Esterification in CSTRs in Series with Aspen Plus® V8.0

1. Lesson Objectives

- Use Aspen Plus to determine whether a given reaction is technically feasible using three continuous stirred tank reactors in series.

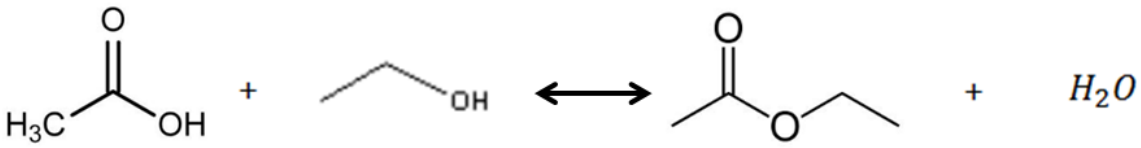
2. Prerequisites

- Aspen Plus V8.0
- Basic knowledge of reaction rate laws

3. Background

Consider the reversible liquid phase esterification of acetic acid shown below.

Homogeneous Reaction:



Acetic acid + ethanol ⟷ ethyl acetate + water

Reaction Kinetics:

Forward Reaction $k_f = 8\ x\ 10^{-6}\ m^3 kmol^{-1} s^{-1}$

Reverse Reaction $k_r = 2.7\ x\ 10^{-6}\ m^3 kmol^{-1} s^{-1}$

The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

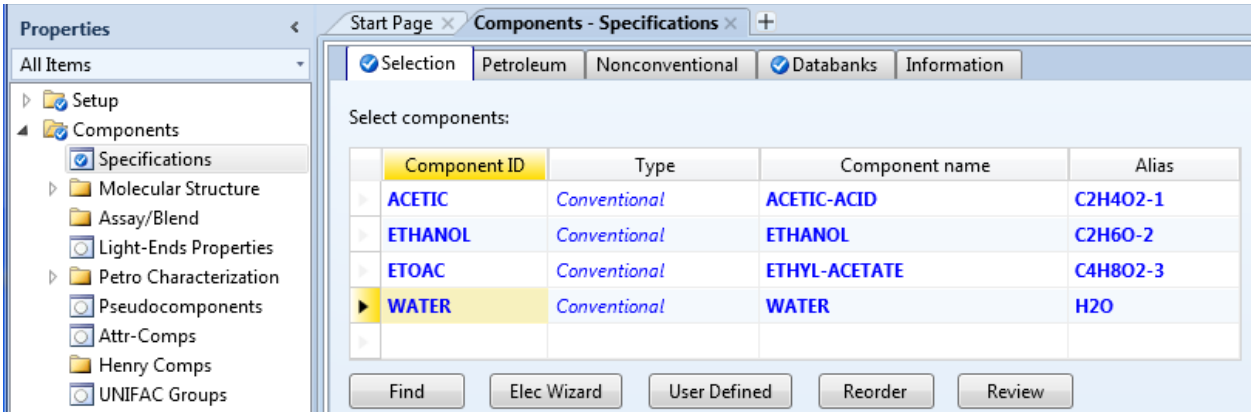
4. Problem Statement and Aspen Plus Solution

It is desired to produce 9,000 kg/day of ethyl acetate product from a feed stream consisting of 13 mole % acetic acid, 35 mole % ethanol, and 52 mole % water. This feed stream is available at 100,000 kg/day. Three 2,600 L

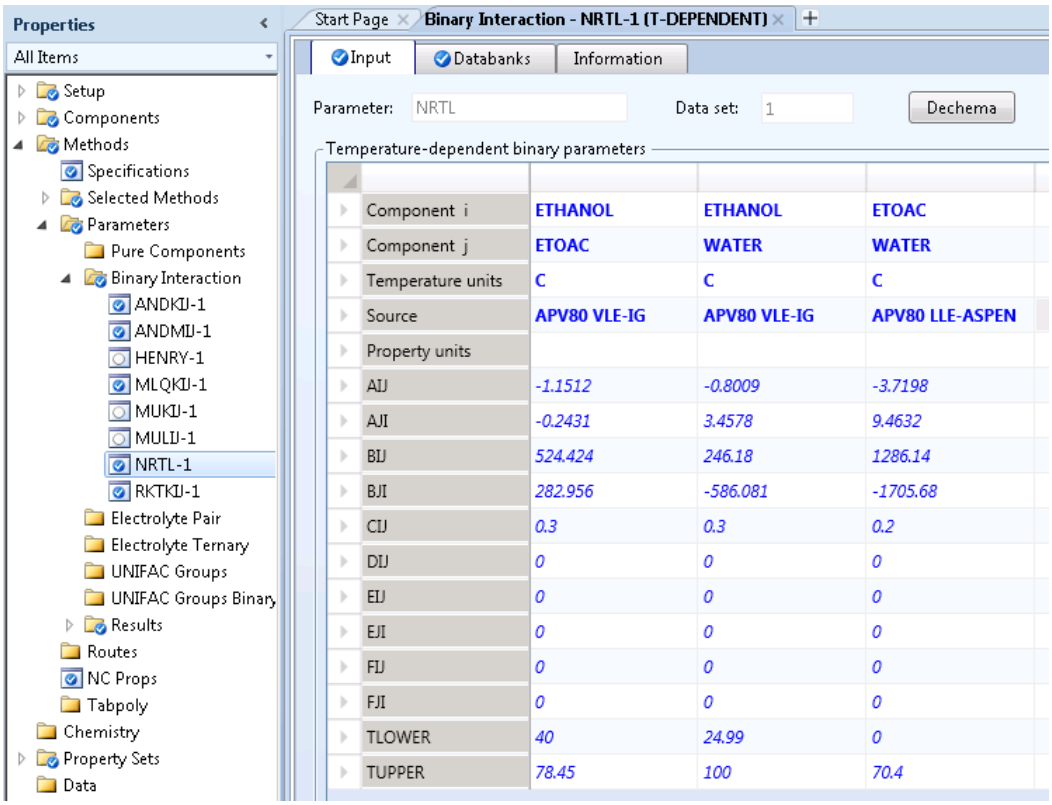
CSTRs are available to use for this process. Determine if it is possible to achieve the desired production rate of ethyl acetate by operating these three reactors in series.

4.01. Start **Aspen Plus V8.0**. Select **New | Chemical Processes | Chemicals with Metric Units**. Click **Create**.

4.02. Define Components. On the navigation pane go to **Components | Specifications**. This form should open by default after starting a new file. Use the **Find** button to select acetic acid, ethanol, ethyl acetate, and water. You may rename the **Component ID's** if you wish.

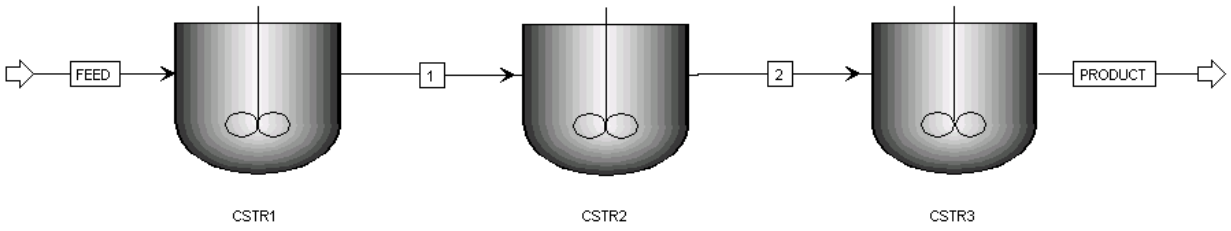


4.03. Populate the binary interaction parameters by going to **Methods | Parameters | Binary Interaction | NRTL-1**.

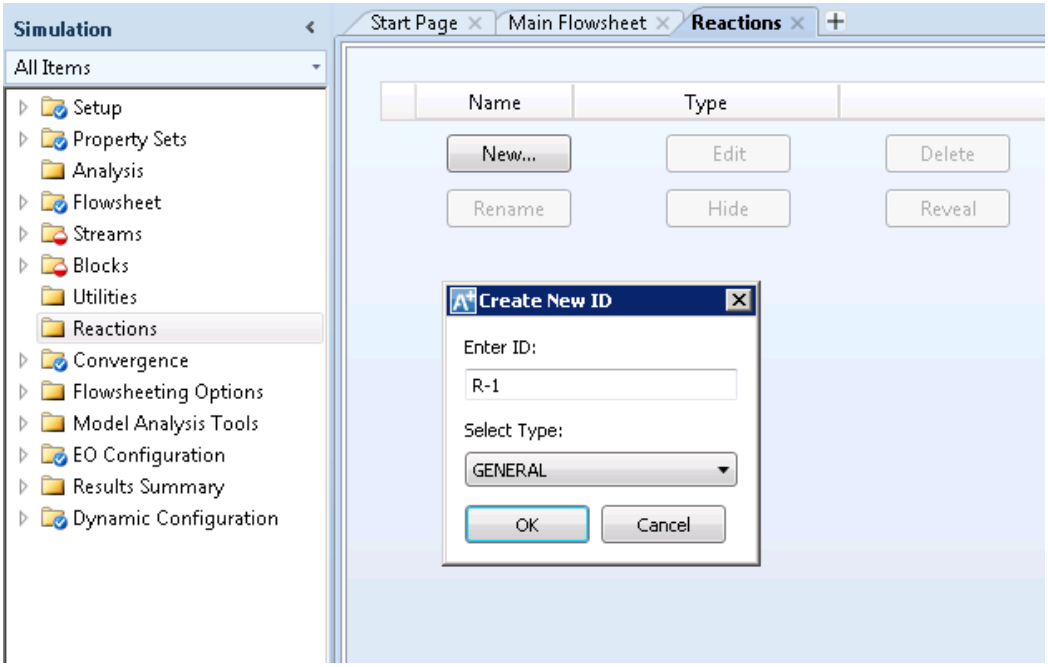


4.04. Create flowsheet. Move to the Simulation environment by clicking the Simulation button in the bottom left corner of the screen.

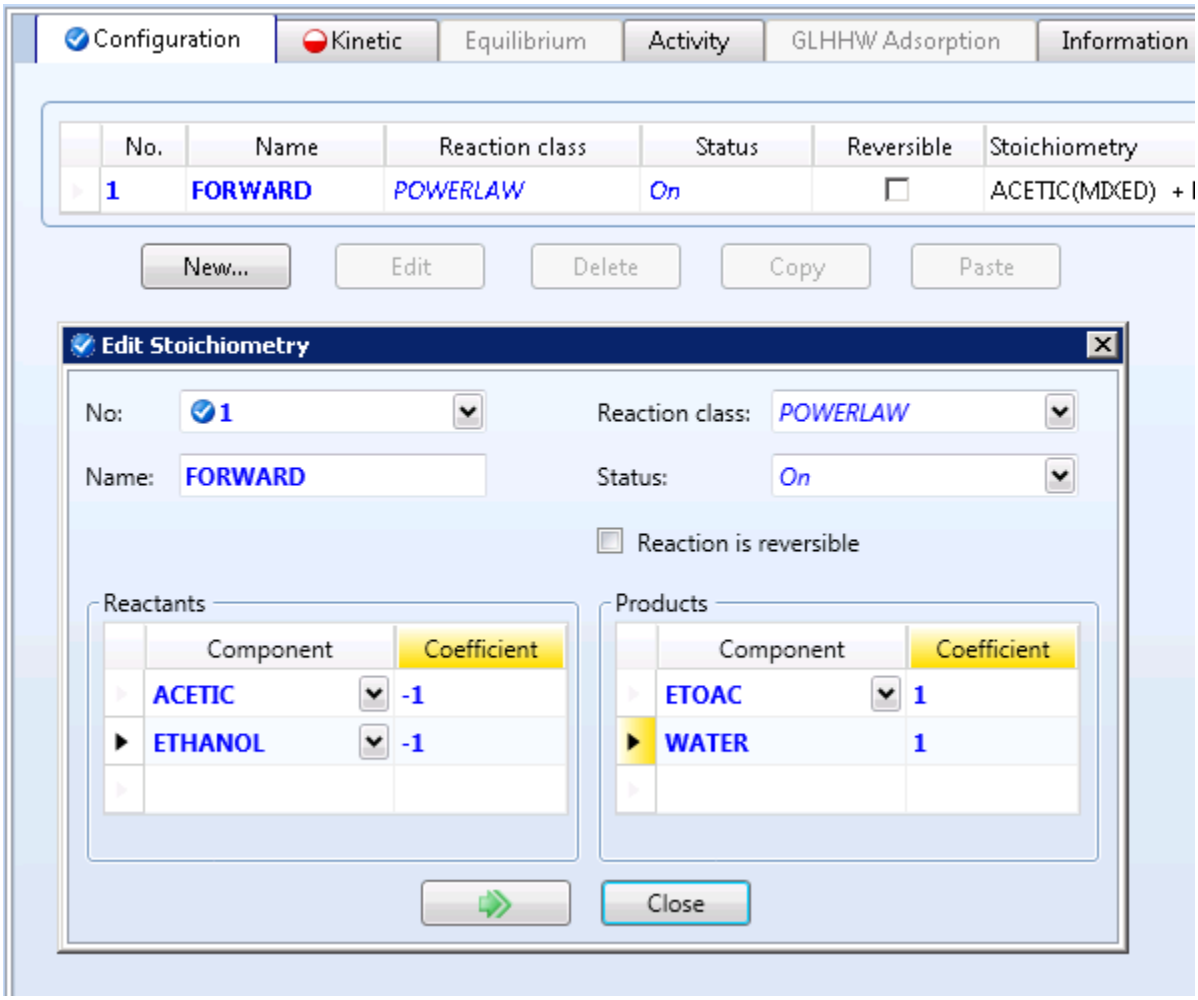
4.05. Place three **RCSTR** blocks onto the flowsheet from the **Reactors** tab in the **Model Palette**. The RCSTR block models a continuously stirred tank reactor with user-provided stoichiometry and kinetics. Connect the required ports with material streams.



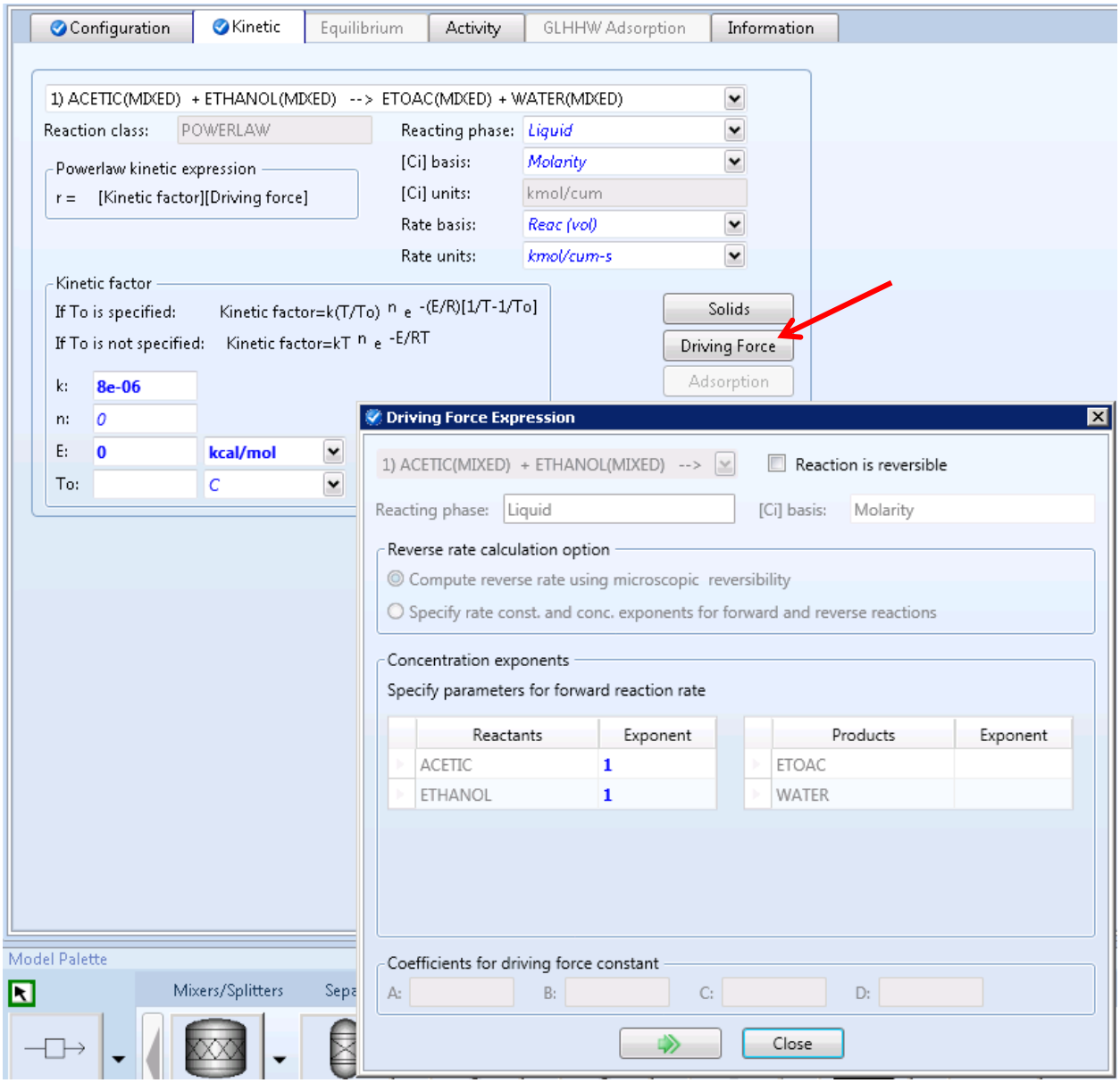
4.06. Define Reactions. On the navigation pane go to **Reactions** and click **New**. A default reaction ID **R-1** will be created, select **GENERAL** for type.



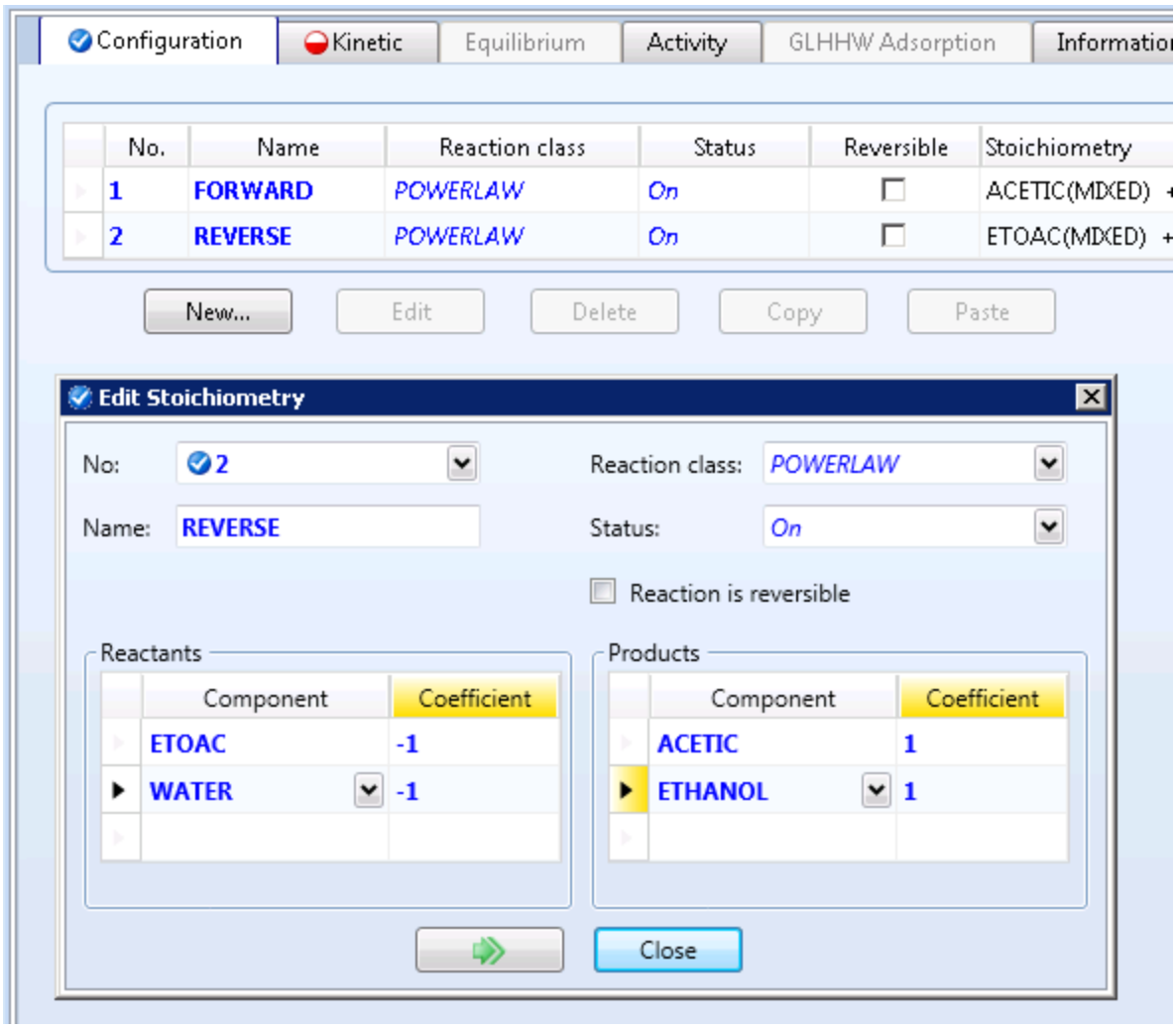
4.07. Once **R-1** is created, specify the reaction by clicking **New** in the **R-1 | Configuration** tab. For reversible reactions it is often useful to enter the forward and reverse reactions as separate reactions within the same reaction group. Start with the forward reaction. Name the reaction, select reactants and products, and enter the stoichiometric coefficients.



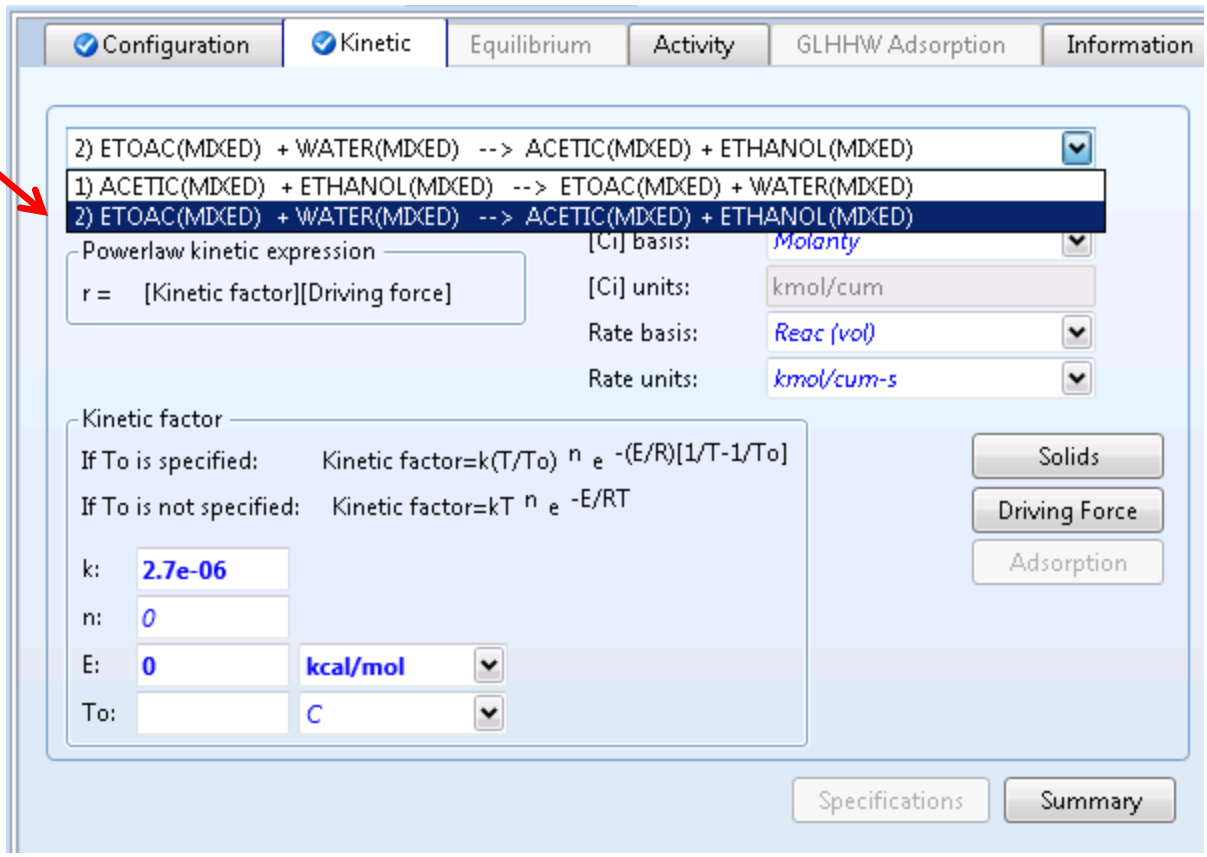
4.08. Click on the **Kinetic** tab and enter **k = 8e-06** and **E = 0**. Click on **Driving Force** and enter **1** for the reactant concentration exponents.



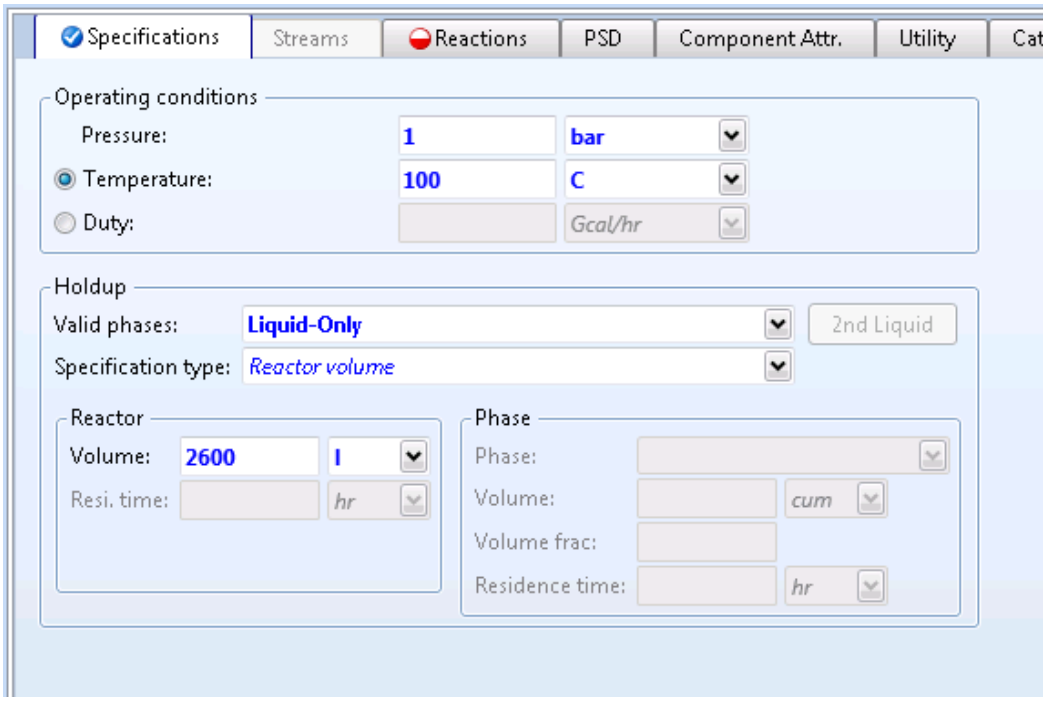
4.09. For the reverse reaction, click **Reactions | R-1 | Configuration | New**. Name the reaction, select reactants and products, and enter the stoichiometric coefficient.



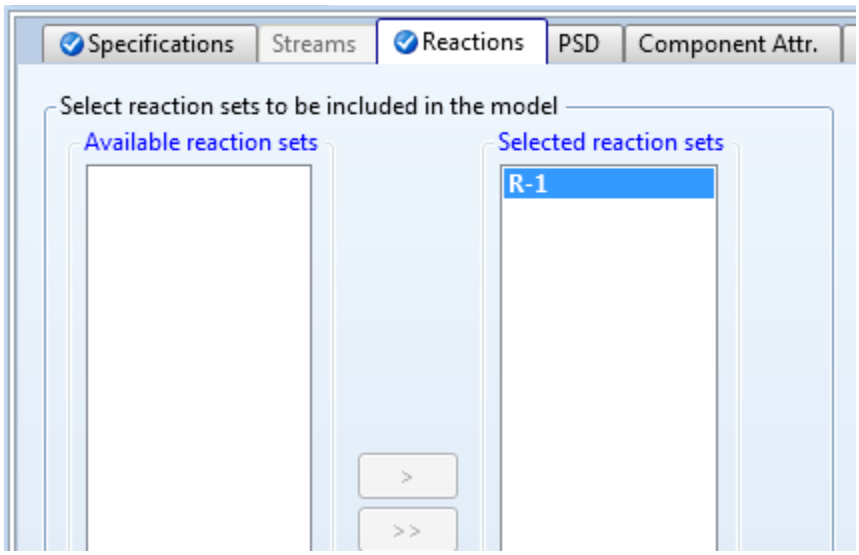
4.10. Click on the **Kinetics** tab and select reaction **2**. Enter **k = 2.7e-06**, **E = 0**. Click on **Driving Force** and enter **1** for the reactant concentration exponents.



4.11. Specify reactor operating conditions. Go to **Blocks | CSTR1 | Setup**. Enter **Pressure = 1 bar**, **Temperature = 100°C**, **Valid phases = Liquid-Only**, **Specification Type = Reactor Volume**, **Reactor Volume = 2600 L**.

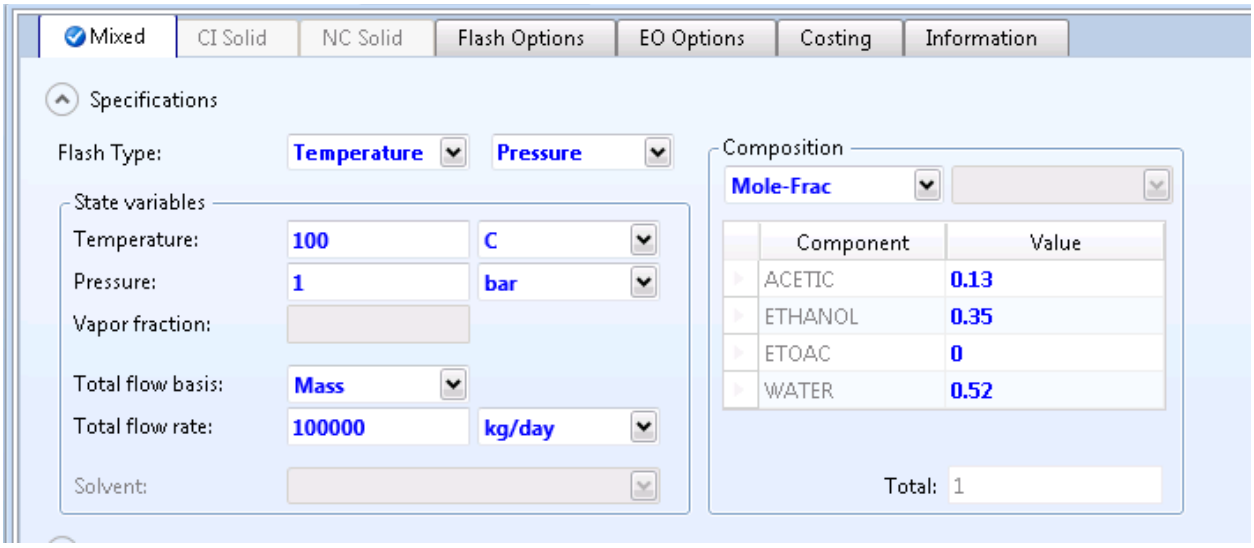


4.12. In the **Reactions** tab, move reaction set **R-1** to the selected reaction sets column.

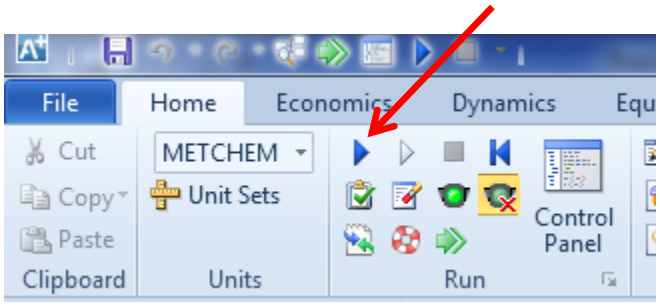


Repeat for the other two reactors. Enter the same conditions for temperature, pressure, valid phases, specification type, volume, and selected reactions.

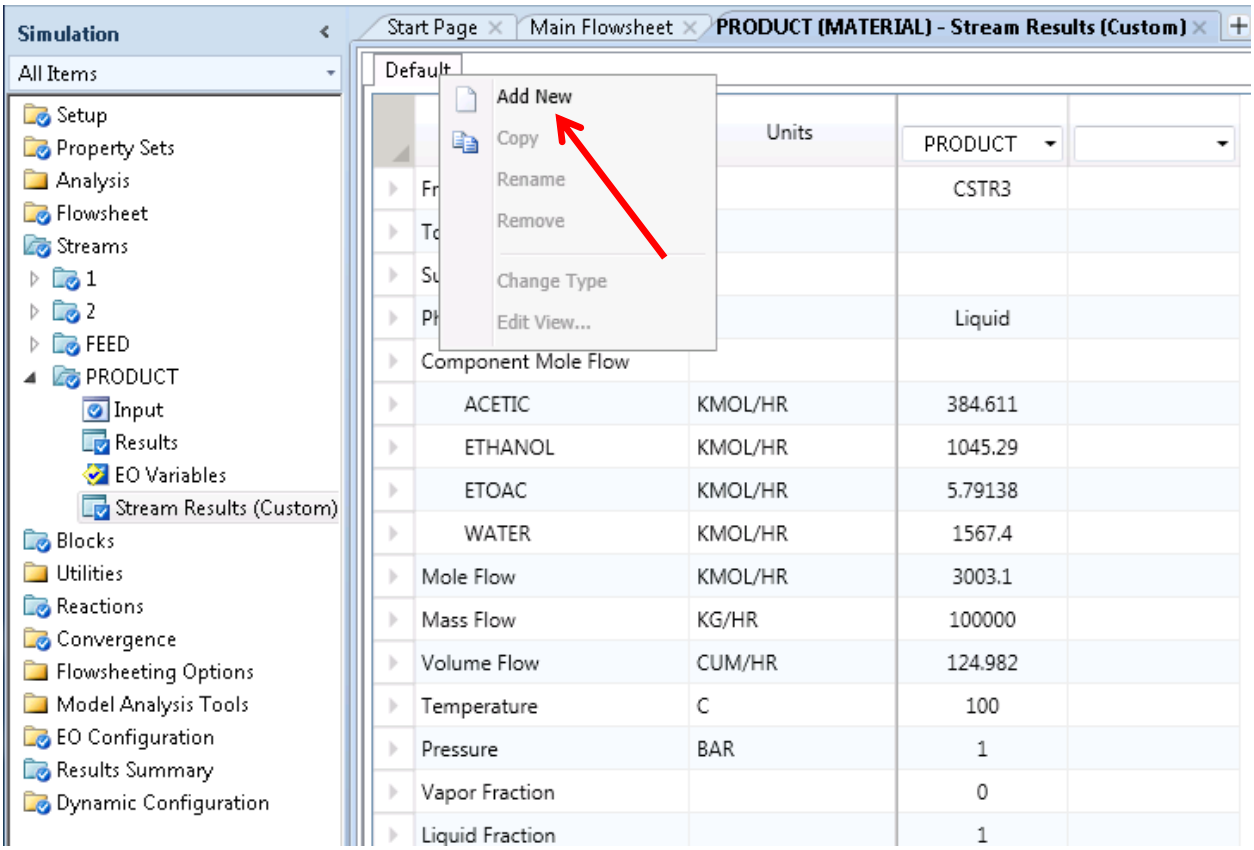
4.13. Specify the feed stream. Go to **Streams | FEED | Input**. Choose **Mole Frac** for **Composition** type and enter **Acetic Acid = 0.13**, **Ethanol = 0.35**, **Ethyl Acetate = 0**, and **water = 0.52**. Enter **Temperature = 100°C** and **Pressure = 1 bar**. Select **Mass** as the **Total flow basis** and enter **100,000 kg/day**.



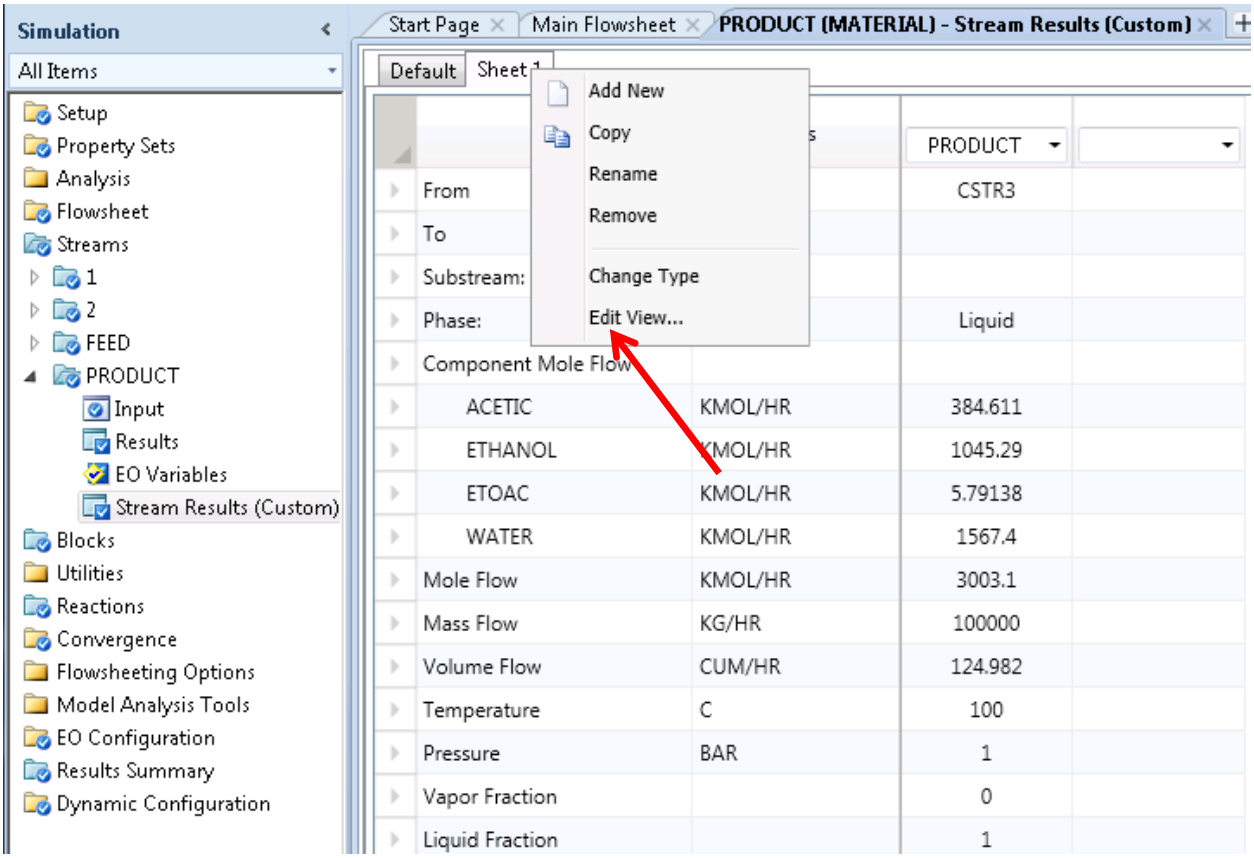
4.14. Open the **Control Panel** and run the simulation (**F5**).



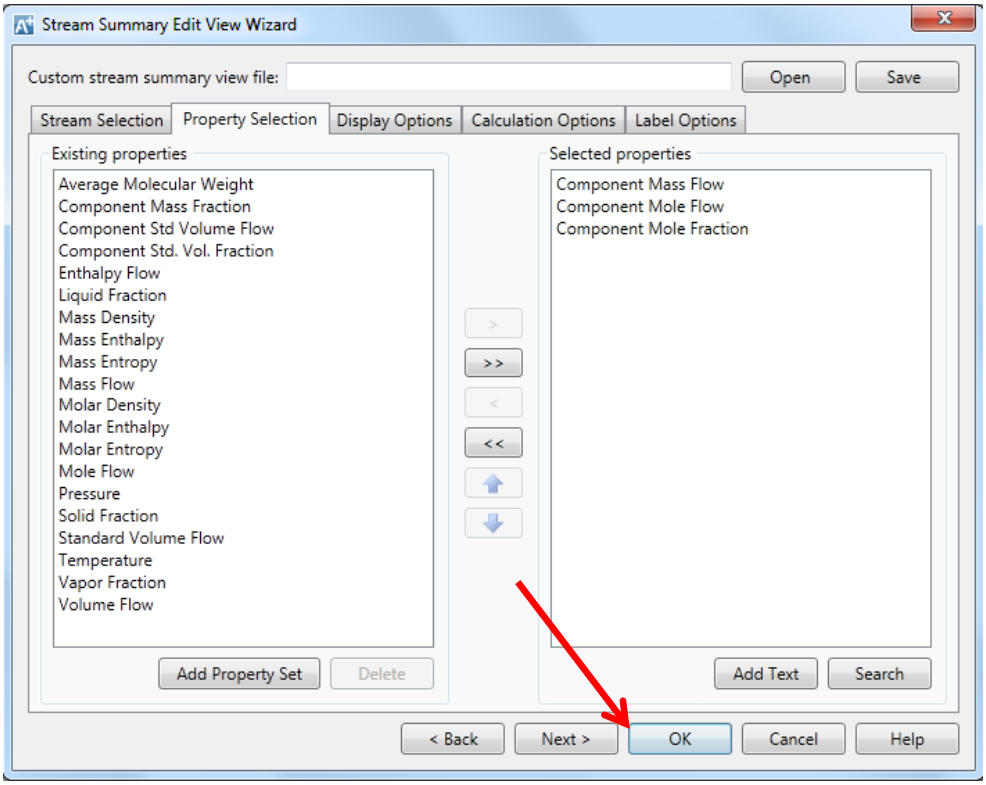
4.15. Check results. Go to **Streams | PRODUCT | Stream Results (Custom)**. In custom stream results you can create data sheets that display only the results that you choose. A default sheet will appear with various stream results. Note that you can change the units and add new streams to the data table. To create a new data table, right click on the **Default** tab. Select **Add New**.



4.16. A dialogue box will appear, asking you to enter the name of the new data sheet. Once you name the new sheet, a new table will appear. You can customize which results you want to display by right clicking on the table tab and selecting **Edit View**.



4.17. Selecting **Edit View** will open up a wizard which will allow you to choose which streams you would like to display results for and which stream properties to display. In the **Stream Selection** tab, select both **FEED** and **PRODUCT** streams. In the **Property Selection** tab, begin by moving all properties to the left column. Then move the properties you would like to see displayed over to the right column. For this case, select **Component Mass Flow**, **Component Mole Flow**, and **Component Mole Fraction**.



4.18. In the **Display Options** tab in **the Stream Summary Edit View Wizard**, you can select the default units for each property. For **Component Mass Flow** select **kg/day**, and for **Component Mole Flow** select **kmol/hr**. After clicking **OK** the custom stream table should look like the following.

Default | Sheet 1

	Units	FEED	PRODUCT
From			CSTR3
To		CSTR1	
Substream: MIXED			
Phase: All			
Component Mass Flow			
ACETIC	KG/DAY	23444.7	17648.9
ETHANOL	KG/DAY	48422.5	43976.2
ETOAC	KG/DAY	0	8503.36
WATER	KG/DAY	28132.9	29871.6
Component Mole Flow			
ACETIC	KMOL/HR	16.2668	12.2454
ETHANOL	KMOL/HR	43.7952	39.7738
ETOAC	KMOL/HR	0	4.02135
WATER	KMOL/HR	65.0671	69.0885
Component Mole Fraction			
ACETIC		0.13	0.0978623
ETHANOL		0.35	0.317862
ETOAC		0	0.0321376
WATER		0.52	0.552138

This table shows that the flowrate of ethyl acetate is under 9,000 kg/day. Therefore this reactor setup is not capable of meeting the desired production rate.

5. Conclusion

The CSTRs cannot be used in series to make the target amount of product. Aspen Plus can be used to model existing equipment in addition to designing new equipment. Modeling existing equipment lets engineers decide if they can repurpose equipment and improve performance by changing state variables.

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