Isomerization in a batch reactor with Aspen Plus® V8.0

1. Lesson Objectives

- Use chemical reaction kinetics to calculate the time required to reach a desired conversion in a batch reactor
- Use Aspen Plus to confirm the analytical solution

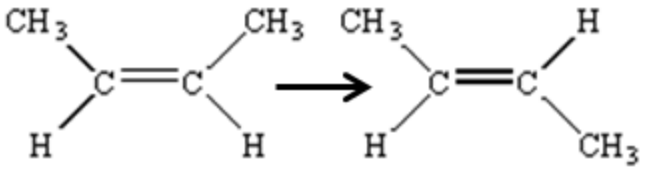
2. Prerequisites

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

3. Background

2-Butene is a four carbon alkene that exists as two geometric isomers: *cis*-2-butene and *trans*-2-butene. The irreversible isomerization reaction with 1st order reaction kinetics is shown below. It is desired to determine the time required to reach 90% reaction conversion in a batch reactor.

Homogeneous reaction



cis-2-Butene *trans-2-Butene*

1st order reaction kinetics $r_A = kC_A, k = 0.23min^{-1} = 0.003833s^{-1}$

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

4. Solution

Analytic Solution:

$$r_A = kC_A = kN_A/V$$

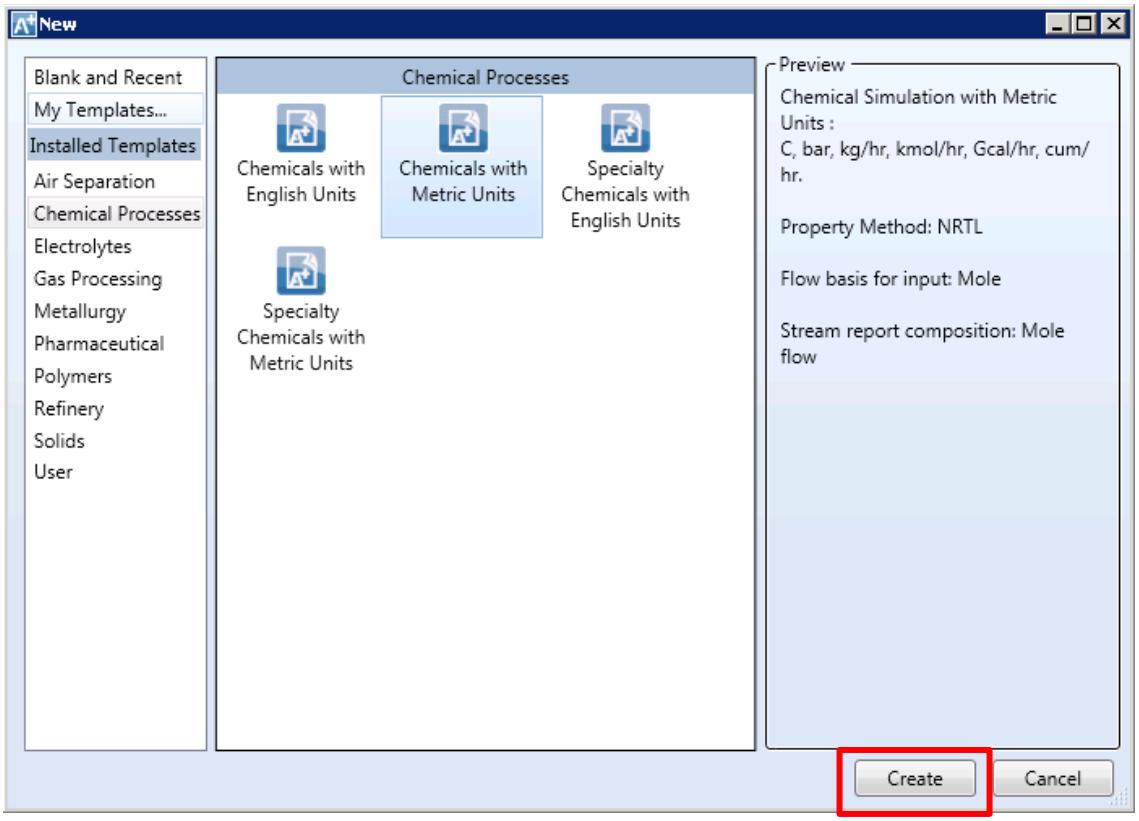
$$\int_0^t dt = -\int_{N_{A0}}^{N_A} \frac{1}{V}\frac{dN_A}{r_A} = -\frac{1}{k}\ln\frac{N_A}{N_{A0}}$$

$$t = -\frac{1}{k}\ln(1 - x_A);\ x_A = 1 - \frac{N_A}{N_{A0}}$$

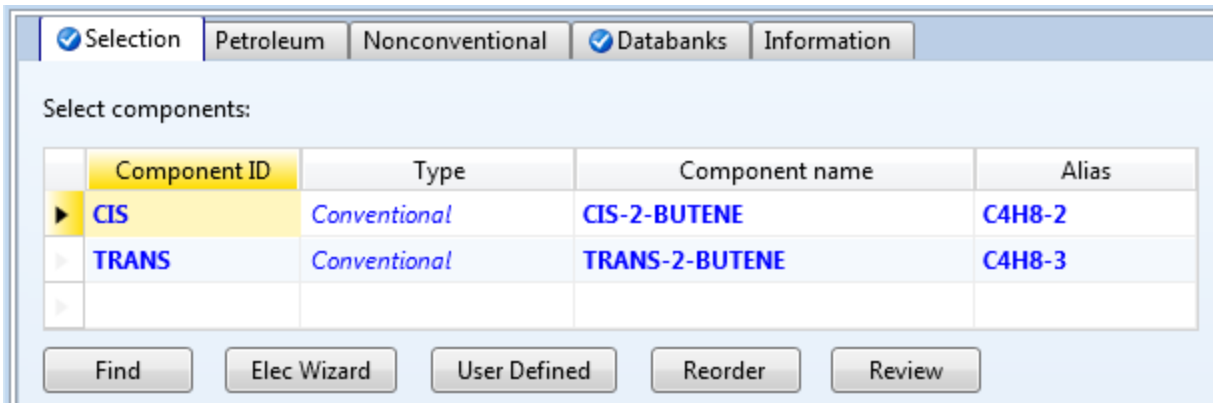
$$\therefore t = -\frac{1}{0.23 min^{-1}}\ln(1 - 0.9) = 10.01 \text{ min}$$

Aspen Plus Solution:

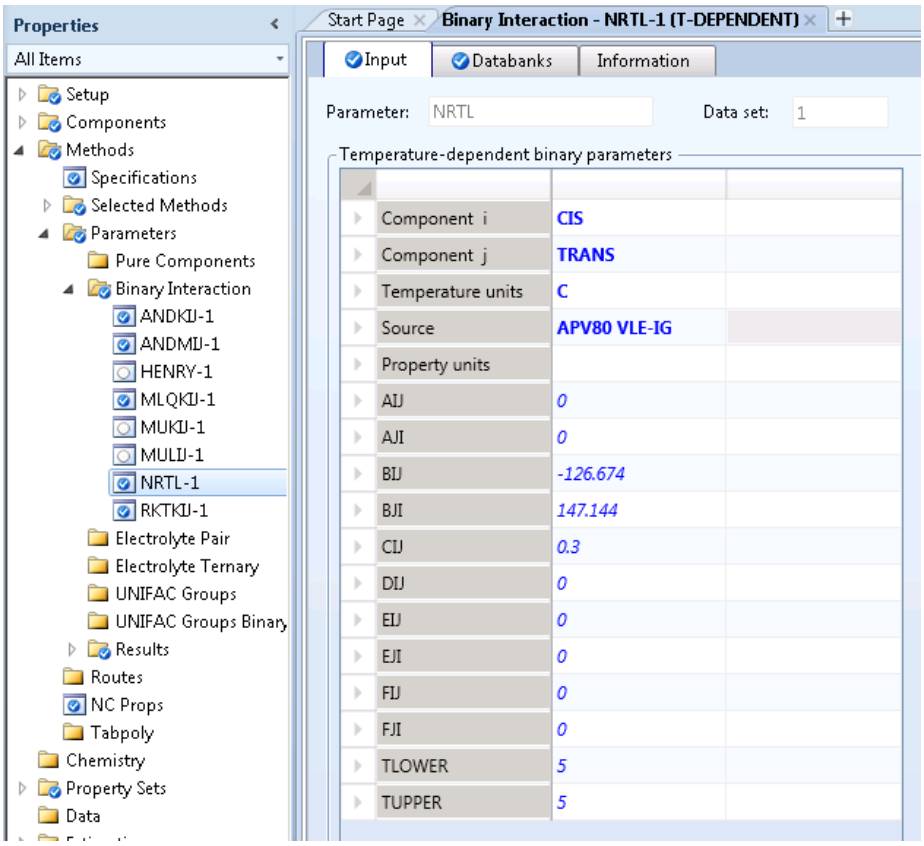
4.01. Start **Aspen Plus V8.0**. Create a new simulation by clicking **New** on the **Start Page**. Select the template by clicking **Chemical Processes | Chemicals with Metric Units**. Click **Create** to begin.



4.02. Define components. After creating a new simulation, Aspen Plus should open to the **Components | Specifications** form. To define components enter **CIS-2-BUTENE** and **TRANS-2-BUTENE** for **Component name** and enter **CIS** and **TRANS** as **Component ID's**. A warning message will appear saying that this change will cause the parameters to be updated. Click **Yes**.



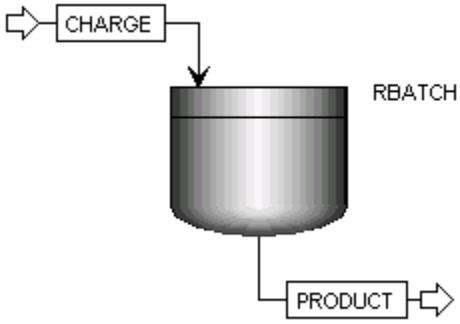
4.03. Populate the binary interaction parameters. Since a template was chosen to create the simulation, the property method is already chosen, in this case NRTL. However, since components have been added, the binary interaction parameters must be populated. Go to **Methods | Parameters | Binary Interaction | NRTL-1.**



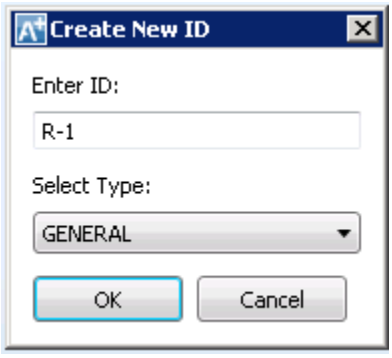
4.04. We are now ready to create the flowsheet. Move to the simulation environment by clicking the **Simulation** button at the bottom left of the screen.

4.05. In the simulation environment add an **RBatch** reactor model to the main flowsheet. Go to the **Reactors** tab of the **Model Palette**, select **RBatch** and drop it to the flowsheet. Connect two **Material streams** for batch charge and reactor product. You can rename the streams and the reactor block by using **Ctrl+M**.

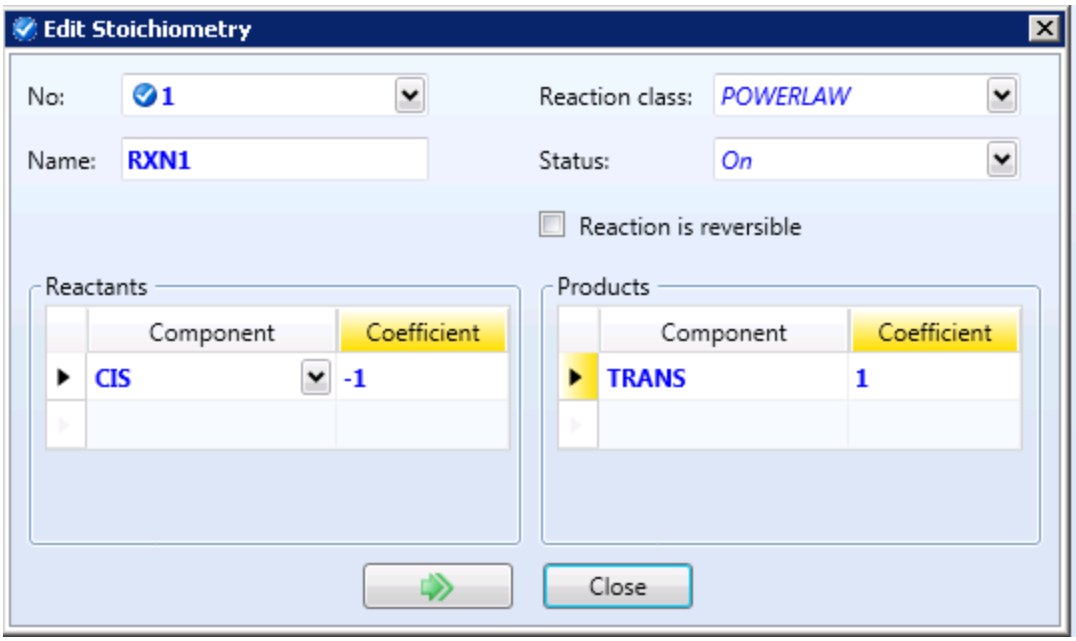
Note: The RBatch block models a specified reaction using the kinetic data and specified residence time. However, it is still a steady state model, and so a realization of the model would require many batch reactors in parallel with staggered start and end times.



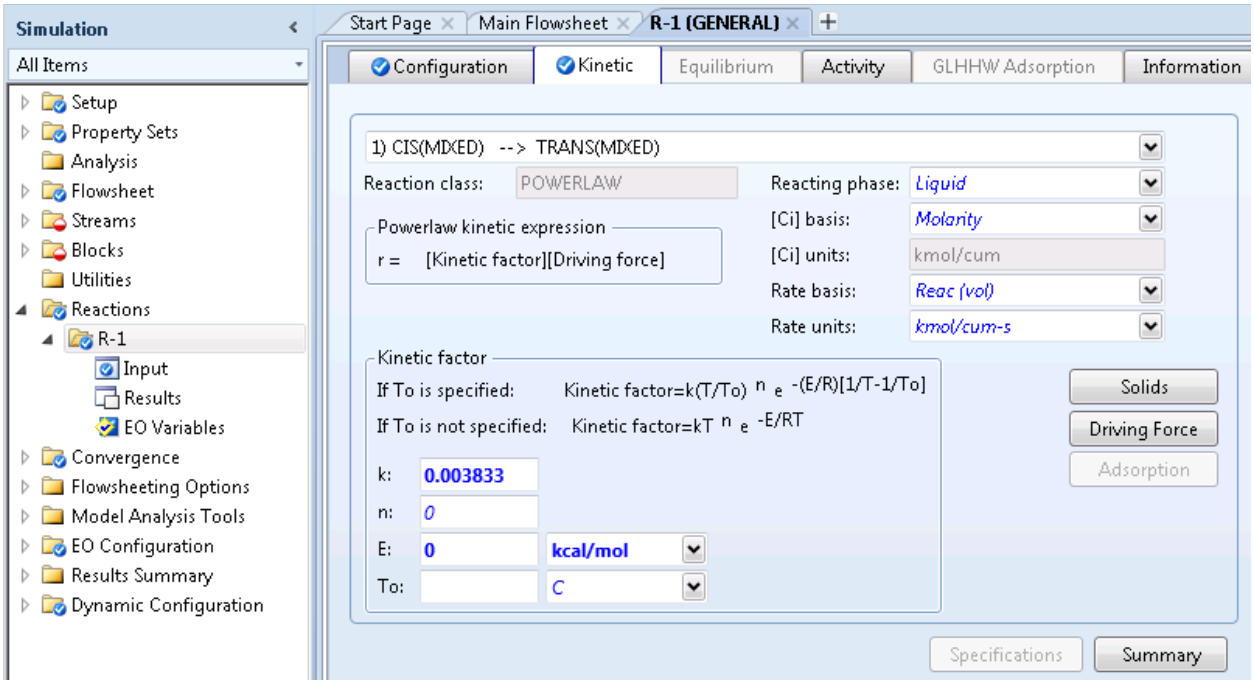
4.06. Define Reaction. In the navigation pane go to **Reactions | New**. Select **GENERAL** for reaction type. By default, reaction ID **R-1** will be created or you can create a new ID. Click **OK**.



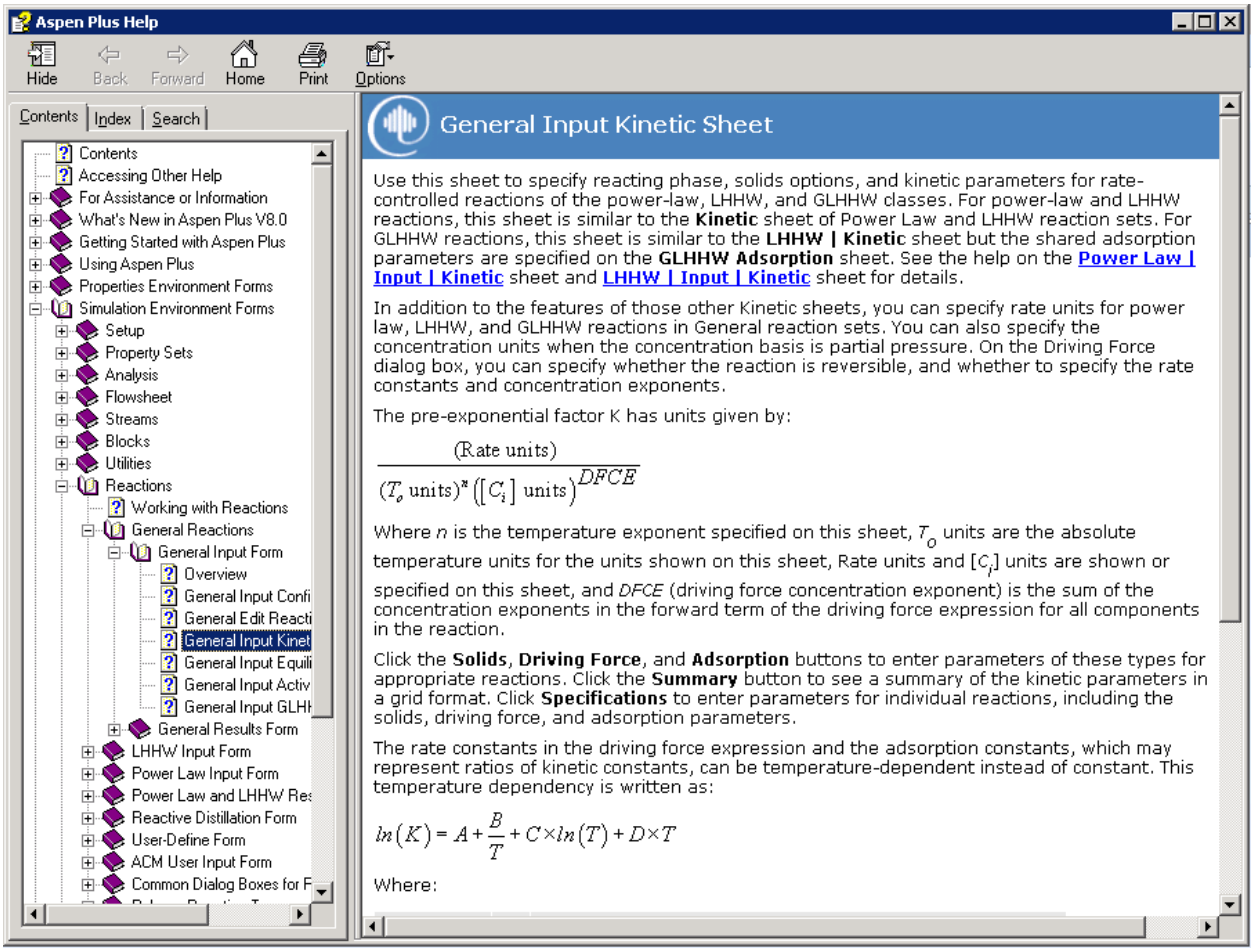
4.07. Go to **Reactions | R-1** and click **New**. Enter **RXN1** as the reaction name. Select **CIS** for the reactant component and **TRANS** for the product component, as well as the reactant and product stoichiometric coefficients (both **1** in this case). Notice that the coefficient for the reactants automatically becomes negative. Click **Close** when complete.



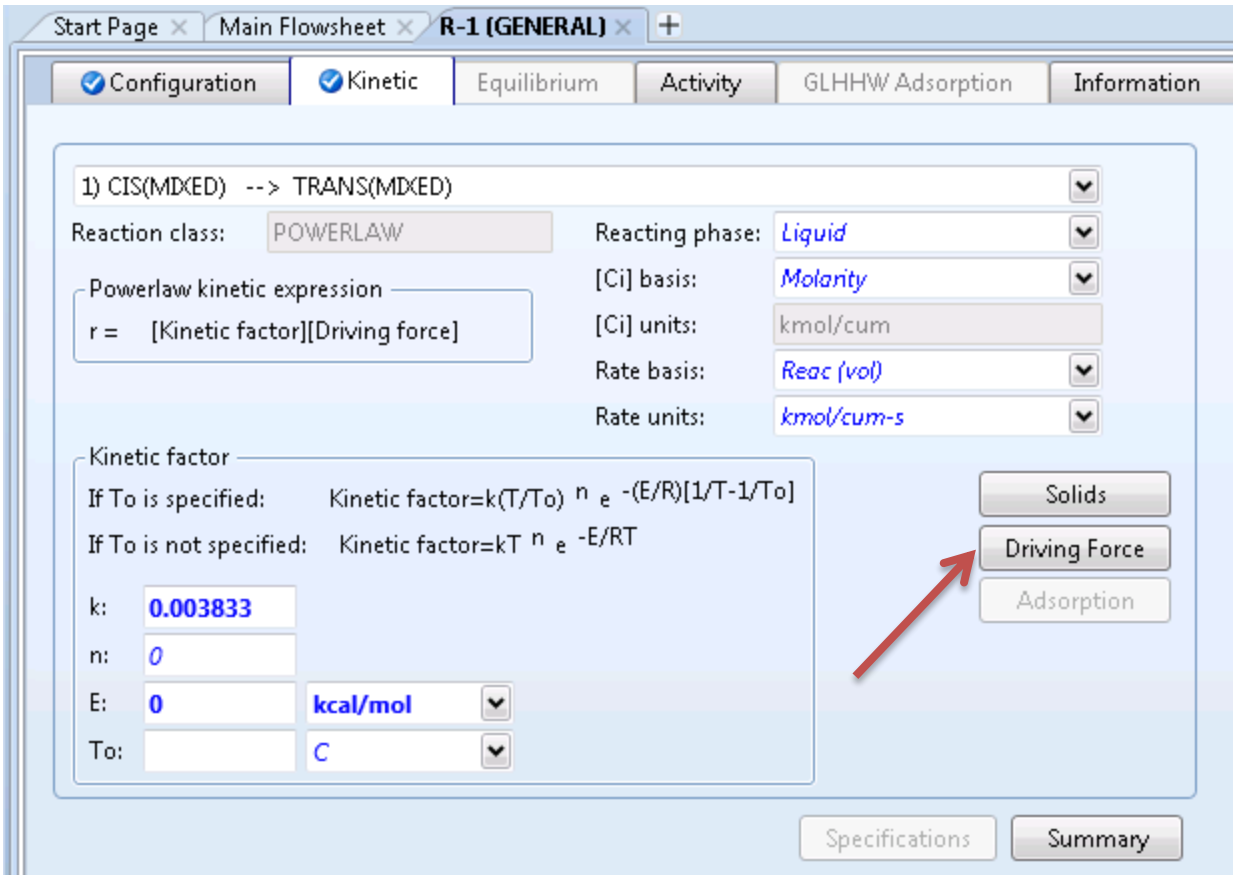
4.08. Define reaction kinetics. In Reaction group R-1, go to the **Kinetic** tab. Enter **k = 0.003833** and enter **E = 0** (as this is isothermal). Note that the default units for rate constant are inverse seconds.

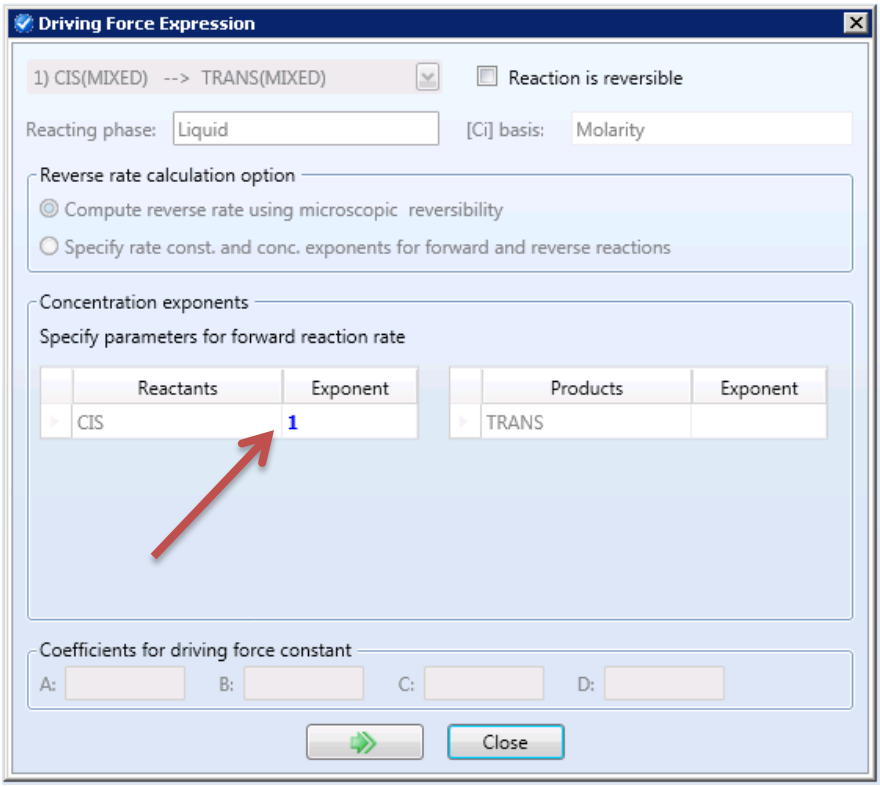


4.09. Hovering the mouse over an input field will show hover text giving information about it. Clicking into the field and pressing **F1** brings up the **Aspen Plus Help** page on the topic. Doing this in the field for k shows the help page about the pre-exponential factor which shows the equation in which it is used.



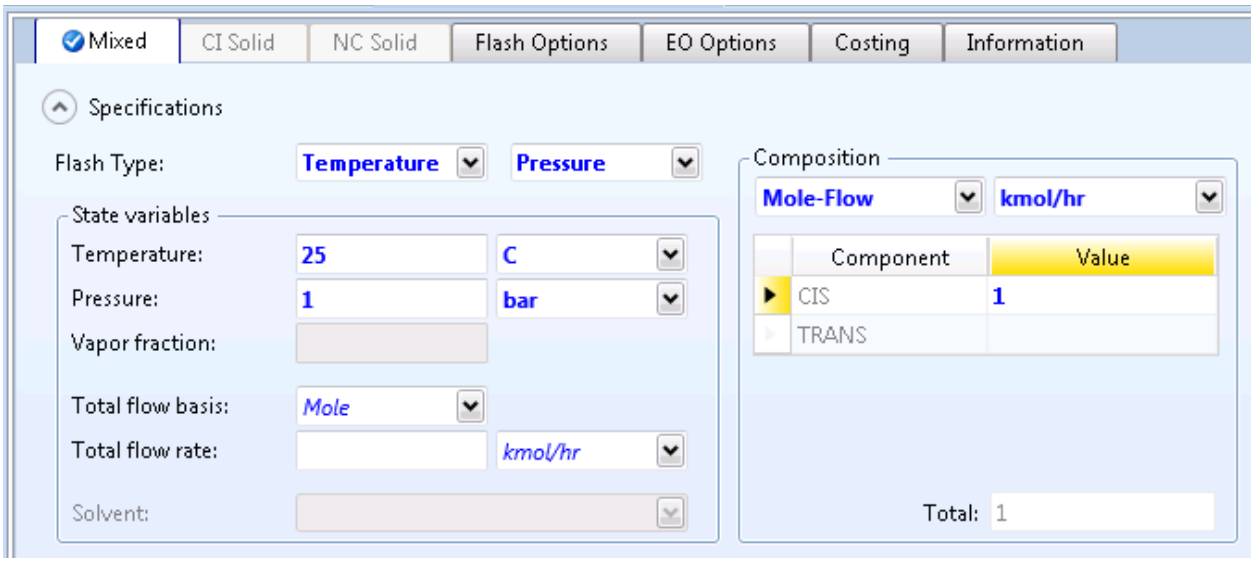
4.10. Next, select the **Driving Force** button. Enter **1** as the exponent for cis-2-butene. Click **Close** when complete.


Start Page
Main Flowsheet
R-1 (GENERAL)
Configuration
Kinetic
Equilibrium
Activity
GLHHW Adsorption
Information
1) CIS(MIXED) --> TRANS(MIXED)
Reaction class: POWERLAW
Reacting phase: Liquid
[Ci] basis: Molarity
[Ci] units: kmol/cum
Rate basis: Reac (vol)
Rate units: kmol/cum-s
Powerlaw kinetic expression
r = [Kinetic factor][Driving force]
Kinetic factor
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: 0.003833
n: 0
E: 0 kcal/mol
To: C
Solids
Driving Force
Adsorption
Specifications
Summary


Driving Force Expression
1) CIS(MIXED) --> TRANS(MIXED)
Reaction is reversible
Reacting phase: Liquid
[Ci] basis: Molarity
Reverse rate calculation option
Compute reverse rate using microscopic reversibility
Specify rate const. and conc. exponents for forward and reverse reactions
Concentration exponents
Specify parameters for forward reaction rate
Reactants
Exponent
CIS
1
Products
Exponent
TRANS
Coefficients for driving force constant
A:
B:
C:
D:
Close

4.11. Define reactor feed stream. In the navigation pane go to **Streams | CHARGE | Input**. Enter **25°C** for **Temperature**, **1 bar** for **Pressure**, and a **Mole-Flow** of **1 kmol/hr** for component **CIS**.

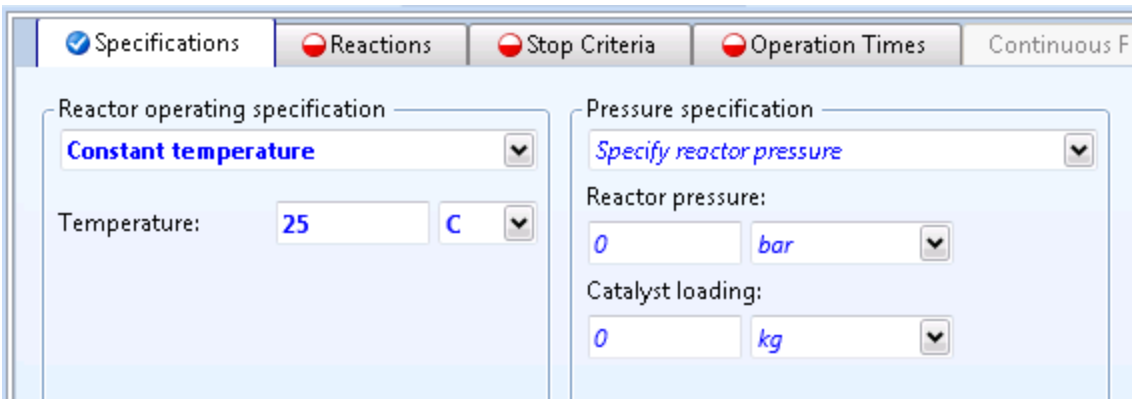
Note: If you enter a flow into the composition section, you are not required to enter any additional flow data.



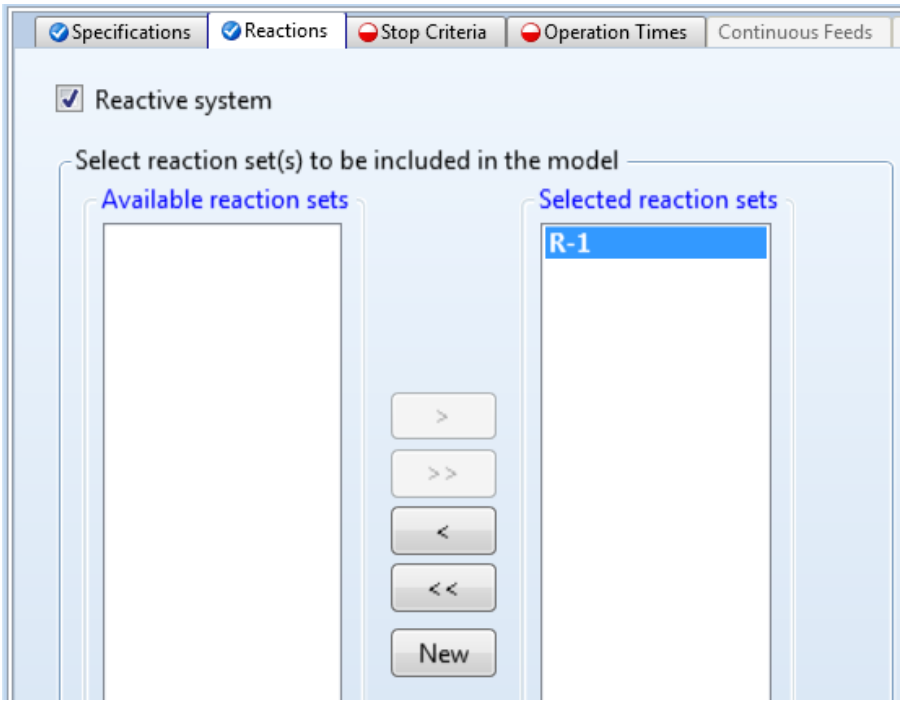
(FAQ) Useful Option To Know: Modeling batch reactors in steady state simulations

Aspen Plus models batch reactors in steady state, so a real-world plant running batch reactors would need several reactors in parallel with staggered start and end times to approximate steady state operation.

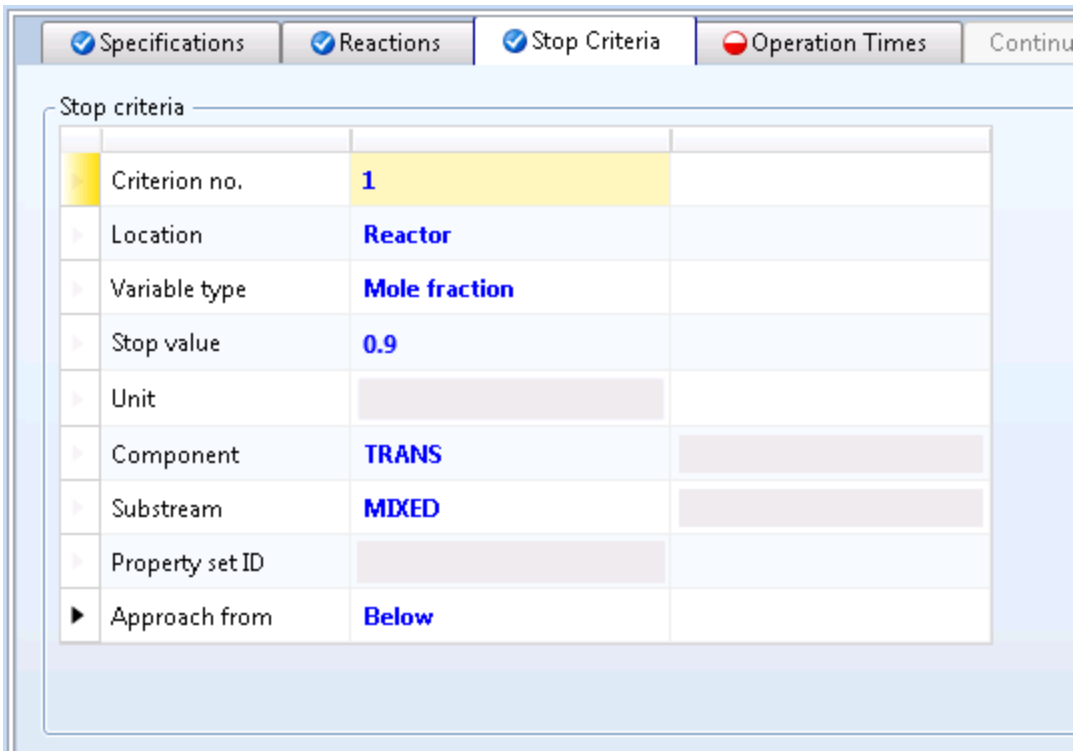
4.12. Specify reactor conditions. Go to **Blocks | RBATCH | Setup**. In the **Reactor operating specification** field select **Constant temperature** and enter a temperature of **25°C**. Note that this is not a realistic reactor temperature; however, since our kinetics are not temperature dependent it is acceptable for this simplified example. Next, enter the reactor operating pressure. You may enter the operating pressure by entering a pressure greater than zero, or you can specify the pressure drop through the reactor by entering a number less than or equal to zero. In this case enter **0** for **Reactor pressure**, which means that this reactor will not experience any pressure losses and will operate at the given feed pressure of 1 bar.



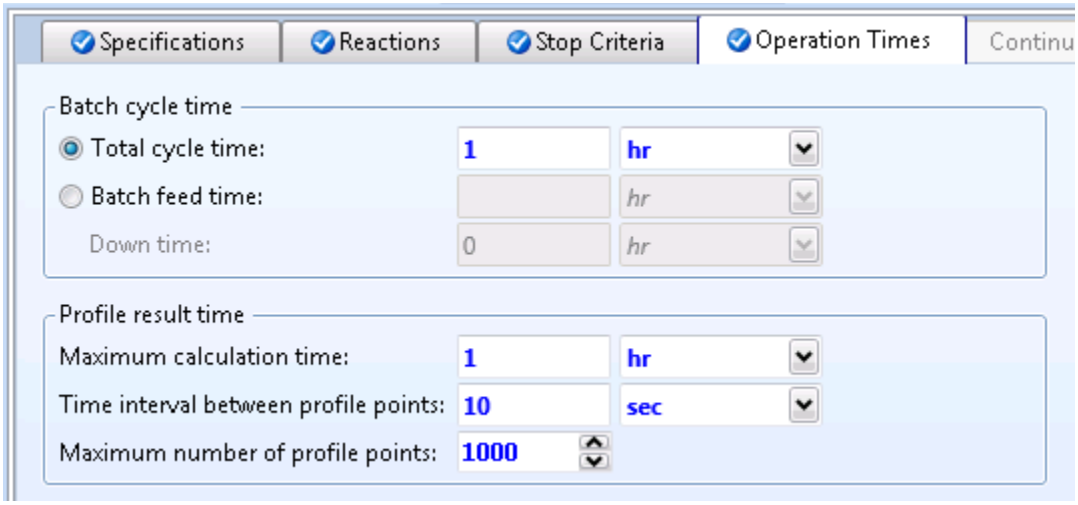
4.13. Choose the reaction set. In the **Reactions** tab, specify **R-1** as the selected reaction set.



4.14. Specify Stop Criteria in order to stop Aspen Plus computation when the conversion reaches a designated number. In this case, when the mole fraction of trans-2-butene in the reactor reaches 0.9, Aspen Plus will stop reactor computations and the product stream will represent the composition of the reactor at this designated stop time. In the **Stop Criteria** tab, complete the input fields as shown below.

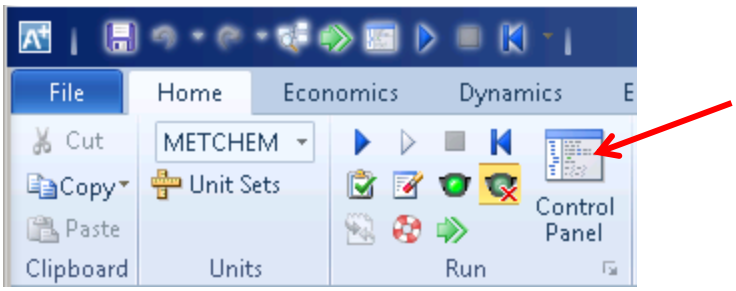


4.15. Define Operation Times in order to create result tables and plots. Complete the input fields in the **Operation Times** tab as shown below.

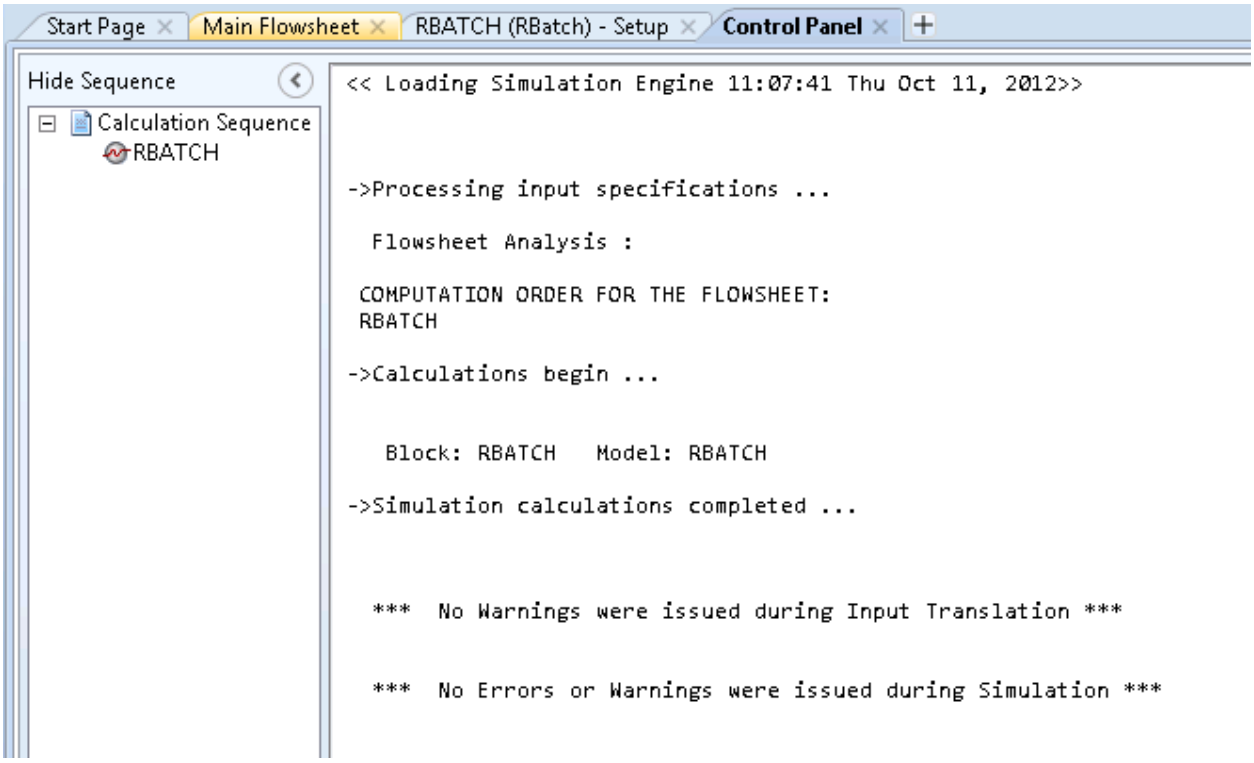


4.16. Save your Aspen Plus simulation file (use .bkp format, for example **Reactor_Batch_CIStoTRANS.bkp**)

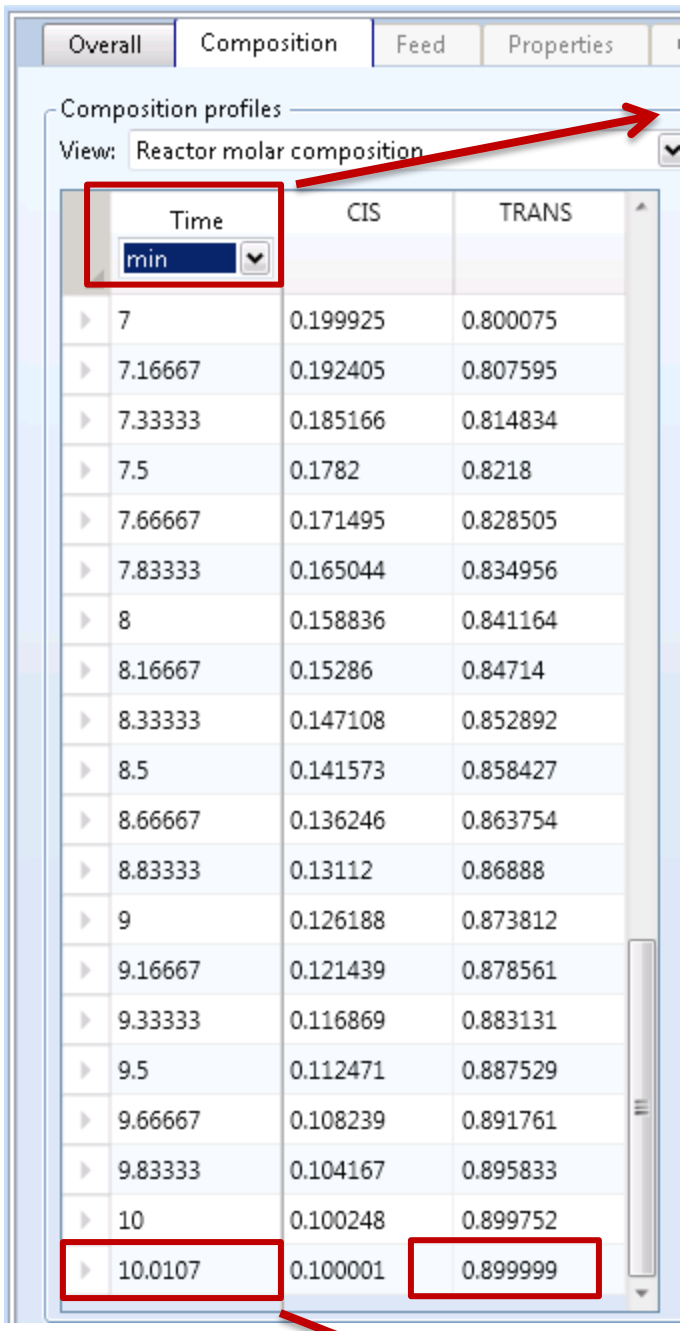
4.17. All the input required to run the simulation has been entered. On the **Home** tab of the ribbon, click the **Control Panel** button. It is a good habit to open the control panel before running the simulation.



4.18. Run the simulation (**F5**). The simulation should run to completion with no errors or warnings.



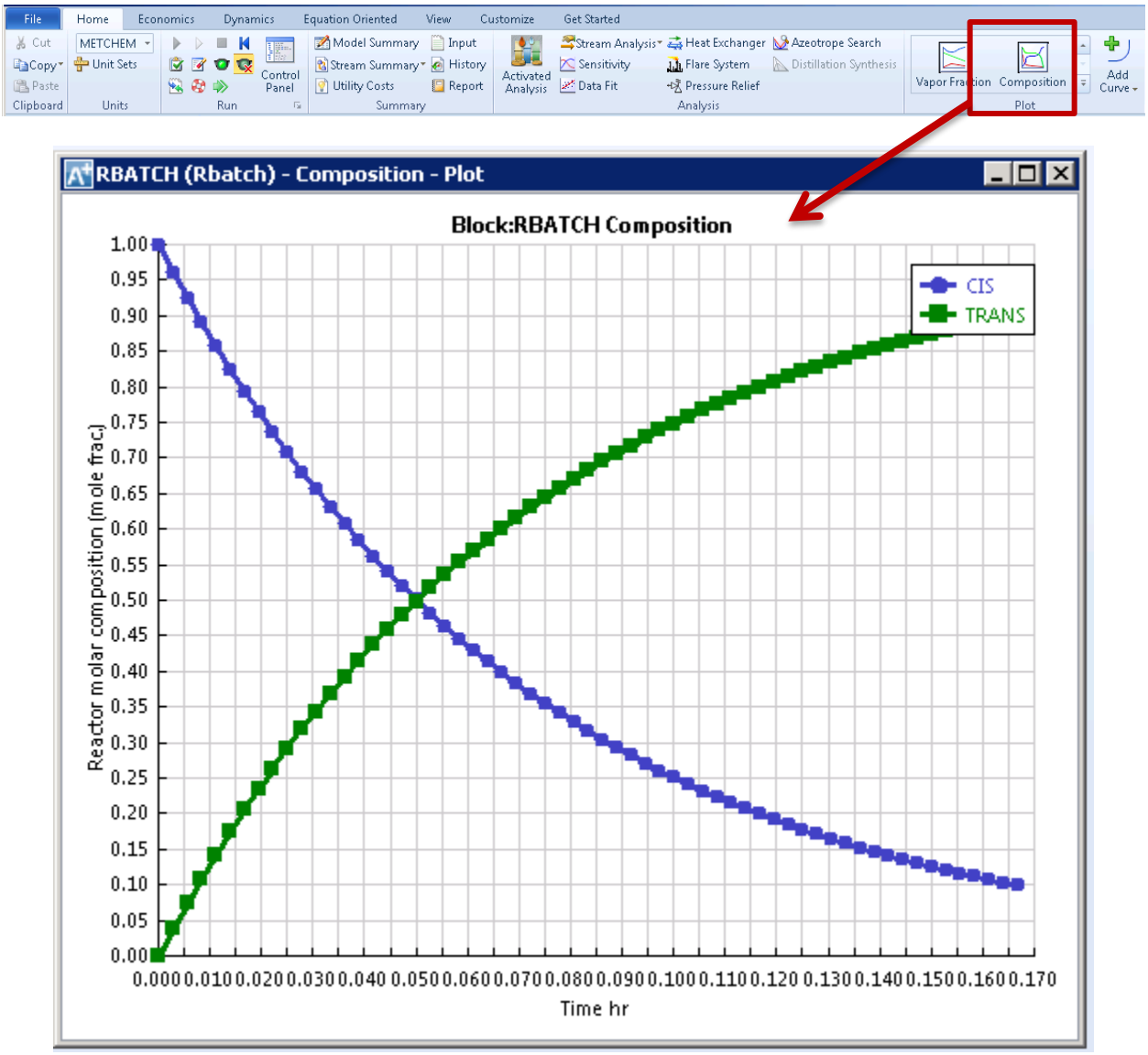
4.19. Check the result table. Go to the **Blocks | RBATCH | Profiles | Compositions** tab. The computed time at which the TRANS mole fraction is 0.9 is **10.01 min**., which is identical to the analytic solution.



You can change the time unit

The required reaction time to reach 90% conversion for component A

4.20. Check the result plot. Select **Composition Plot** in the Ribbon.



4.21. Optional calculation in Aspen Plus

a. Increase the Stop value in the Stop Criteria (as shown in Step 9) so that you can see more results for a longer time

b. What would happen if you changed the reaction constant k (e.g. k = 0.1 or 0.001 1/s)

c. It would be interesting to simulate the batch reactor behavior when the reaction is complex with additional reacting components. As we could imagine, an analytic solution won't be available if the reaction is complex with multi-components, but we can still simulate it in Aspen Plus. You just need to add more components and change reaction data. That is sufficient for any batch reactor simulation.

5. Conclusion

Both the analytical solution and stop criteria in Aspen Plus result in a residence time of 10.01 min. for 90% conversion. The ordinary differential equation (ODE) solution yields an exponential function, and the composition plot has an exponential shape. Using RBatch allows for more advanced calculations. It will model complex reaction systems including parallel and series reactions which lead to coupled systems of ODEs.

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