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

1. Lesson Objectives

- Use component mass balances to calculate the reaction conversion achieved with two continuous stirred tank reactors in series.
- Use Aspen Plus to confirm the analytical solution

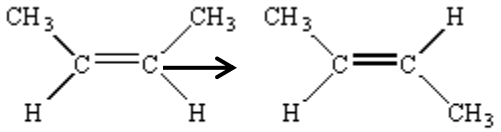
2. Prerequisites

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

3. Background

2-Butene is a four carbon alkene that exists as two geometric isomers: *cis*-2-butene and *trans*-2-butene. The irreversible liquid phase isomerization reaction with 1st order reaction kinetics is shown below.

Homogeneous reaction



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

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

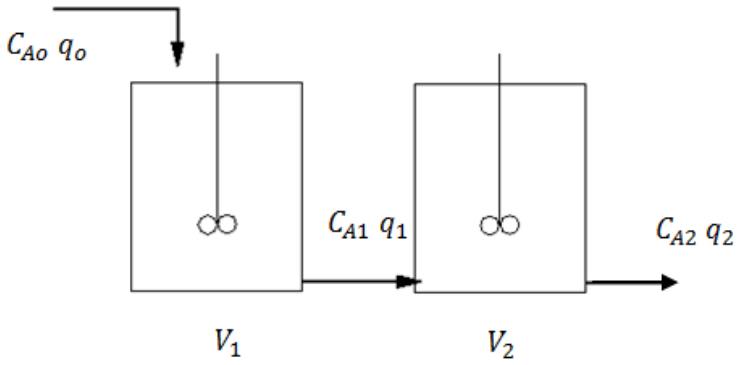
The examples presented are solely intended to illustrate specific concepts and principles. They may not reflect an industrial application or real situation.

4. Problem Statement and Solutions

Problem #1

Determine the conversion achieved if two CSTRs are used in series. Each CSTR has a residence time of 20 min. Assume steady state.

Analytic Solution:



First Reactor Component A Balance

$$V_1 \frac{dC_A}{dt} = C_{Ao}q_o - C_{A1}q_1 - kC_{A1}V_1 = 0$$

$$C_{A1} = \frac{C_{Ao}q_0}{q_1 + KV_1}$$

Second Reactor Component A Balance

$$V_2 \frac{dC_A}{dt} = C_{A1}q_1 - C_{A2}q_2 - kC_{A2}V_2 = 0$$

$$C_{A2} = \frac{C_{A1}q_1}{q_2 + kV_2} = \frac{C_{Ao}q_1q_0}{(q_1 + kV_1)(q_2 + kV_2)}$$

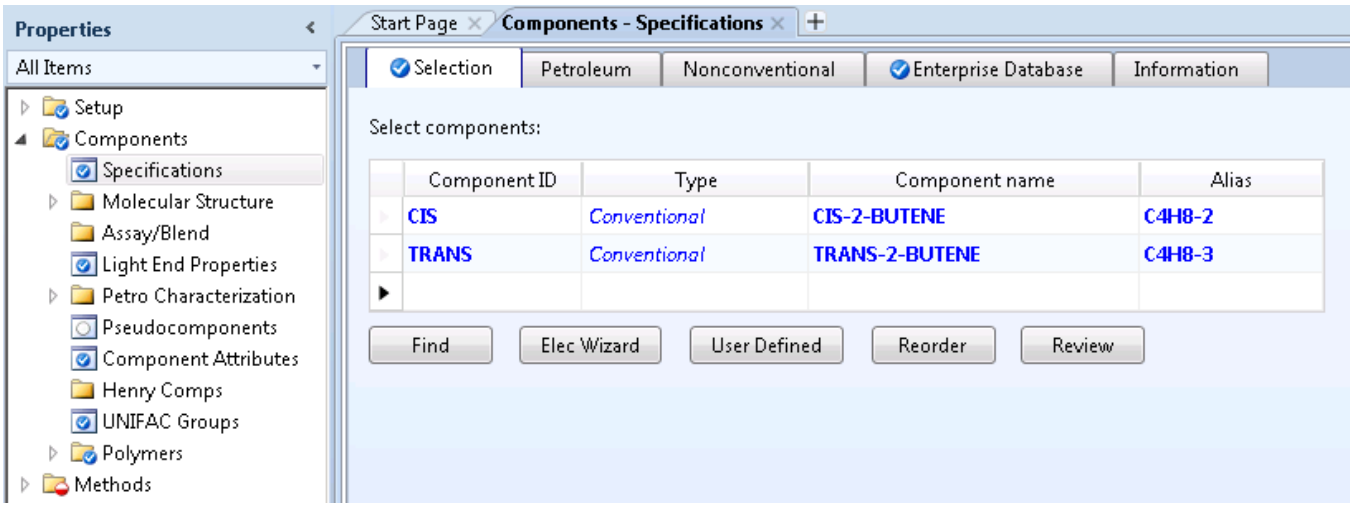
Conversion

$$X = 1 - \frac{C_{A2}}{C_{Ao}} = 1 - \frac{1}{(1 + k\tau_1)(1 + k\tau_2)} = 1 - \frac{1}{\left(1 + (0.23min^{-1})(20min)\right)^2} = \mathbf{0.968112}$$

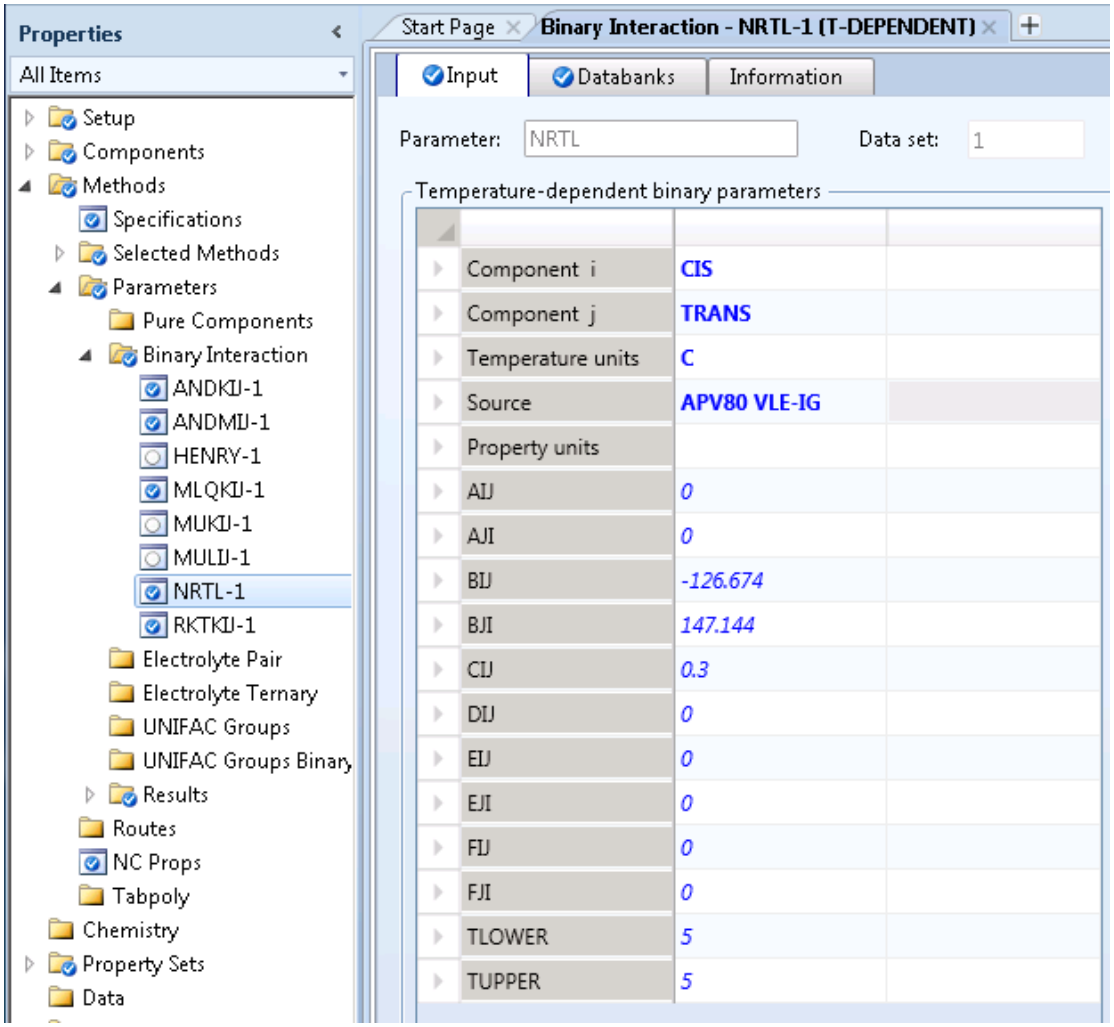
Aspen Plus Solution:

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

4.02. Begin by defining the components in the **Components | Specifications | Selection** tab. Enter **CIS-2-BUTENE** and **TRANS-2-BUTENE** for **Component name** and enter **CIS** and **TRANS** as the **component ID's**. A window will appear stating that this change will cause parameters to be updated. Click **Yes**.

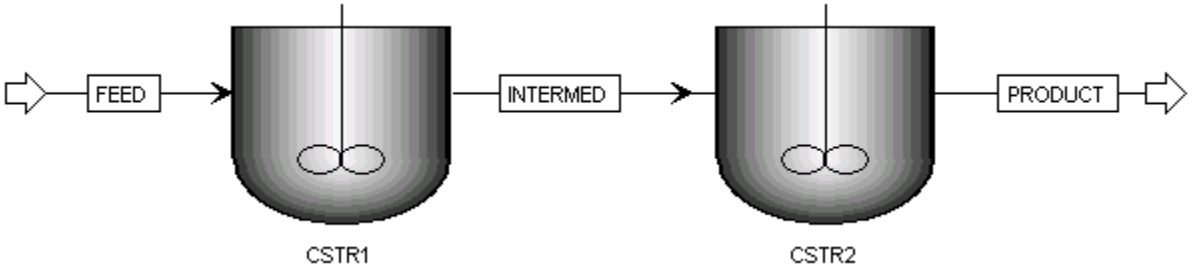


4.03. Populate the binary interaction parameters by going to **Methods | Parameters | Binary Interaction | NRTL-1**.

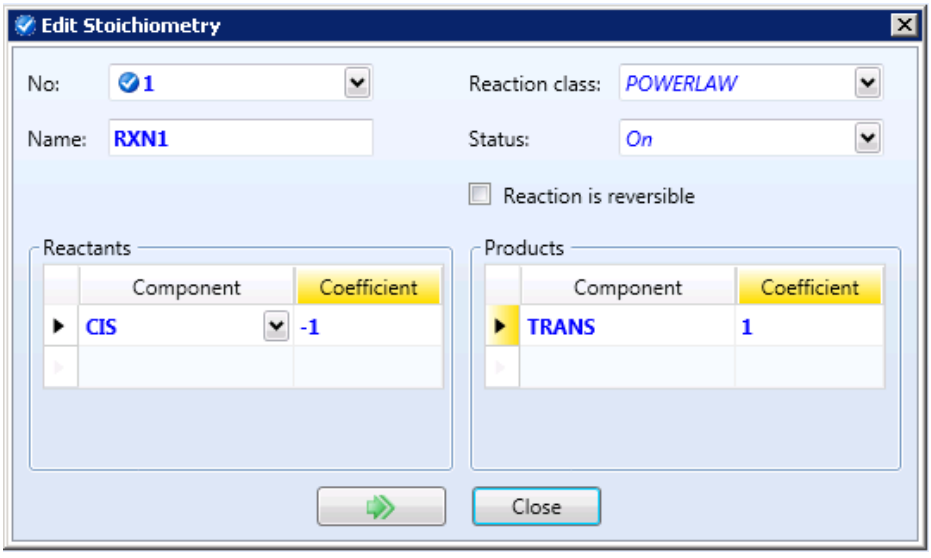


4.04. To create the flowsheet, move to the simulation environment by clicking the **Simulation** button in the bottom left of the screen.

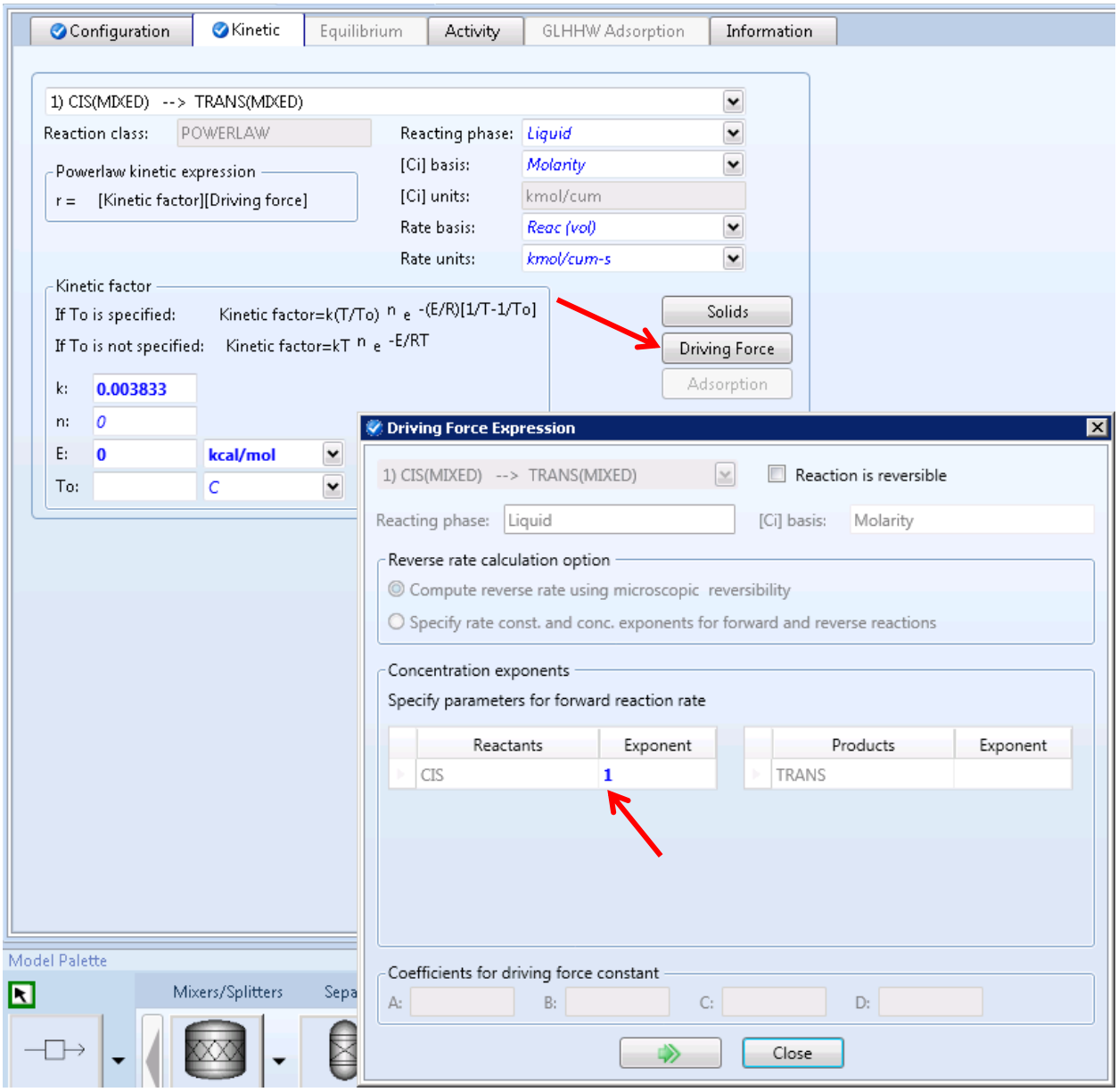
4.05. From the **Model Palette** add two **RCSTR** models to the main flowsheet. The RCSTR model is located under the **Reactors** tab. The RCSTR block models a continuously stirred tank reactor with user-provided stoichiometry and kinetics. Place 2 CSTRs in series and connect the necessary ports with material streams.



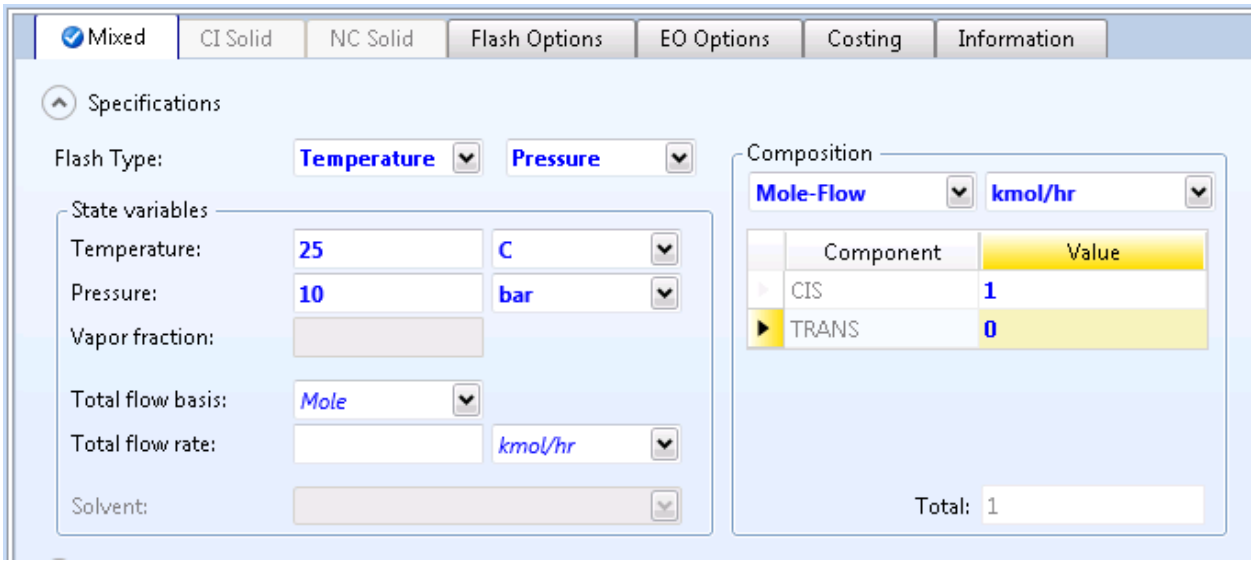
4.06. Define the reactions. Go to **Reactions** in the navigation pane and click **New**. The default reaction ID **R-1** will be created, and select **GENERAL** for reaction type. In **R-1**, click **New** which will open a stoichiometry window. Give the reaction a name, select the reactants and products for this reaction and specify the stoichiometric coefficients.



4.07. Click on the **Kinetic** tab and enter **k = 0.003833** and **E = 0**. Next click **Driving Force** and enter **1** for the **CIS** reactant exponent.

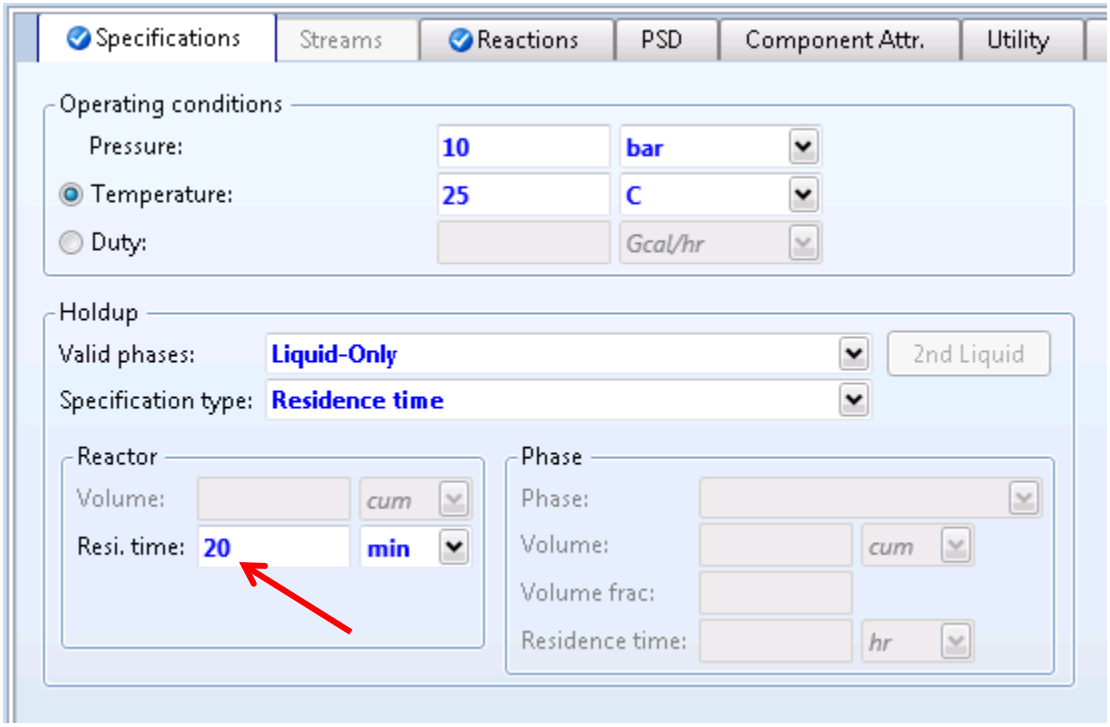


4.08. Specify the feed stream. Go to **Streams | FEED | Input**. Under **Composition** select **Mole-Flow** and enter a value of **1 kmol/hr** for **CIS** and **0** for **TRANS**. Under the **State variables** enter **T = 25°C**, and **P = 10 bar**. (Note that we will be specifying residence time in the reactor block therefore the calculated conversion will be the same for any given flowrate.)

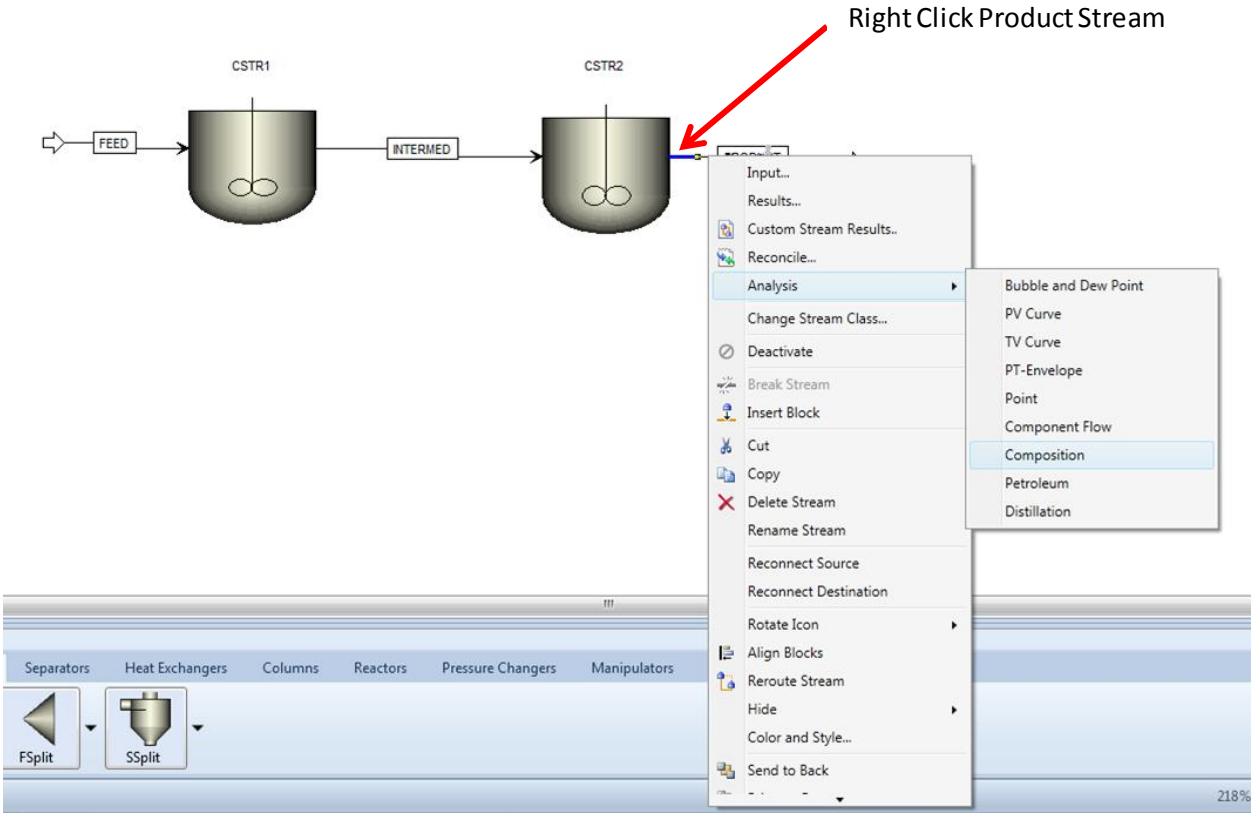


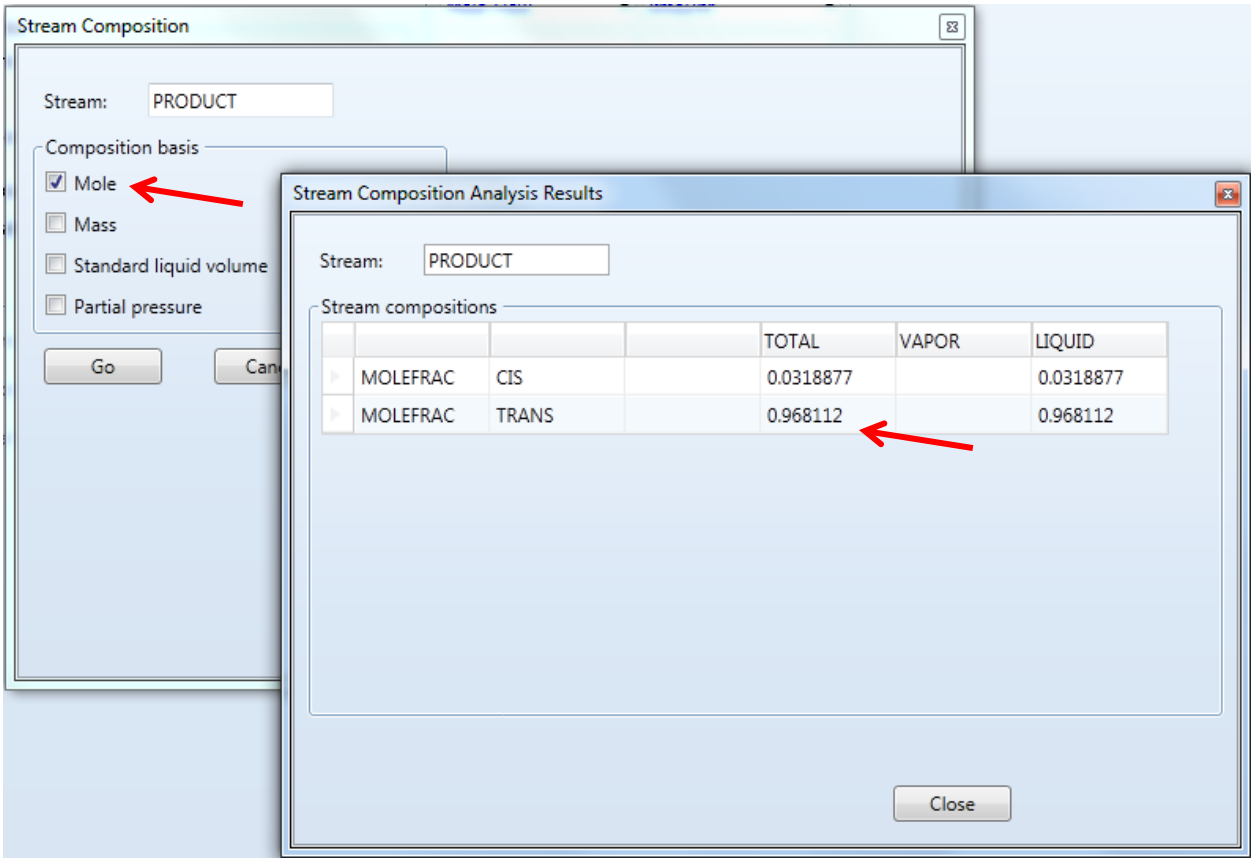
4.09. Specify the operating conditions of the CSTRs. Go to **Blocks | CSTR1 | Setup**. Enter **Pressure = 10 bar**, **Temperature = 25°C**, **Valid Phases = Liquid Only**, and **Specification Type = Residence time**. Enter a residence time of **20 min** and select **R-1** in the **Reactions** tab.

Repeat this for the second CSTR.



4.10. Open the **Control Panel** and run the simulation (**F5**). Go to the main flowsheet and right click on the **PRODUCT** stream. Click **Analysis | Composition** and check **Mole** then click **Go**. The mole fraction of trans-2-butene in the product stream is **0.968112**. This means the reaction conversion is 0.968112, which is identical to the analytical solution.

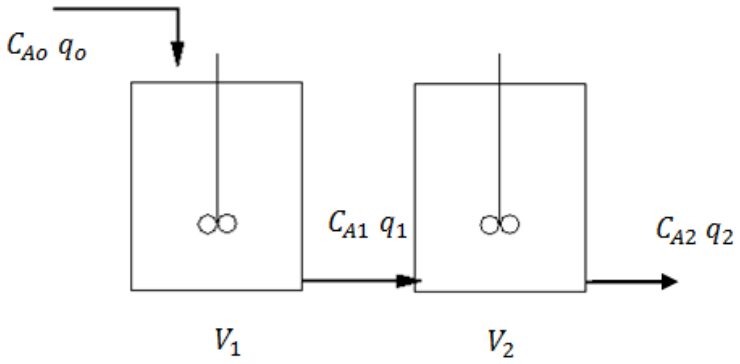




Problem #2

Consider the same 1st order reaction, except this time using two CSTRs of different sizes. Calculate the conversion achieved if the first reactor has a residence time of 30 min and the second reactor has a residence time of 10 min. Assume steady state.

Analytic Solution:



First Reactor Component A Balance

$$V_1 \frac{dC_A}{dt} = C_{Ao} q_o - C_{A1} q_1 - k C_{A1} V_1 = 0$$

$$C_{A1} = \frac{C_{Ao} q_0}{q_1 + K V_1}$$

Second Reactor Component A Balance

$$V_2 \frac{dC_A}{dt} = C_{A1} q_1 - C_{A2} q_2 - k C_{A2} V_2 = 0$$

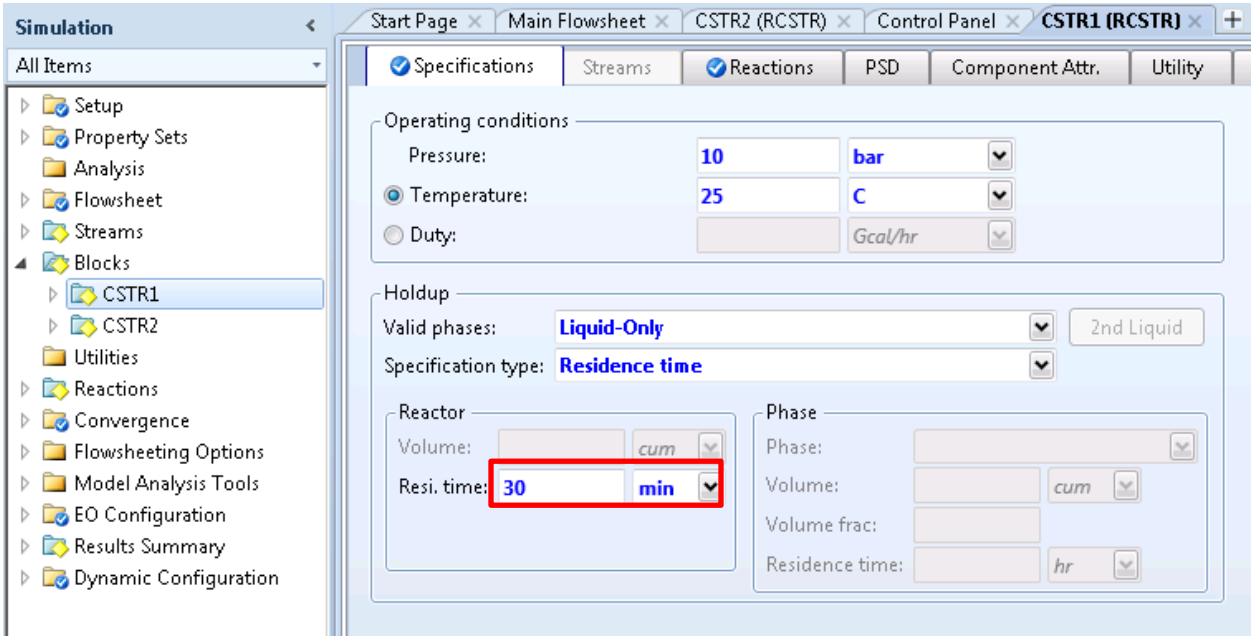
$$C_{A2} = \frac{C_{A1} q_1}{q_2 + k V_2} = \frac{C_{Ao} q_1 q_0}{(q_1 + k V_1)(q_2 + k V_2)}$$

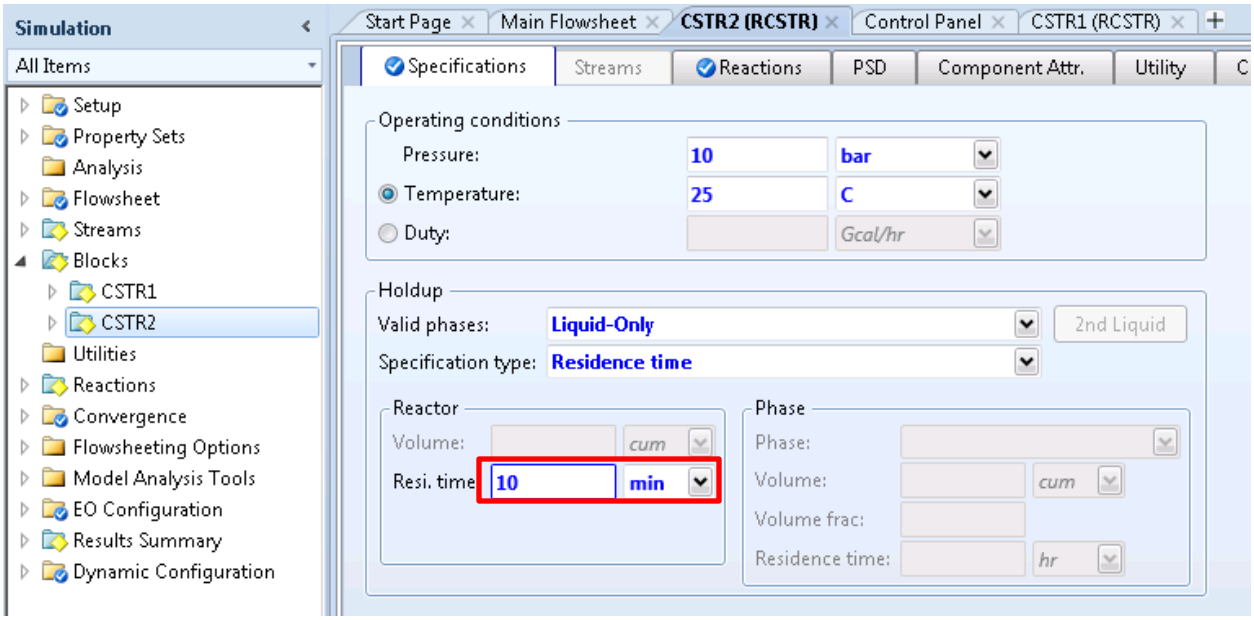
Conversion

$$X = 1 - \frac{C_{A2}}{C_{Ao}} = 1 - \frac{1}{(1+k\tau_1)(1+k\tau_2)} = 1 - \frac{1}{(1+(0.23 min^{-1})(30 min))(1+(0.23 min^{-1})(10 min))} = \mathbf{0.961642}$$

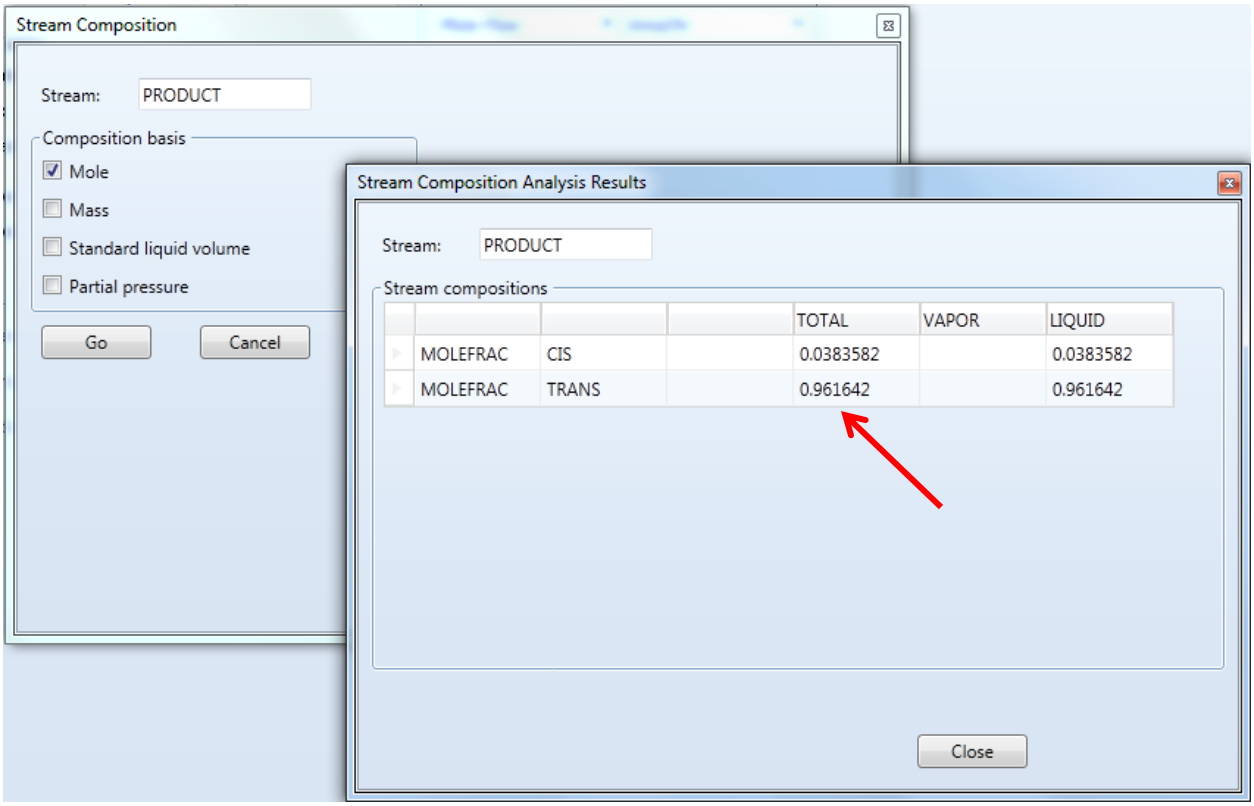
Aspen Plus Solution:

4.11. The same procedure described in the case of two equal volume CSTRs in series should be followed. The only difference being the first CSTR has a residence time of **30 min** and the second CSTR has a residence time of **10 min**.





4.12. Run the simulation. The mole fraction of trans-2-butene in the product stream is 0.**961642**, thus the conversion is 0.96164. This is identical with the analytic solution.



Note: In this problem, residence time was specified instead of volume because if volume is specified then volumetric flowrate must be calculated to solve for conversion. In this isomerization reaction, the cis and trans forms of 2-butene have different densities, and therefore the volumetric flowrate does not

remain constant throughout the reaction process. This makes it difficult to solve this problem analytically.

5. Conclusion

The conversion is slightly higher when the residence times are the same. When both are 20 min., the conversion is 96.81%, and it is only 96.16% when they are 30 and 10 min. respectively. This is a result of the decreasing dependence of conversion on residence time: the second derivative of conversion with respect to residence time is negative.

$$\frac{d\mathrm{X}^2}{d^2\tau} < 0$$

Total residence time is not sufficient to describe a series system of CSTRs. Multiple CSTRs in series yield higher conversion than a single CSTR that has a residence time equal to the sum of the series arrangement.

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