Isomerization in a PFR with Aspen Plus® V8.0

1. Lesson Objectives

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

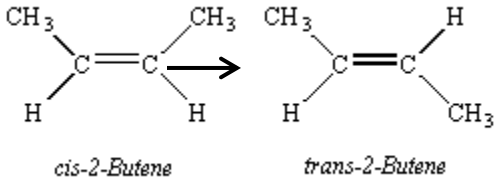
2. Prerequisites

- Aspen Plus V8.0
- Basic knowledge of reaction rate laws and plug flow reactors

3. Background/Problem

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.

Homogeneous reaction



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

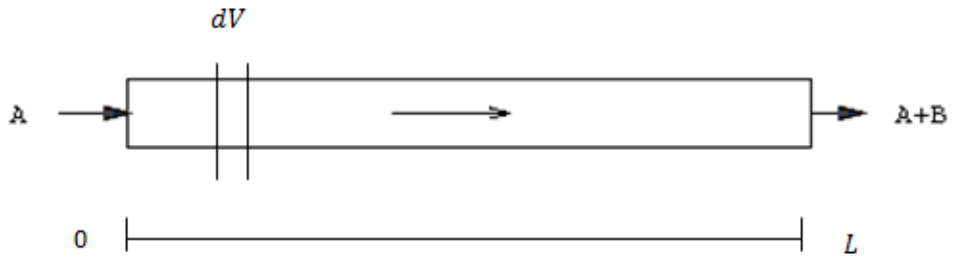
1st order reaction kinetics $r_A = kC_A, k = 0.23min^{-1} = 0.003833s^{-1}$

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 Aspen Plus Solution

Calculate the residence time required to achieve 90% conversion using a plug flow reactor. Assume steady state operation.

Analytic Solution:



$$q\frac{dC_A}{dV} = -kC_A$$

$$q\int_{C_{Ao}}^{C_{A,L}} \frac{dC_A}{C_A} = -k\int_0^L dV$$

$$q ln\frac{C_{A,L}}{C_{Ao}} = -kV$$

$$C_{A,L} = C_{Ao}\exp\left(\frac{-kV}{q}\right)$$

$$\tau = \frac{V}{q} = \frac{1}{k}\ln\left(\frac{C_{Ao}}{C_{A,L}}\right)$$

$$X = 1 - \frac{C_{A,L}}{C_{Ao}}$$

$$\frac{C_{Ao}}{C_{A,L}} = \frac{1}{1-X}$$

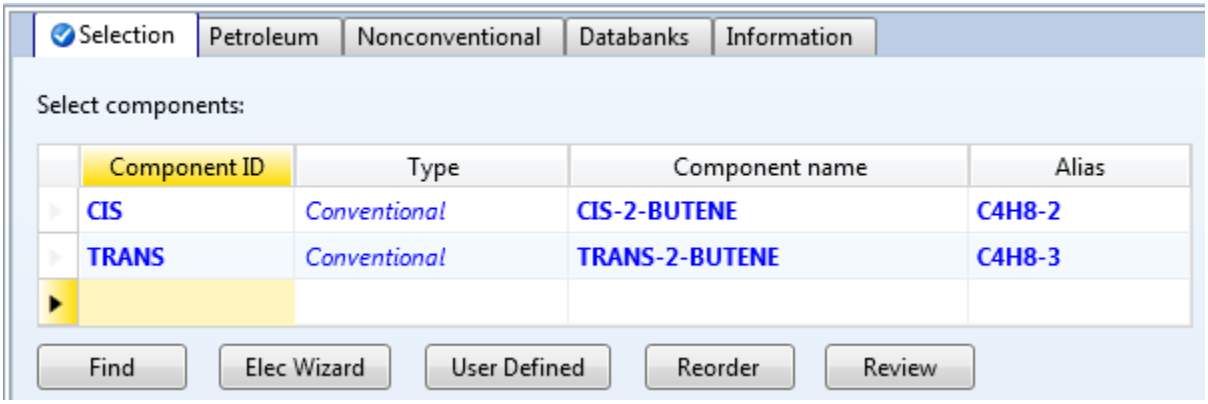
$$\tau = \frac{1}{k}\ln\left(\frac{1}{1-X}\right)$$

$$\tau = \frac{1}{0.23min^{-1}}\ln\left(\frac{1}{1-.9}\right) = \mathbf{10.01\ min}$$

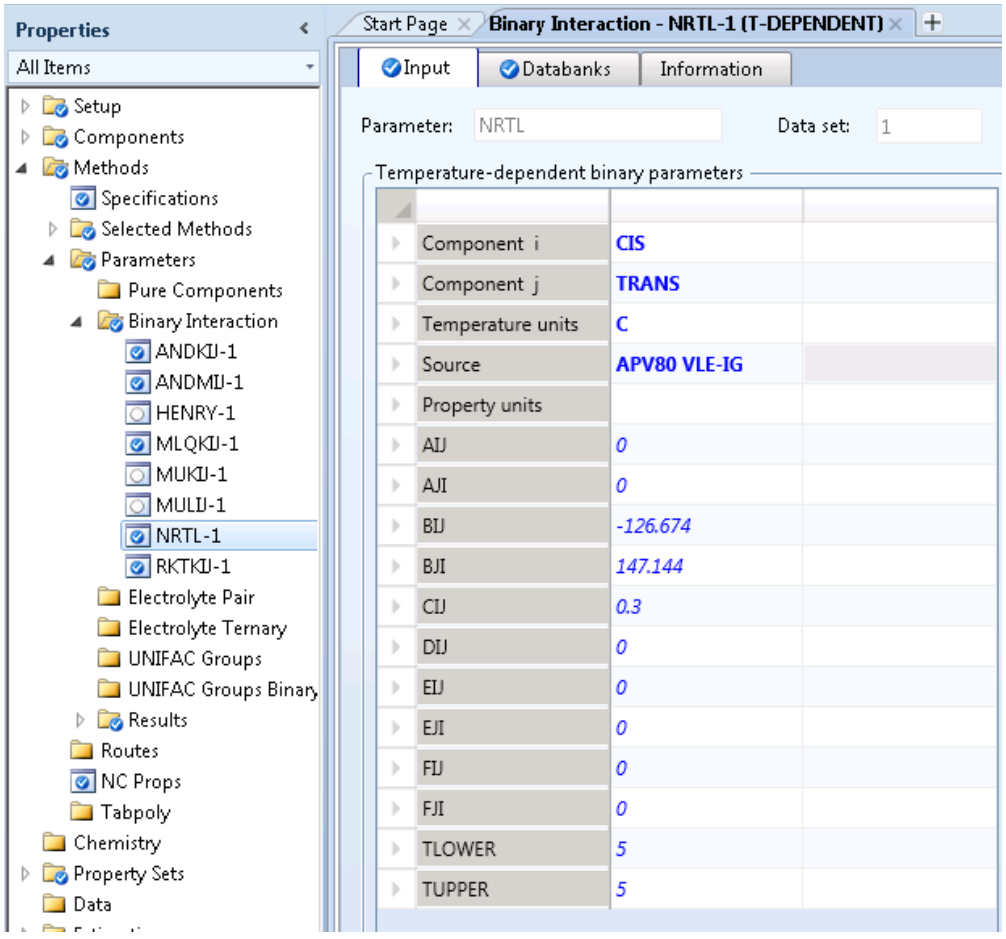
Aspen Plus Solution:

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** as **Component name** and enter **CIS** and **TRANS** as the **Component ID's**. A window will appear stating that these changes will cause parameters to be updated. Click **Yes**.

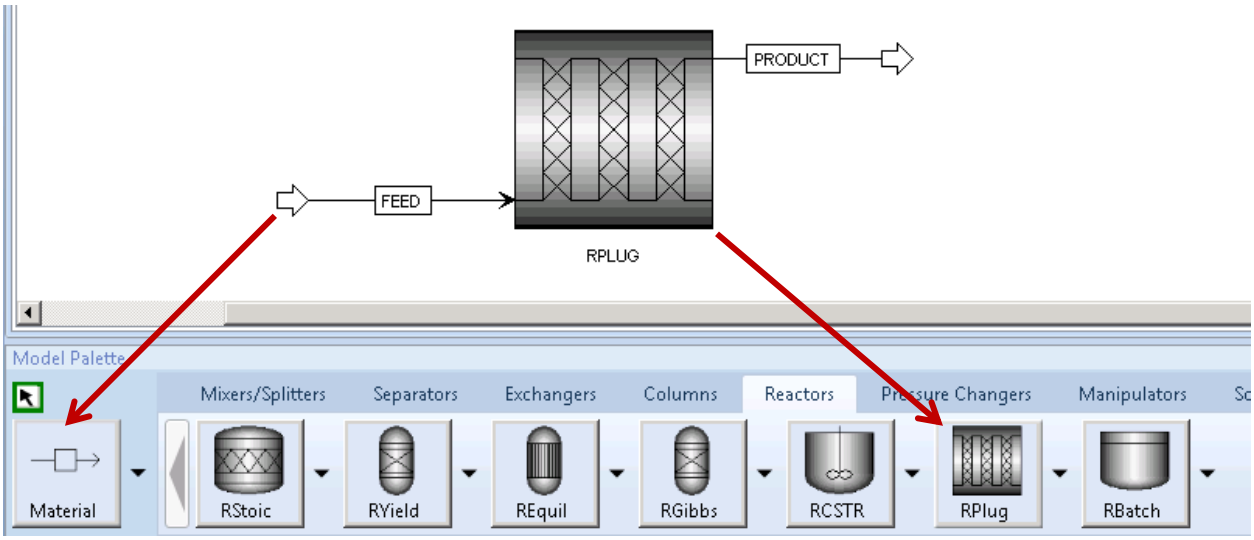


4.03. To populate the binary interaction parameters go to **Methods | Parameters | Binary Interaction | NRTL-1**.

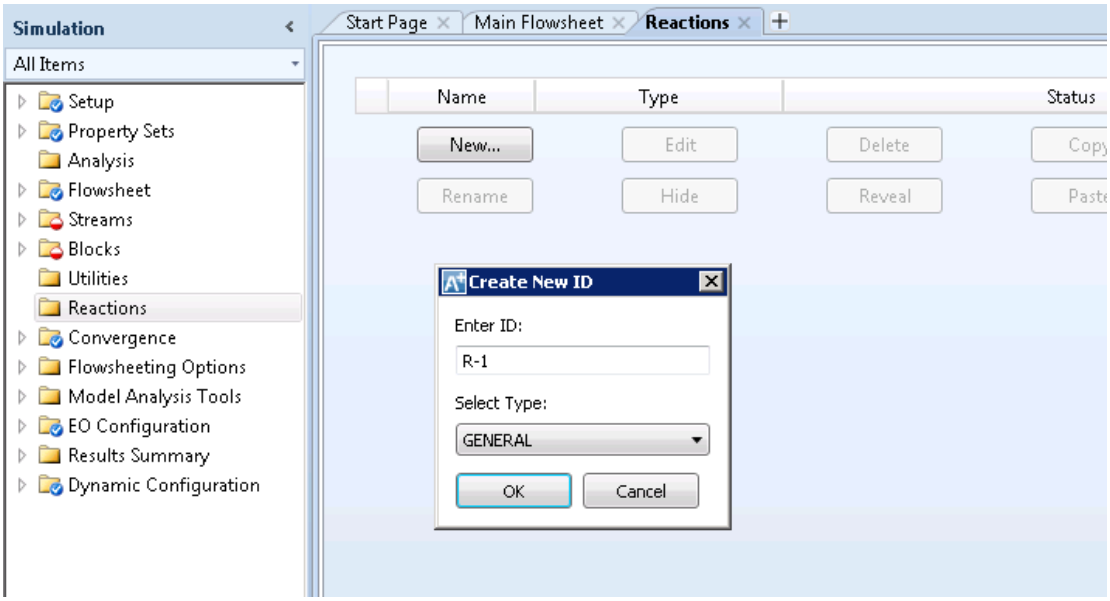


4.04. Go to the simulation environment by clicking the **Simulation** button in the bottom left of the screen.

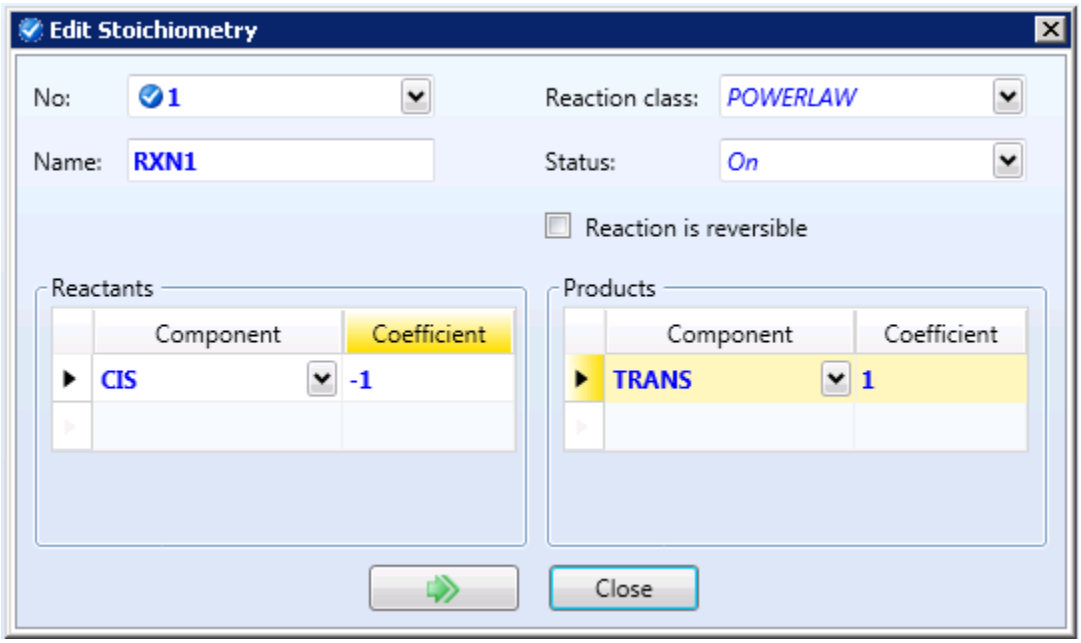
4.05. Create the process flowsheet by selecting an **RPlug** block from the **Model Palette** under the **Reactors** tab. The RPlug block models a plug flow reactor with no axial mixing using the user specified stoichiometry and kinetics. Drop the RPlug block onto the flowsheet and connect the inlet and outlet ports with material streams. Name these streams accordingly, in this case **FEED** and **PRODUCT**.



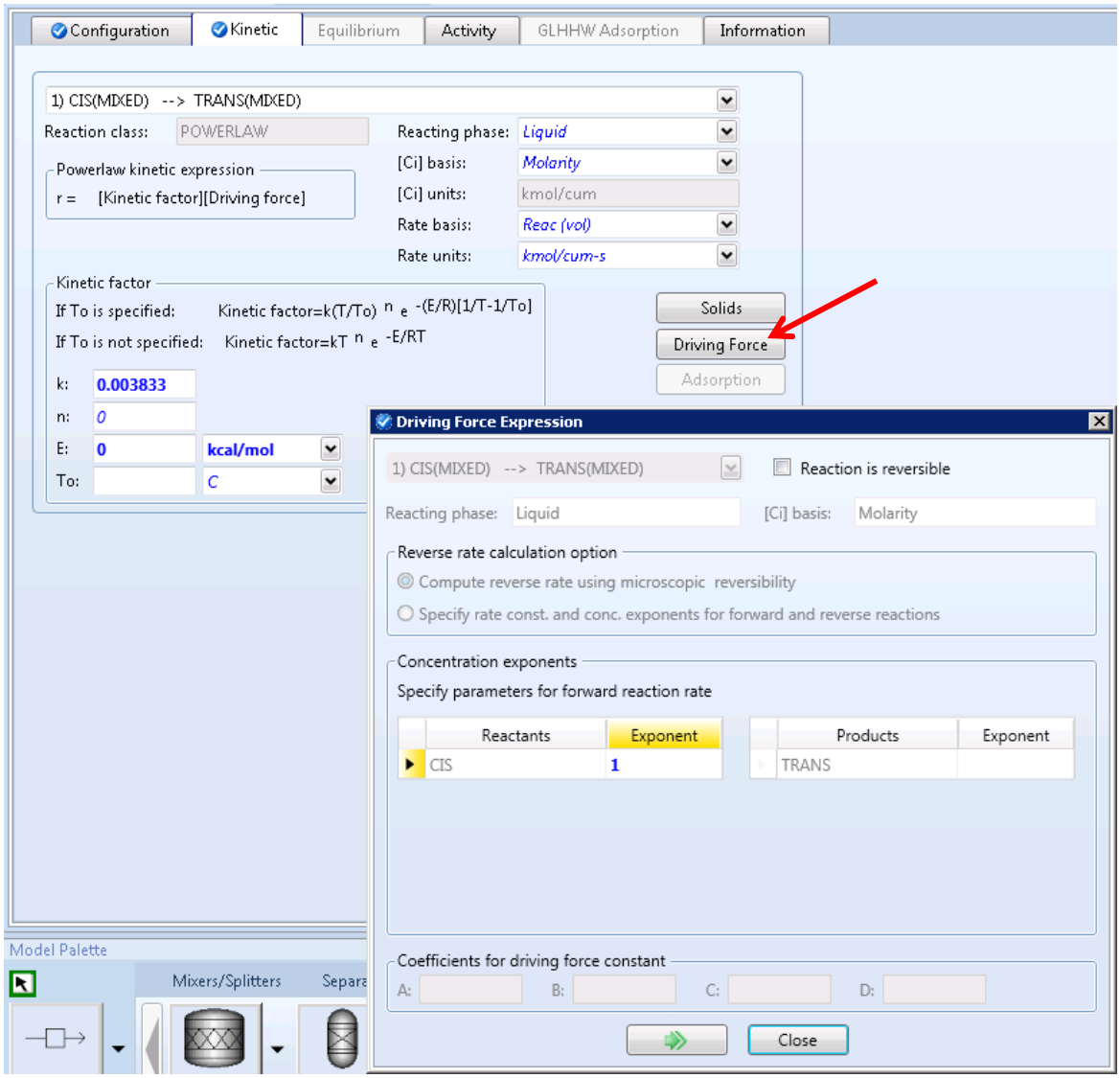
4.06. Define the reaction. Go to **Reactions** in the navigation pane and select **New**. The default reaction ID **R-1** will be created. Select **GENERAL** for reaction type.



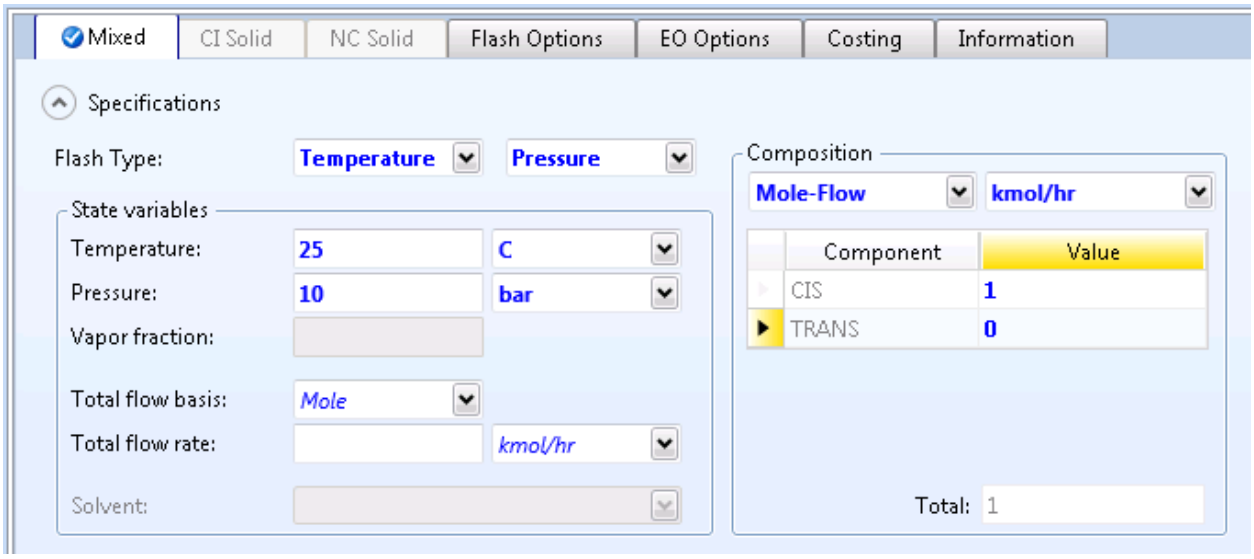
4.07. In the **R-1 | Configuration** tab click **New** which will open a stoichiometry window. Name the reaction, select reactants and products for this reaction and specify the stoichiometric coefficients.



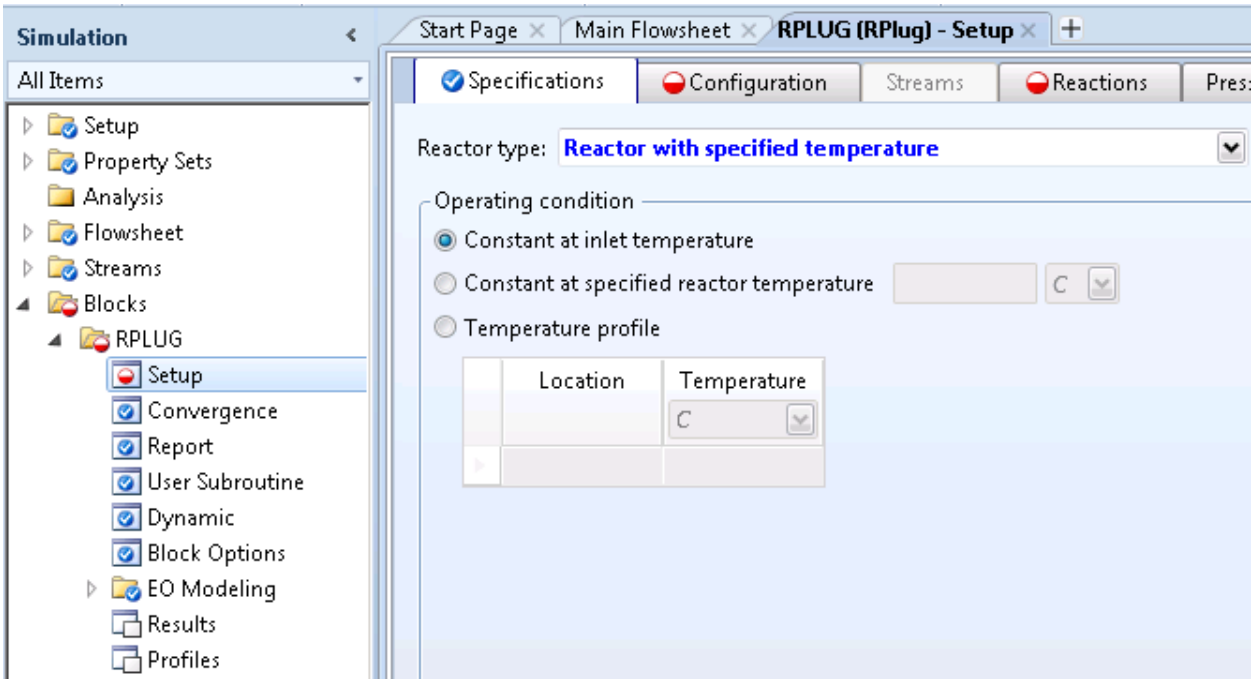
4.08. Click on the **Kinetic** tab and enter **k = 0.003833** and **E = 0**. Next click **Driving Force** and enter **1** for the **CIS** reactant exponent.



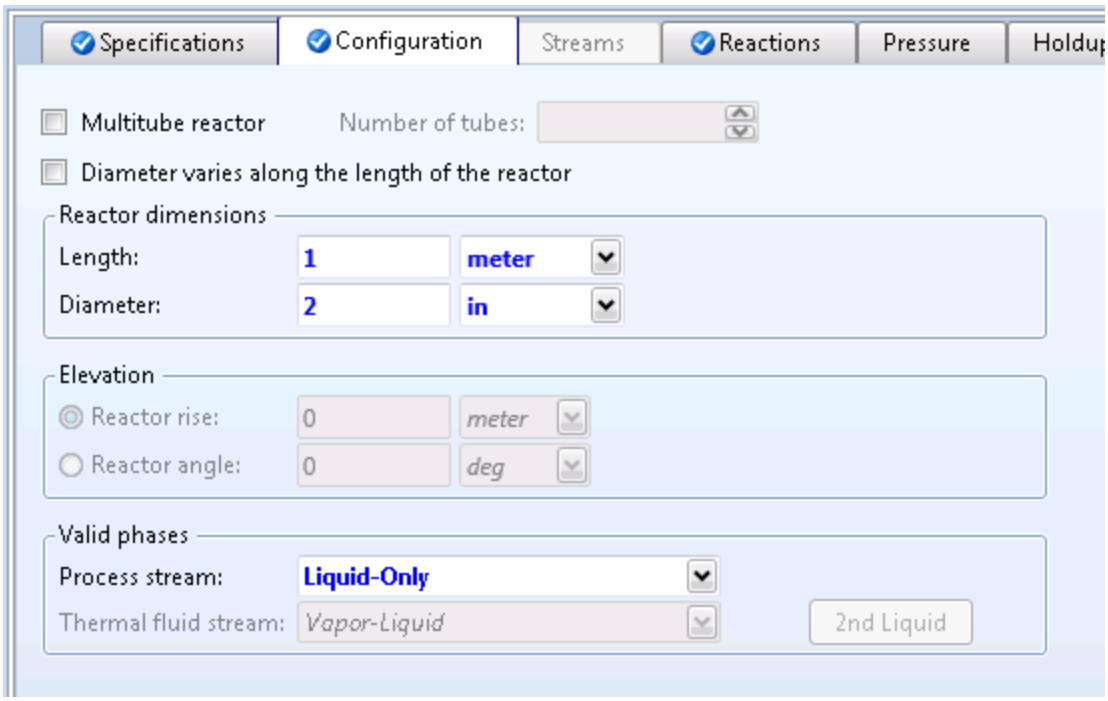
4.09. Specify the feed Stream. Go to **Streams | FEED | Input**. Under **Composition** select **Mole-Flow** and enter a value of **1 kmol/hr** for **CIS** and **0** for **TRANS**. Under the **State variables** enter **T = 25°C**, **P = 10 bar**. (Note that the required residence time will be the same regardless of flowrate.)



4.10. Specify the PFR operating conditions by clicking **Blocks | RPLUG | Setup**. Select **Reactor with specified temperature** as the **Reactor type**, with the operating condition of **Constant at inlet temperature**.

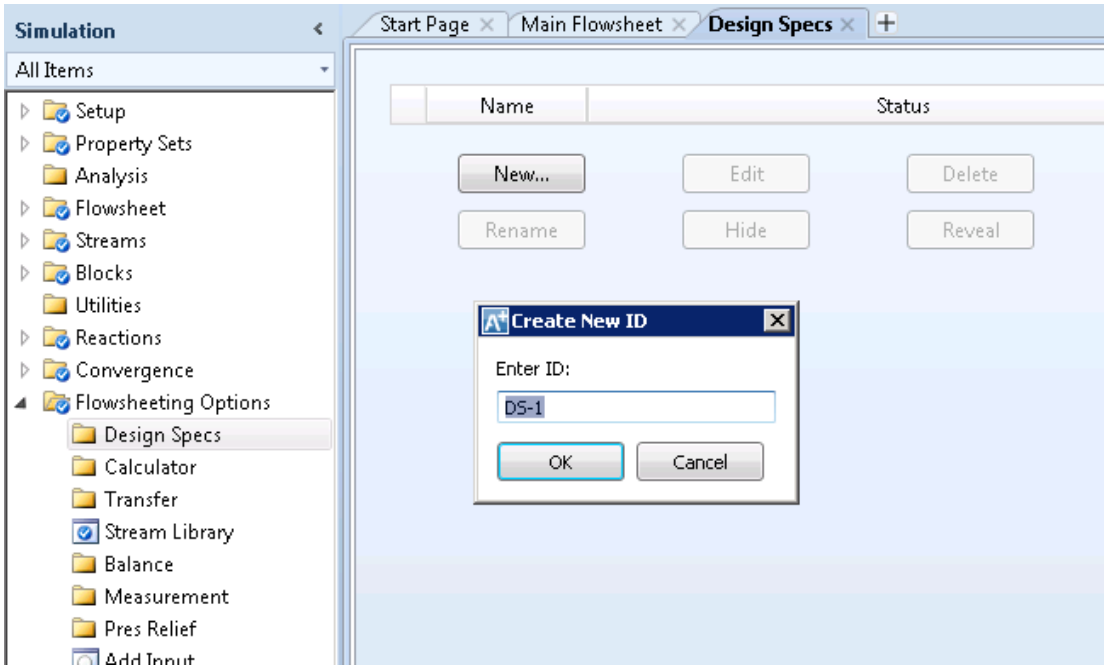


4.11. Click the **Configuration** tab and enter **Length = 1 meter** and **Diameter = 2 inches** (this geometry is just an initial guess and will be iterated to find the solution in the flowsheet design spec shown in step 8). Select **Liquid-Only** for **Valid phases**. In the **Reactions** tab, select **R-1** to be included in the **Selected reaction sets**.

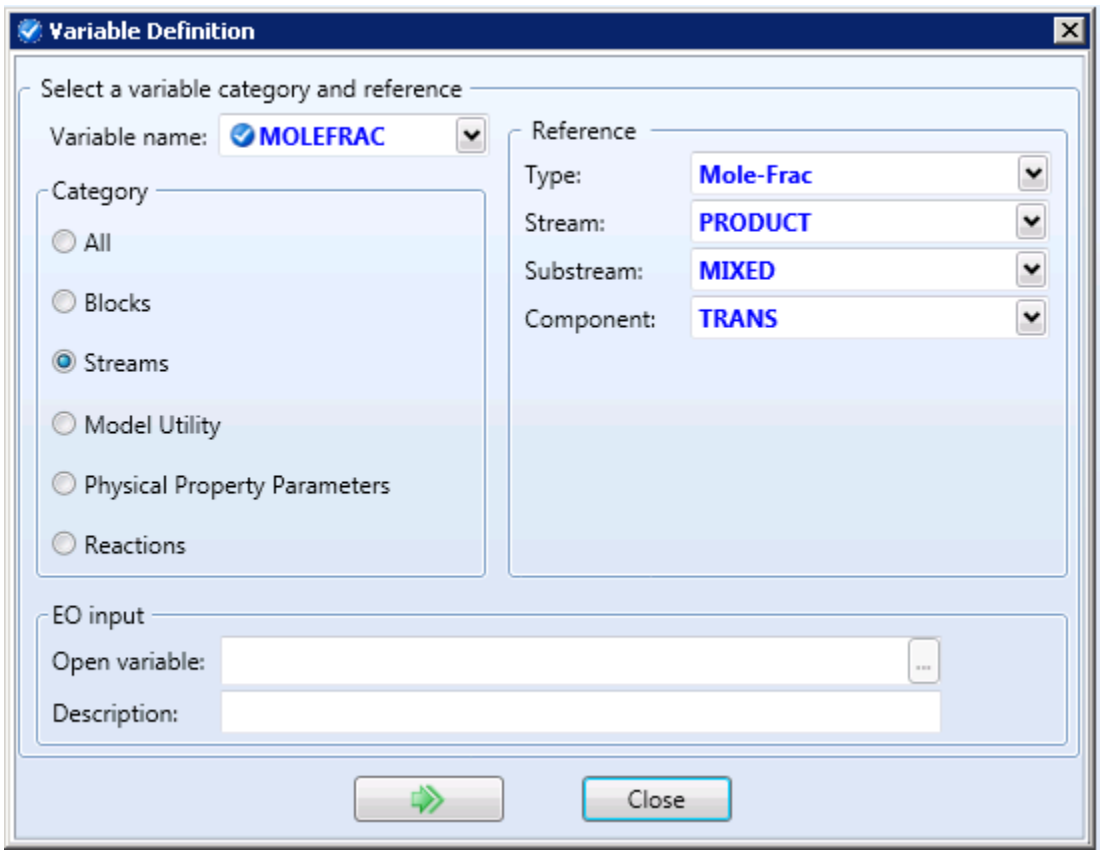


Often times plug flow reactors are designed to contain multiple tubes. This is common for reactions that require a high surface area to volume ratio, such as an exothermic reaction where efficient cooling is necessary. For future use, note where to select **Multitube reactor** and enter **Number of tubes**. For this example we will just assume a single tube.

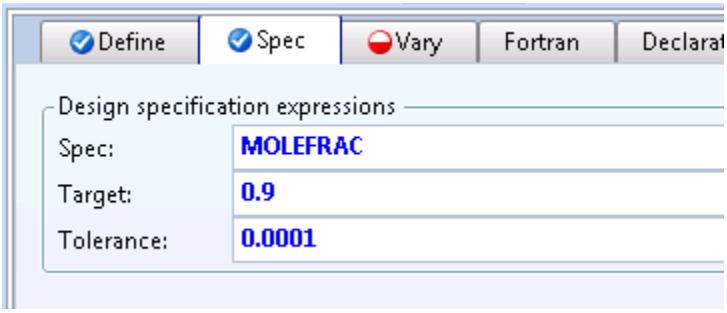
4.12. Create a design specification to determine the residence time required to achieve 90% conversion. As stated in the previous exercises, design specs are used to manipulate input variables to achieve a desired operating result. In the navigation pane go to **Flowsheeting Options | Design Spec | New**. A design spec with the default name **DS-1** will be created.



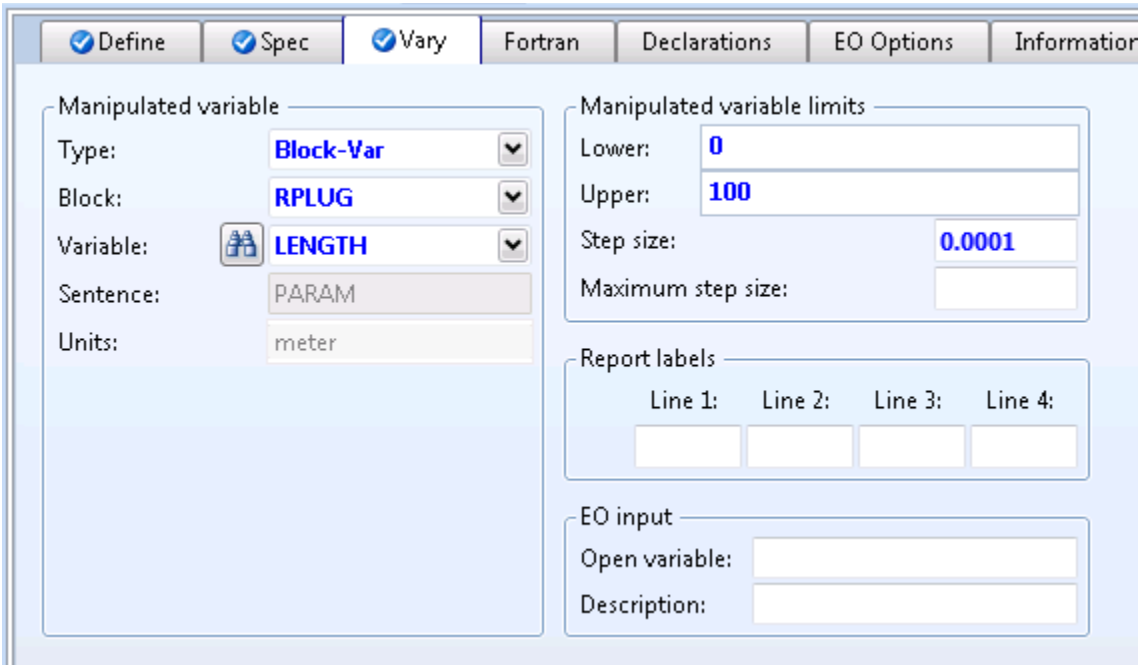
4.13. In the **DS-1 | Define** tab click on **New** and create the variable **MOLEFRAC**. This variable will be defined as the mole fraction of trans-2-butene in the product stream.



4.14. Click on the **Spec** tab and enter **Spec = MOLEFRAC**, **Target = 0.900**, and **Tolerance = 0.0001**.

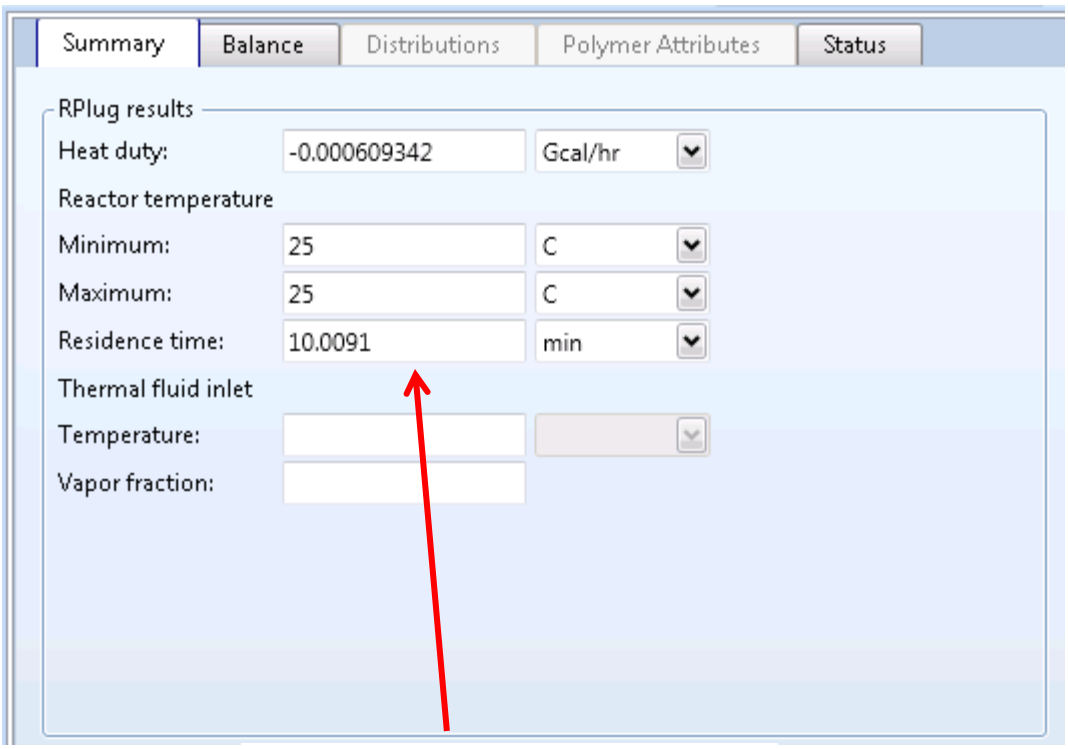


4.15. Click on the **Vary** tab and specify the reactor length to be the manipulated variable.



4.16. Open the **Control Panel** and run the simulation (**F5**). The simulation should complete with no warnings or errors.

4.17. To check results go to **Blocks | RPLUG | Results**. The residence time is equal to approximately 10.01 minutes, identical to the analytical solution.



Required residence time to achieve 90% conversion in the reactor.

5. Conclusion

Both the analytical solution and design spec in Aspen Plus produced the same required residence time of 10.01 min. to achieve 90% reaction conversion in a plug flow reactor. The residence time for a PFR is the same as for a batch reactor. Compare this to the residence time required for a CSTR (RX-003_CSTR_CIStoTRANS). Using RPFR 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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