# Esterification in a batch reactor with Aspen Plus® V8.0

## 1. Lesson Objectives

- Due to complexity of analytical solution, use Aspen Plus to calculate the time required to achieve a desired reaction conversion in a batch reactor

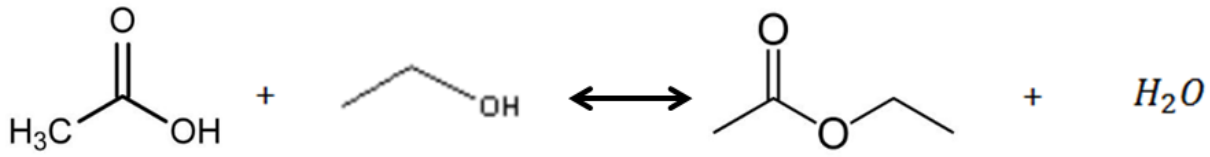
## 2. Prerequisites

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

## 3. Background

Ethyl acetate is manufactured for its use as a solvent due to its low cost of manufacture, low toxicity, and pleasant odor. It is widely produced via the esterification of acetic acid. This is a reversible l iquid phase reaction, 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 $k_r = 2.7\ x\ 10^{-6}\ m^3 kmol^{-1} s^{-1}$

We would like to determine the time required using a batch reactor to achieve 30% reaction conversion given an initial charge of 1,045 kg containing 13 mol % acetic acid, 35 mole % ethanol, and 52 mole % water.

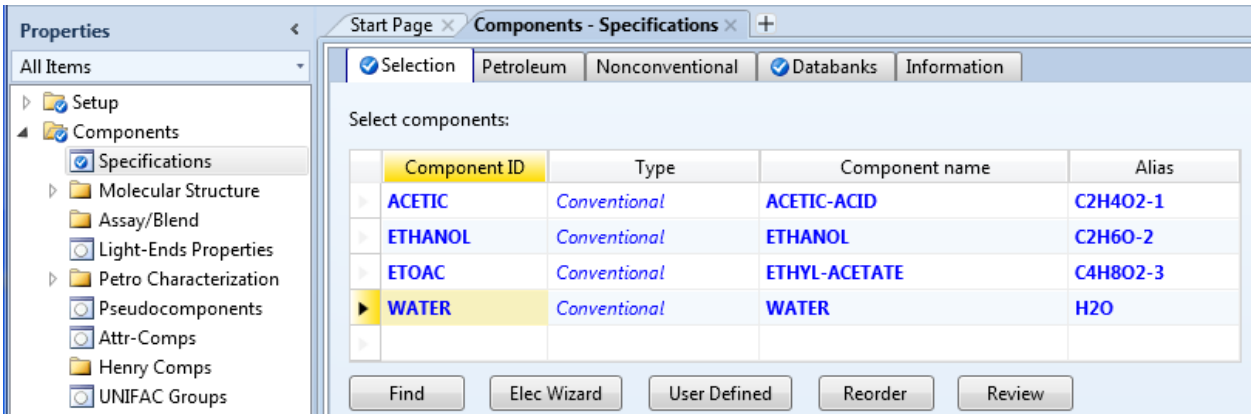
**The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.**

## 4. Solution

Aspen Plus Solution:

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

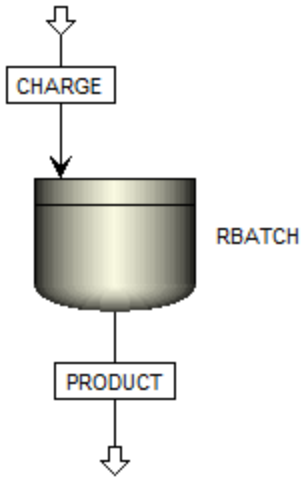
4.02. Define Components. In the properties environment go to **Components | Specifications | Find**. Search for and add **acetic acid**, **ethanol**, **ethyl acetate**, and **water**. You can change the component ID's to match what is shown below, or you can leave the default ID's as they are.



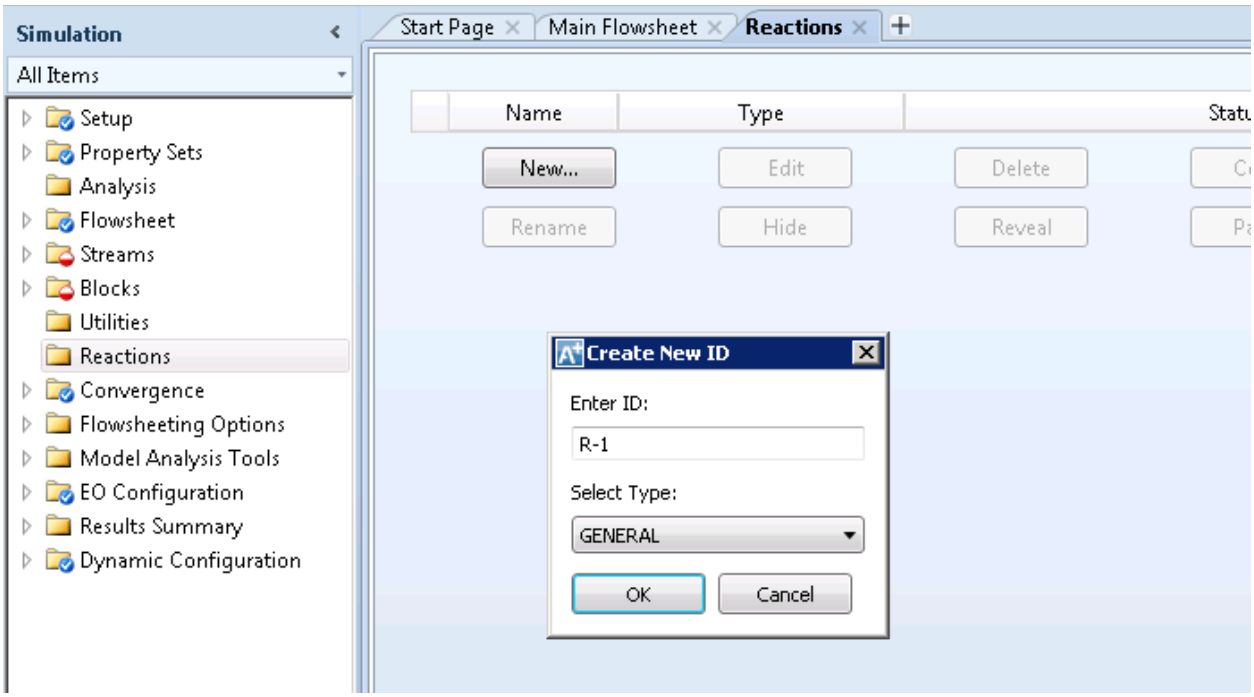

4.03. Populate the binary property model parameters by clicking **Methods | Parameters | Binary Interaction | NRTL-1**.

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

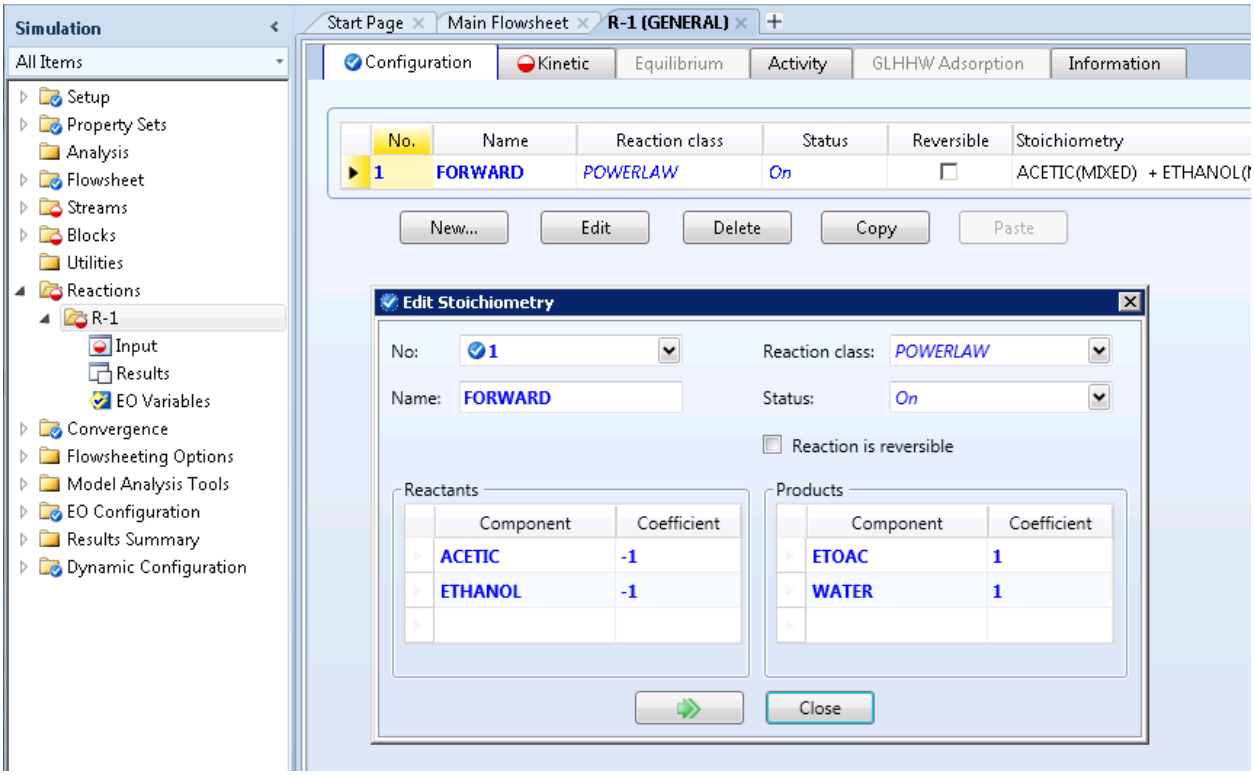

4.05. Place an **RBatch** block onto the flowsheet from the **Reactors** tab in the **Model Palette**. The RBatch block models a specified reaction using the kinetic data and specified residence time. However, it is still a steady state model, and so a realization of the model would require many batch reactors in parallel with staggered start and end times. Connect the required ports with material streams.



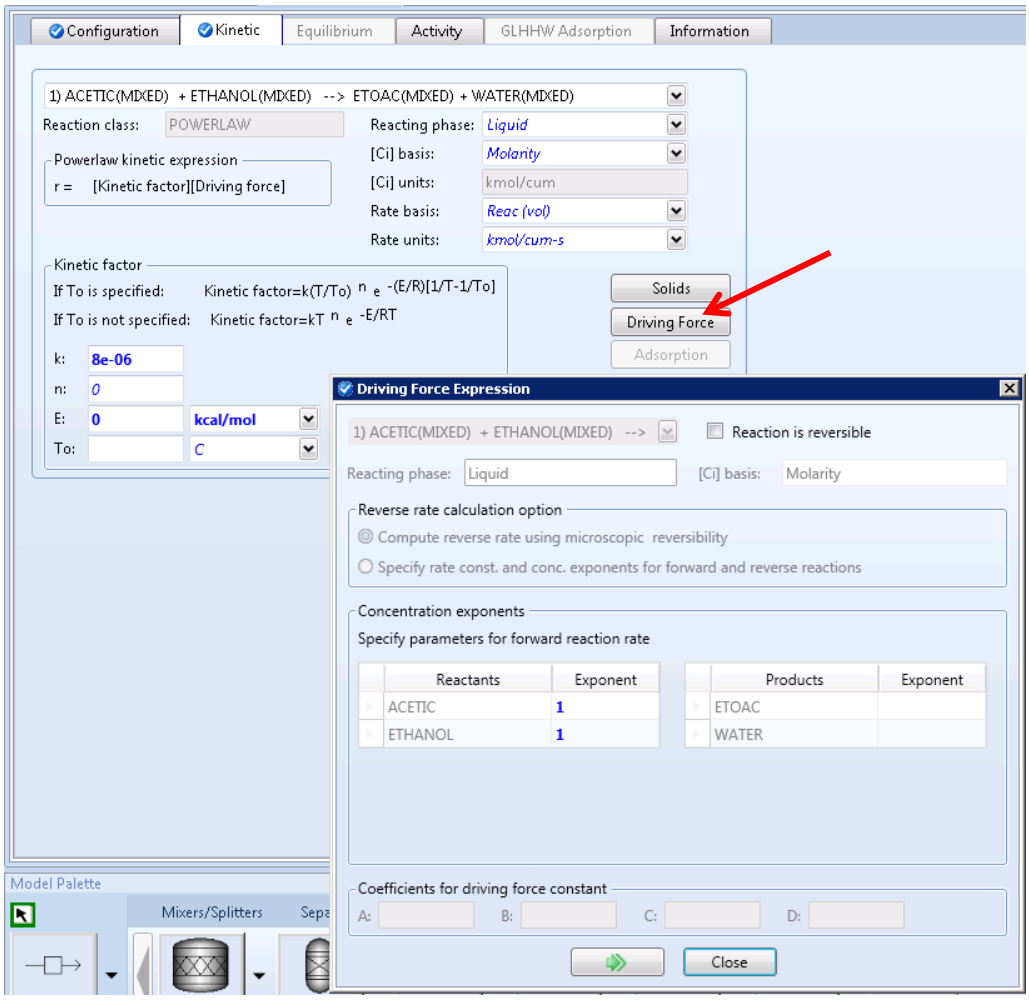

4.06. Define Reactions. In the navigation pane click **Reactions | New**. A default reaction group ID **R-1** will be created, select **GENERAL** for type. Click **OK**.



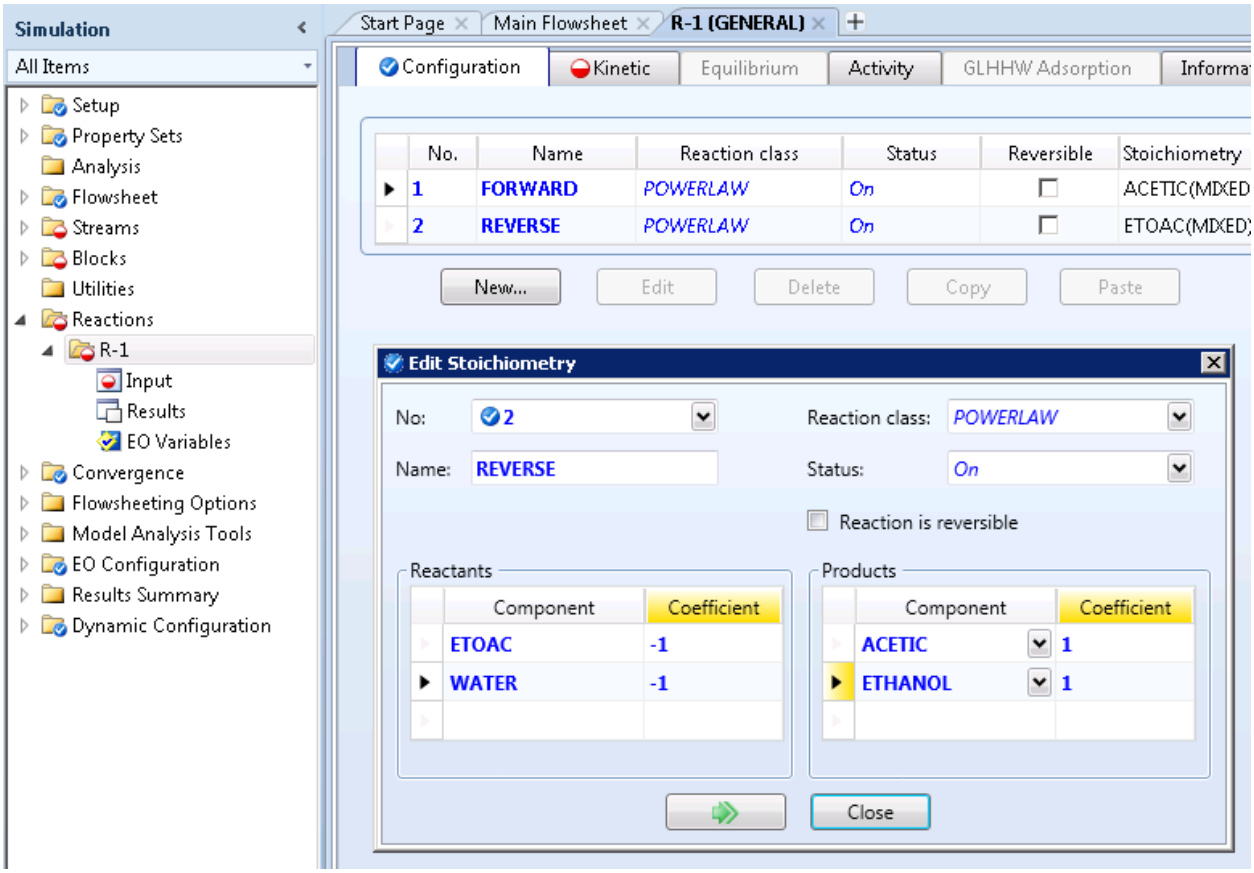

4.07. Once R-1 is created, specify the reaction by clicking **New** in the R-1 folder. For reversible reactions it is often useful to enter the forward and reverse reactions as separate reactions within the same reaction group. Start with the forward reaction. Name the reaction, select reactants and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



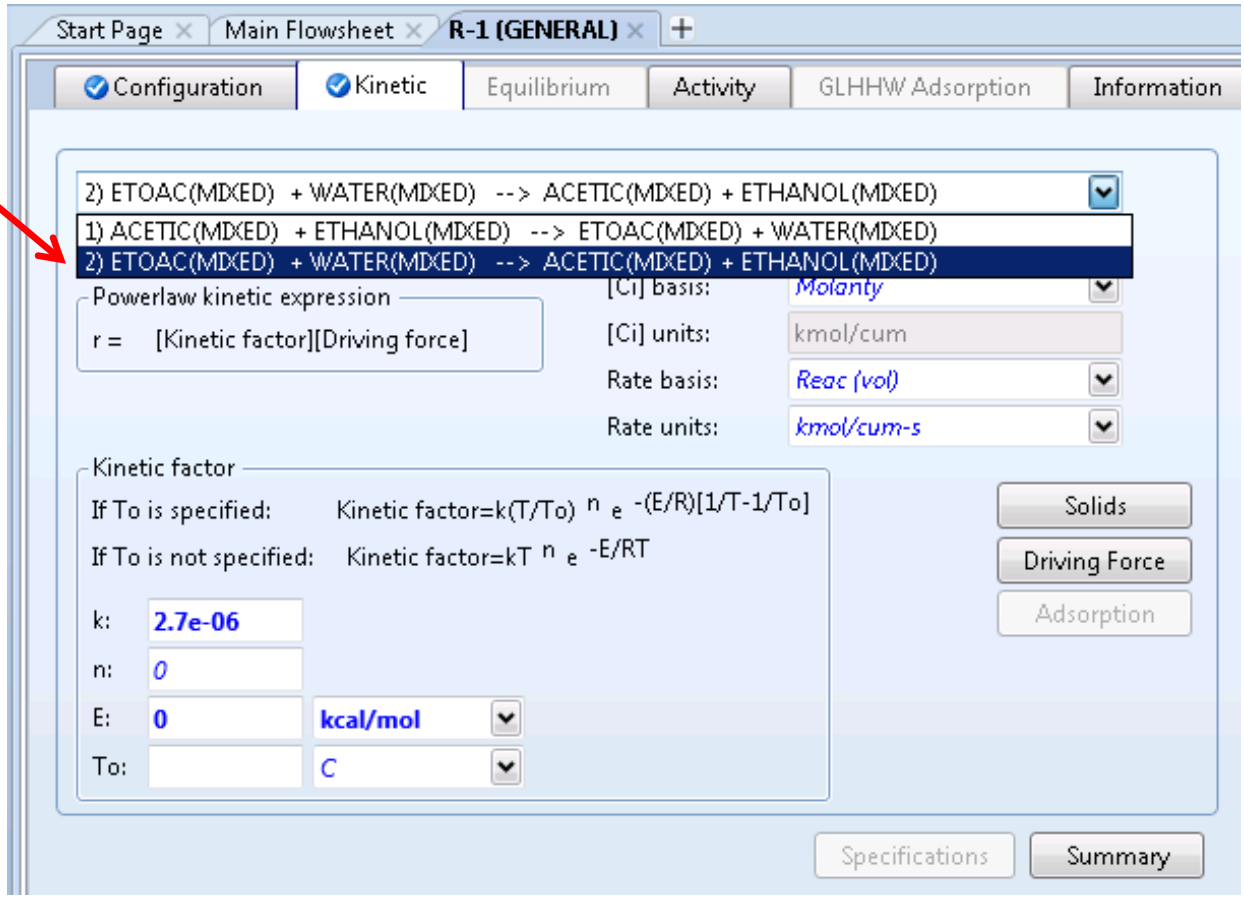

4.08. Click on the **Kinetic** tab and enter **k = 8e-06** and **E = 0**. Click on **Driving Force** and enter **1** for the reactant concentration exponents.



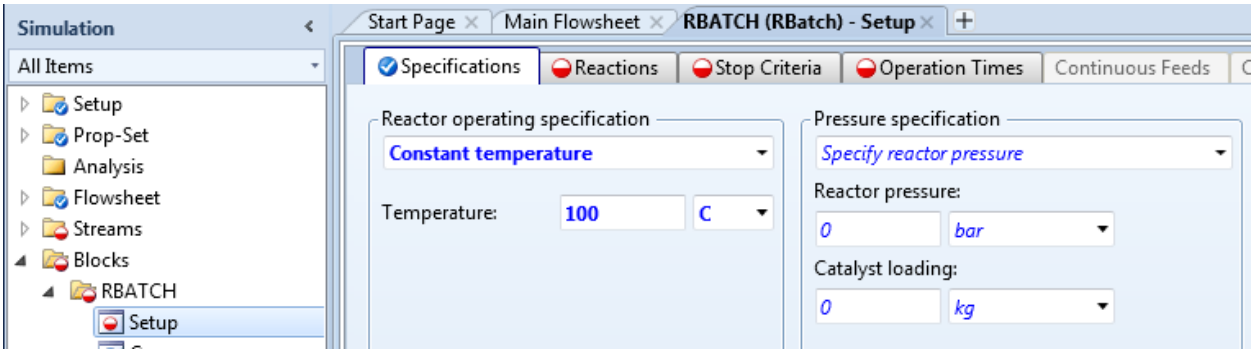

4.09. For the reverse reaction, click **Reactions | R-1 | New**. Name the reaction, select reactants and products, and enter the stoichiometric coefficient.



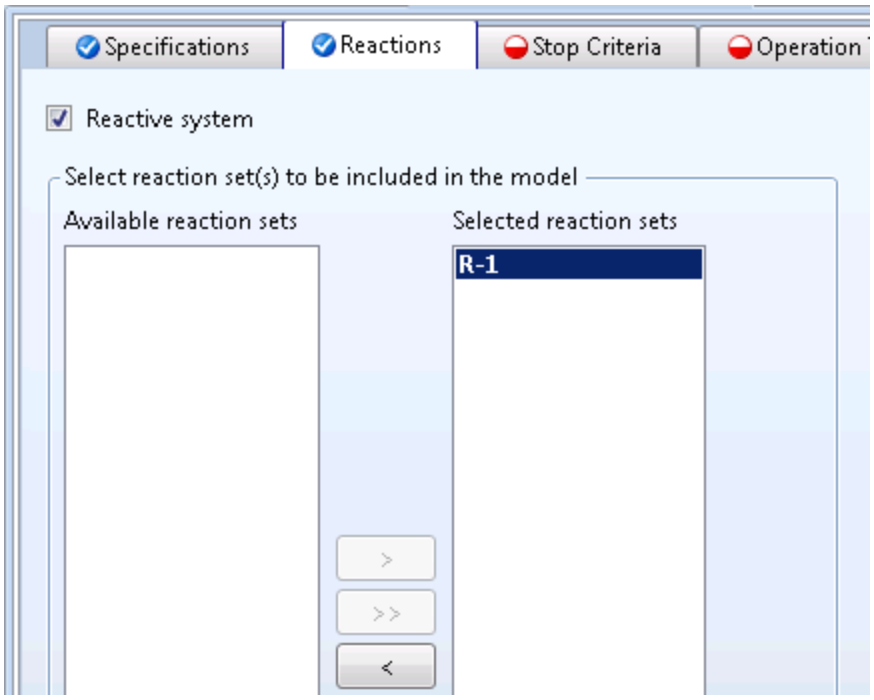

4.10. Click on the **Kinetics** tab and select reaction **2**. Enter **k = 2.7e-06**, **E = 0**. Click on **Driving Force** and enter **1** for the reactant concentration exponents.



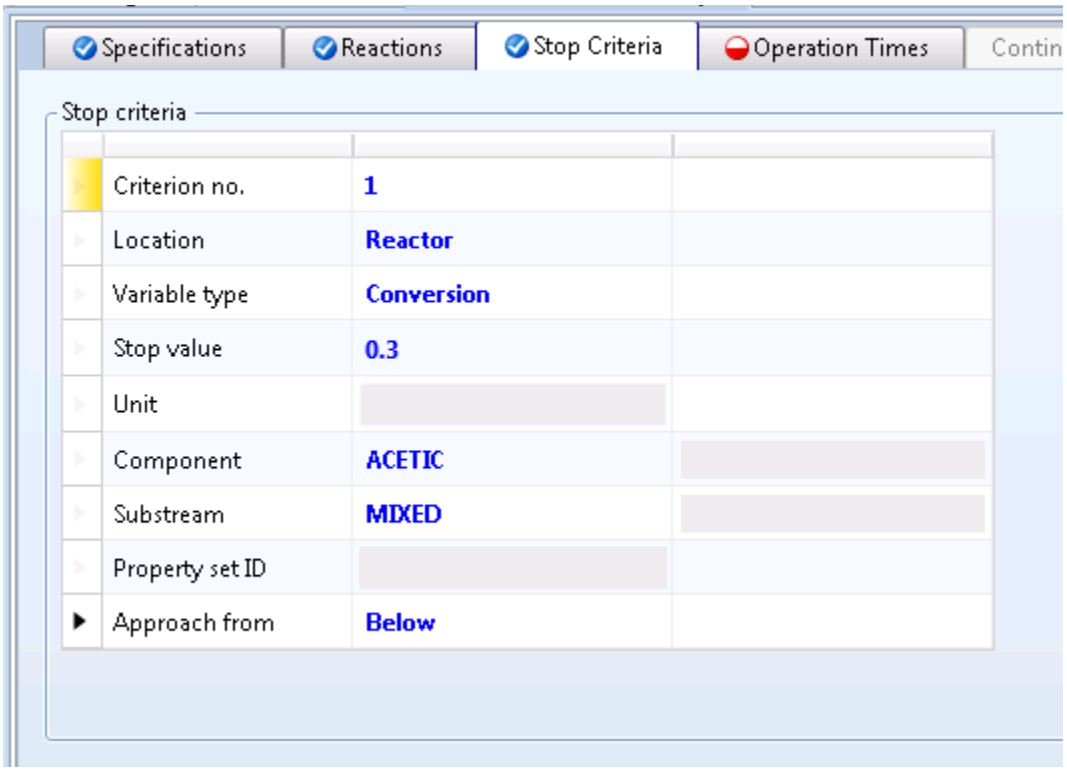

4.11. Specify RBATCH operating conditions. Click **Blocks | RBATCH | Setup**. Select **Constant temperature** and enter **100°C**.



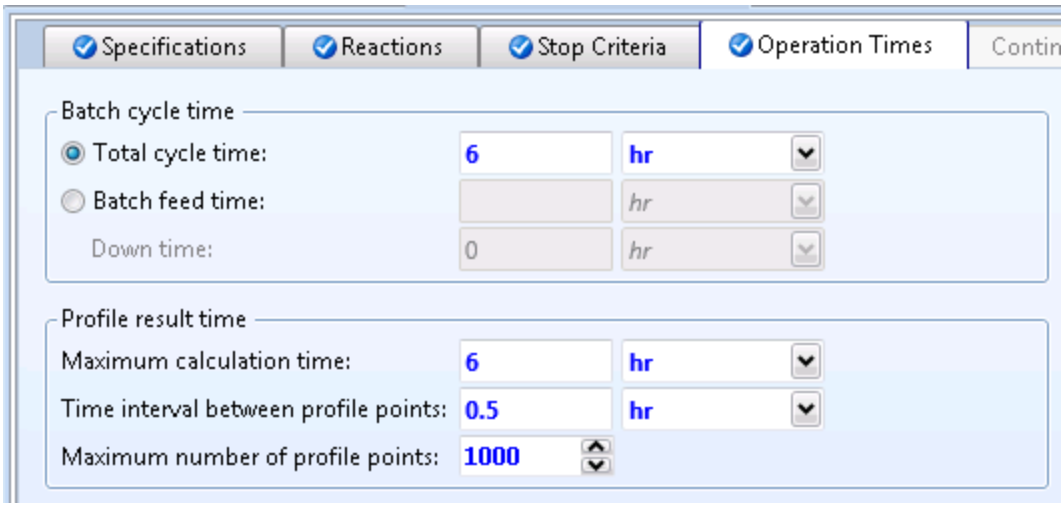

4.12. In the **Reactions** tab, move **R-1** to the **selected reaction sets** area.



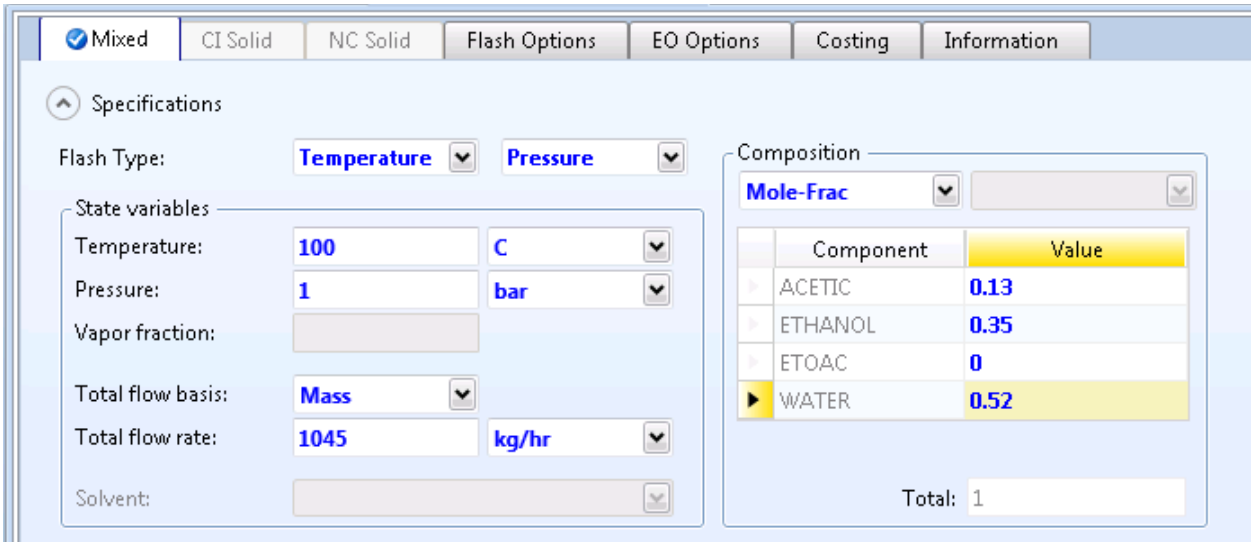

4.13. On the **Stop Criteria** tab, enter the following information.



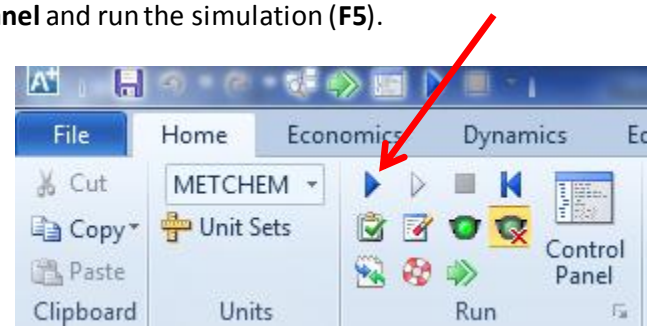

4.14. On the **Operation Times** tab enter the following information.



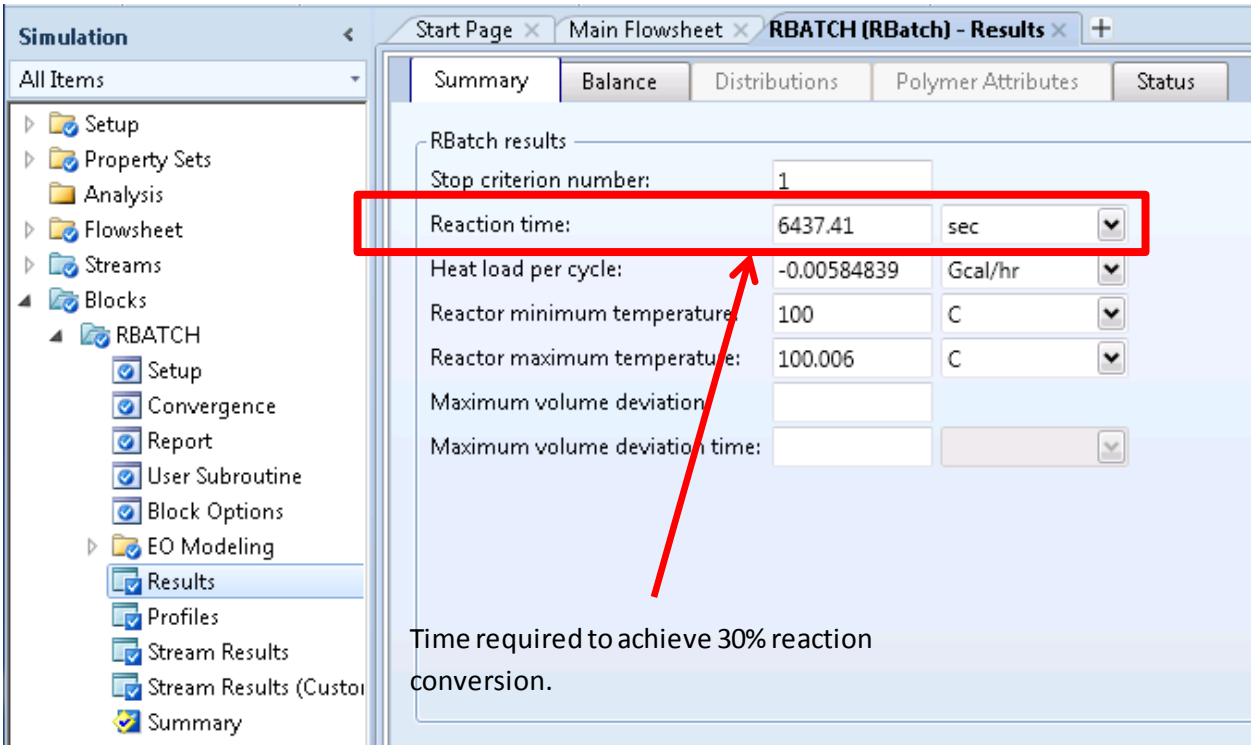

4.15. Specify charge stream. Go to **Streams | CHARGE | Input**. Choose **Mole Frac** for **Composition** type and enter **Acetic Acid = 0.13**, **Ethanol = 0.35**, **Ethyl Acetate = 0**, and **water = 0.52**. Enter **Temperature = 100°C** and **Pressure = 1 bar**. Select **Mass** as the **Total flow basis** and enter **1,045 kg/hr**. Click on the **Flash Options** tab and select **Liquid-Only** in the valid phases drop down menu.




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




4.17. Check results. Go to **Blocks | RBATCH | Results**.




## 5. Conclusion

The RBatch block calculated a residence time of 107.3 min. for 30% conversion. Using these techniques, RBatch can be used to model complex reaction systems including parallel and series reactions which lead to coupled systems of ODEs for analytical solutions.

## 6. Copyright