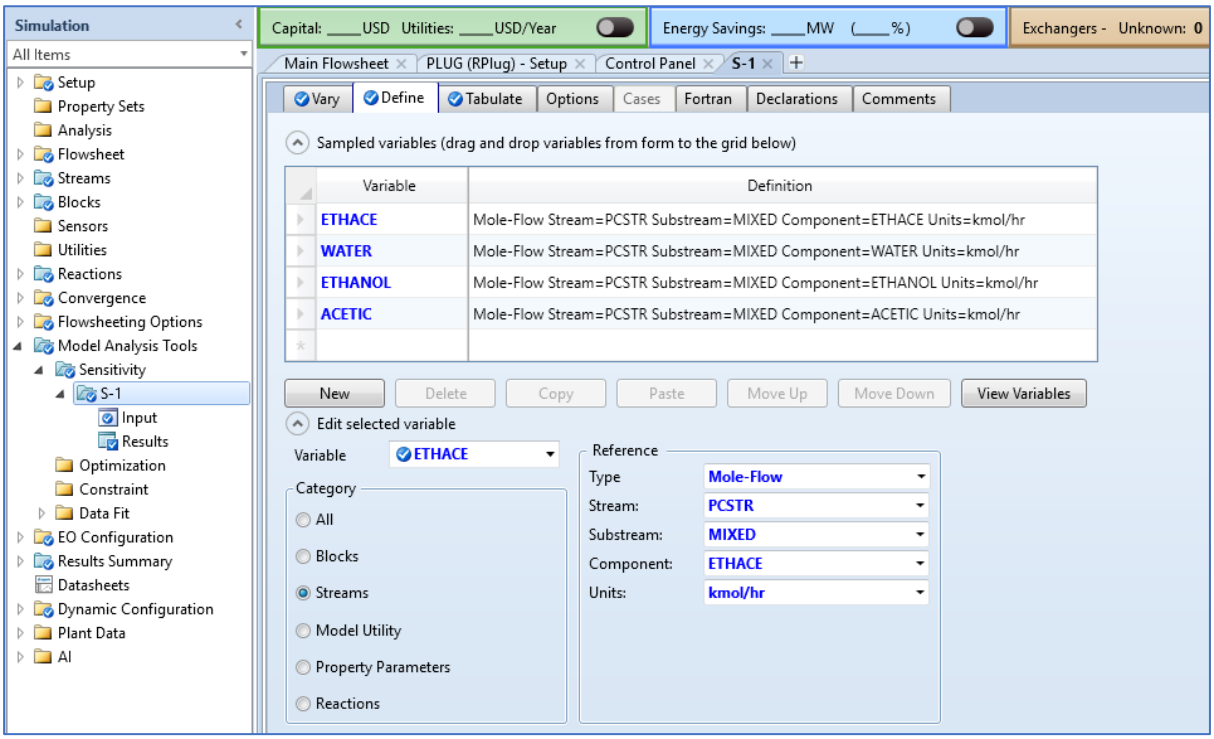
In the *Reactions* tab, check the *Reactive System* checkbox and move the Available Reaction R-1 to the Selected Reaction set.



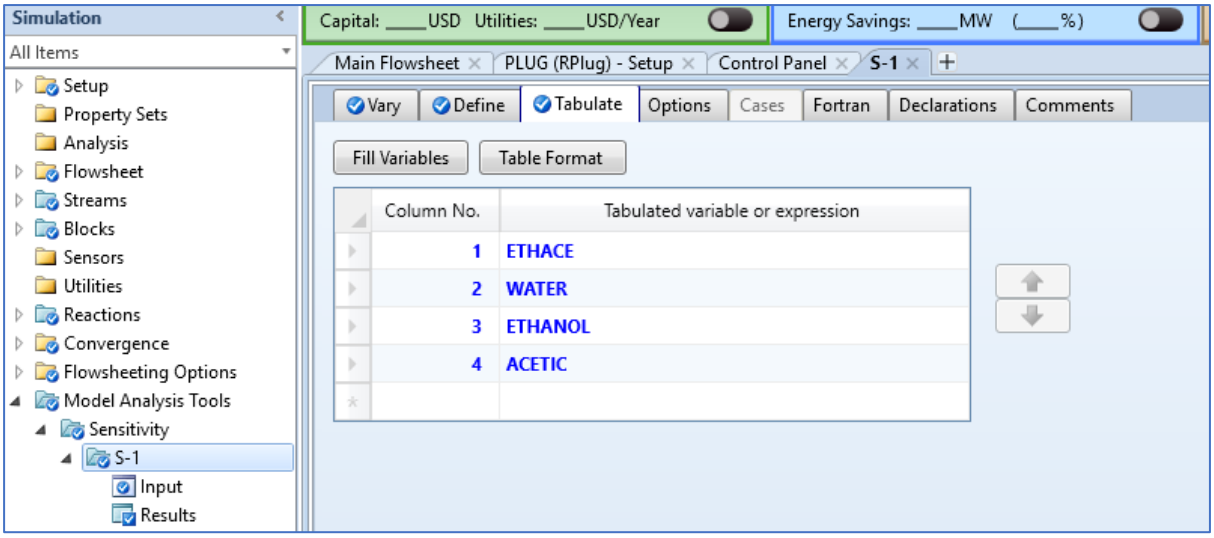
13. Run the simulation. The Control Panel should appear without any error logs. From *Results* tab note the reactor type that produces the maximum amount of Ethyl Acetate in the product stream.
14. In the *Simulation Environment*, on the CSTR block tab, under EO Modelling note the results for the CSTR block. Note the Net Heat Duty value.
15. Under *Model Analysis Tools*, go to Sensitivity and start a new analysis S-1. Enter the variable details as shown.



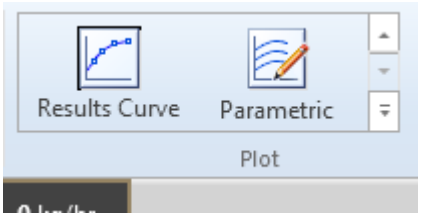
In the *Define* interface, input the CSTR product stream component variables as follows:



In the *Tabulate* interface, fill the variables in the table.



16. Re-run the simulations. The Control Panel should open up without any error logs. Check the Results for S-1 analysis.
17. On the *Home* Ribbon, go to the Plot Option and generate Results Curve.



18. You may also calculate the conversion for desired product by finding the initial and final component concentrations based on your knowledge of Reaction Engineering.