# Isomerization in a CSTR with Aspen Plus® V8.0

## 1. Lesson Objectives

- Use component mass balances to calculate the time required to reach a desired conversion in a continuous stirred tank reactor.
- Use Aspen Plus to confirm the analytical solution

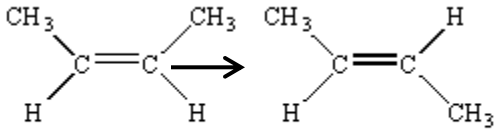
## 2. Prerequisites

- 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. It is desired to determine the time required to reach 90% reaction conversion in a continuous stirred tank reactor. Assume steady state.

Homogeneous reaction



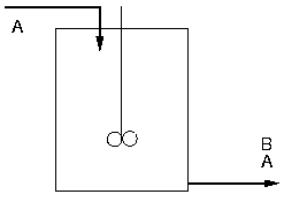

*cis-2-Butene* *trans-2-Butene*

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:




Component A Mole Balance

$$V\frac{dC_A}{dt} = qC_{Ao} - qC_A - kC_AV = 0$$

$$\frac{V}{q} = \frac{C_{Ao}-C_A}{kC_A}$$

Conversion (X)

$$X = 1 - \frac{C_A}{C_{Ao}}$$

$$C_A = C_{Ao}(1 - X)$$

Residence Time (τ)

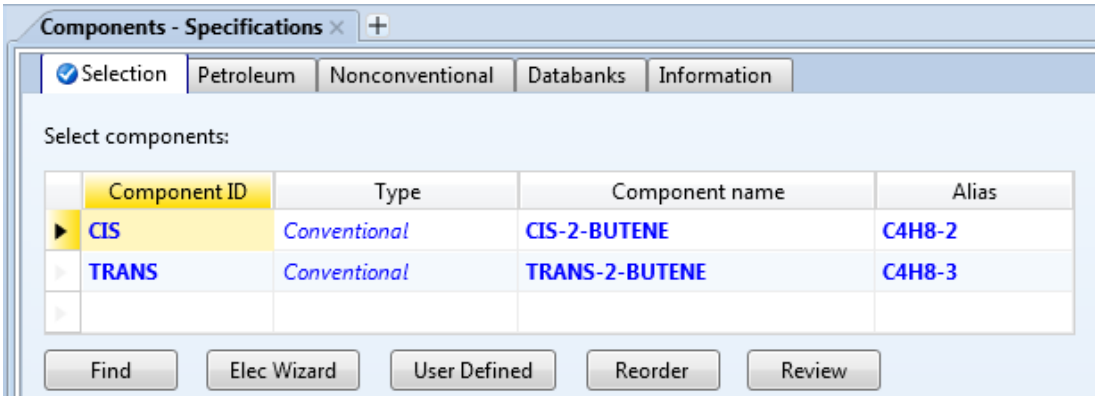
$$\tau = \frac{V}{q}$$

$$\therefore \tau = \frac{X}{k(1-X)} = \frac{0.9}{0.23min^{-1}(1-.9)} = \mathbf{39.13\ min}$$

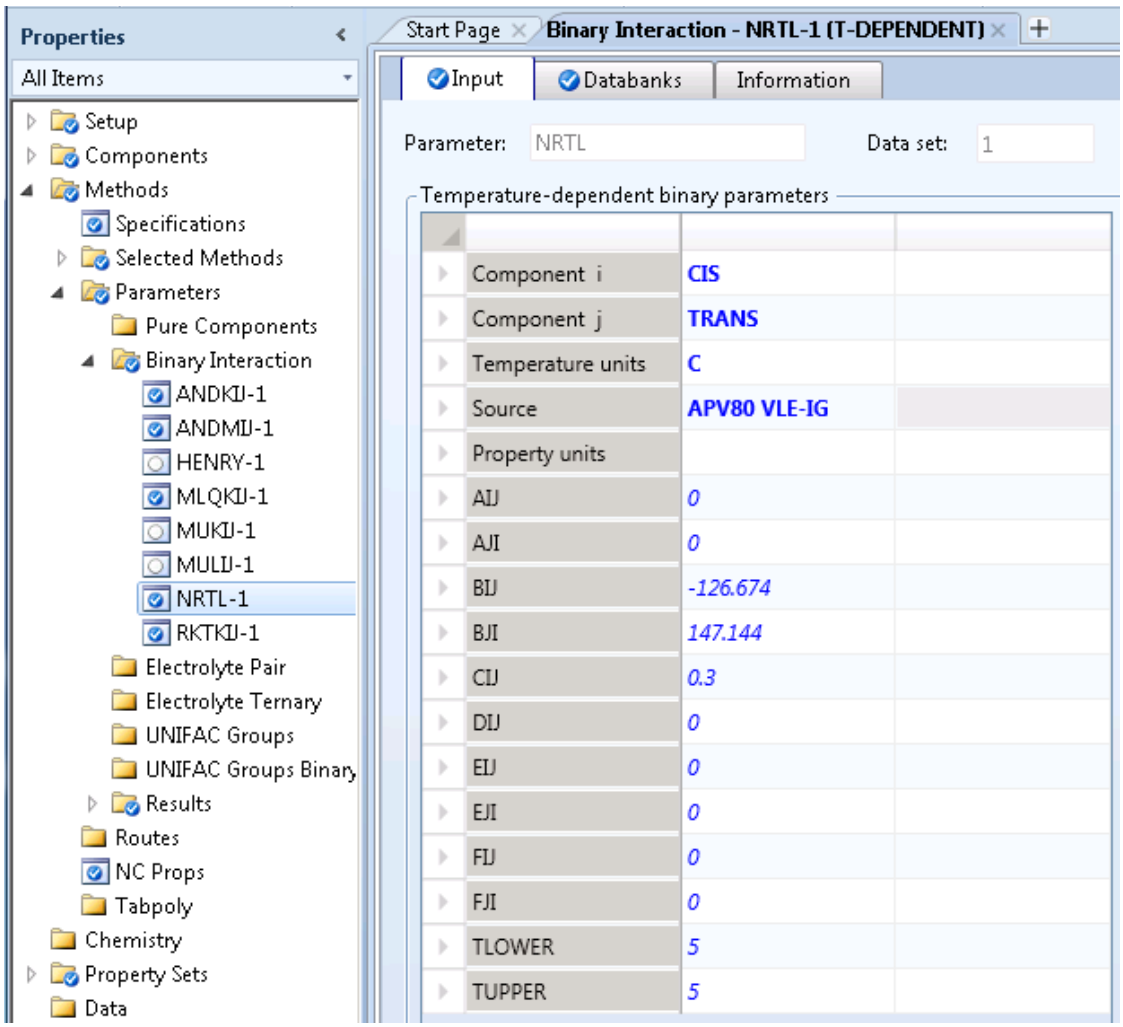
Aspen Plus Solution:

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** for **Component name**. Enter **CIS** and **TRANS** as the **Component ID's**. If a dialogue box appears informing you that parameters will be updated, click **Yes**.

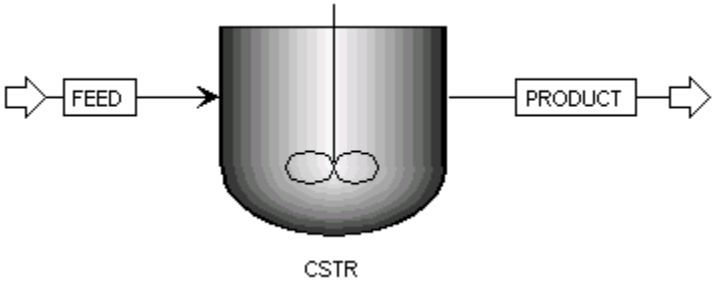



4.03. Populate the binary interaction parameters by going to **Methods | Parameters | Binary Interaction | NRTL-1**. The parameters will be automatically generated.

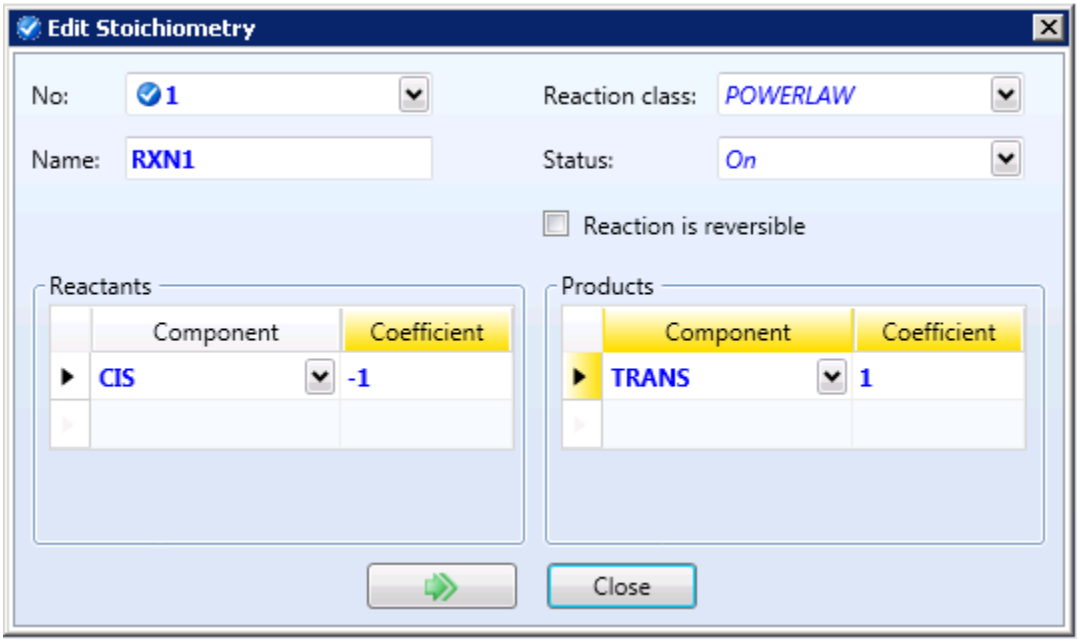



4.04. Move to the simulation environment by clicking the **Simulation** button below the navigation pane on the left of the screen.

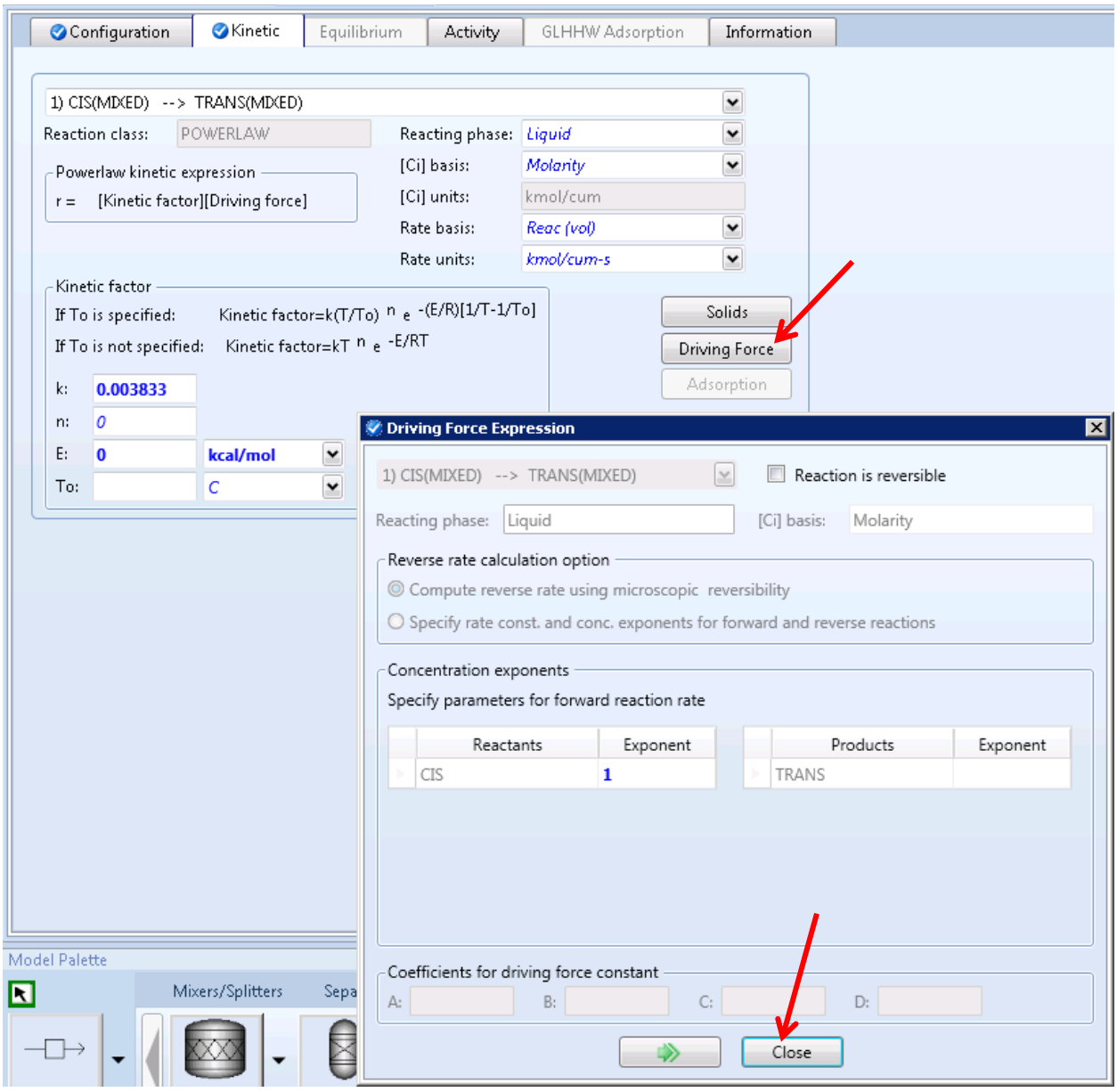

4.05. Place an RCSTR model onto the main flowsheet. In the **Model Palette** under the **Reactors** tab, select an **RCSTR** block and drop it to the flowsheet. The RCSTR block models a continuously stirred tank reactor with user-provided stoichiometry and kinetics. Connect the inlet and outlet ports with material streams and name these streams accordingly, in this case **FEED** and **PRODUCT**. To rename a stream or block, select the item and click **Ctrl + M**.



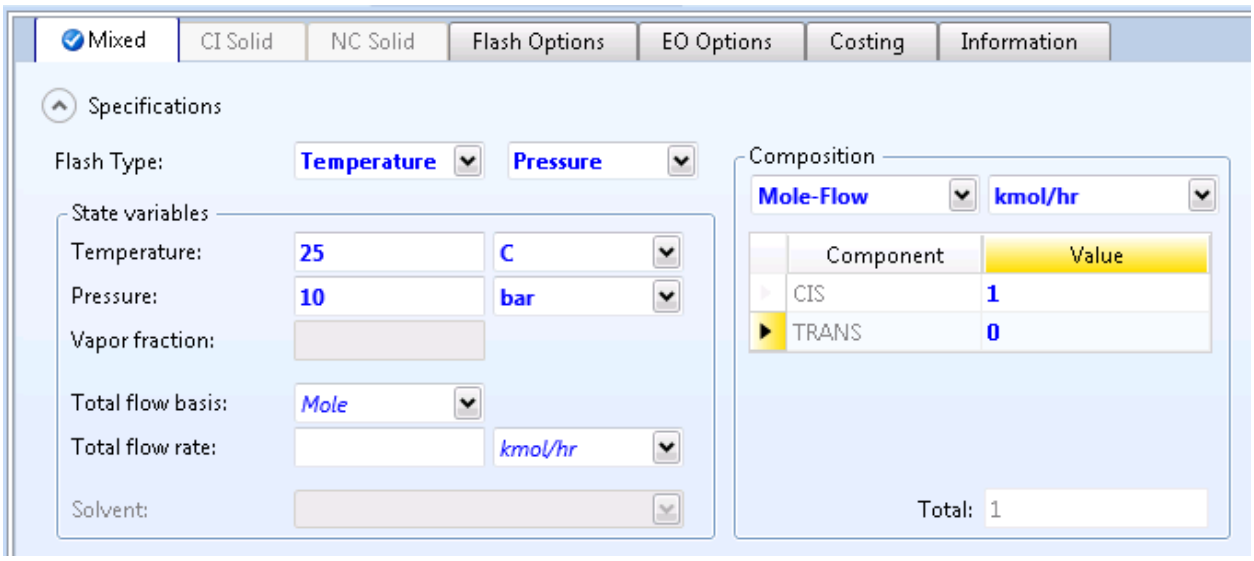

4.06. Now the reactions must be defined. Go to the **Reactions** folder in the navigation pane and click **New**. The default reaction ID **R-1** will be created, and select **GENERAL** for reaction type. In **R-1**, click **New** which will open a stoichiometry window. Give the reaction a name, select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



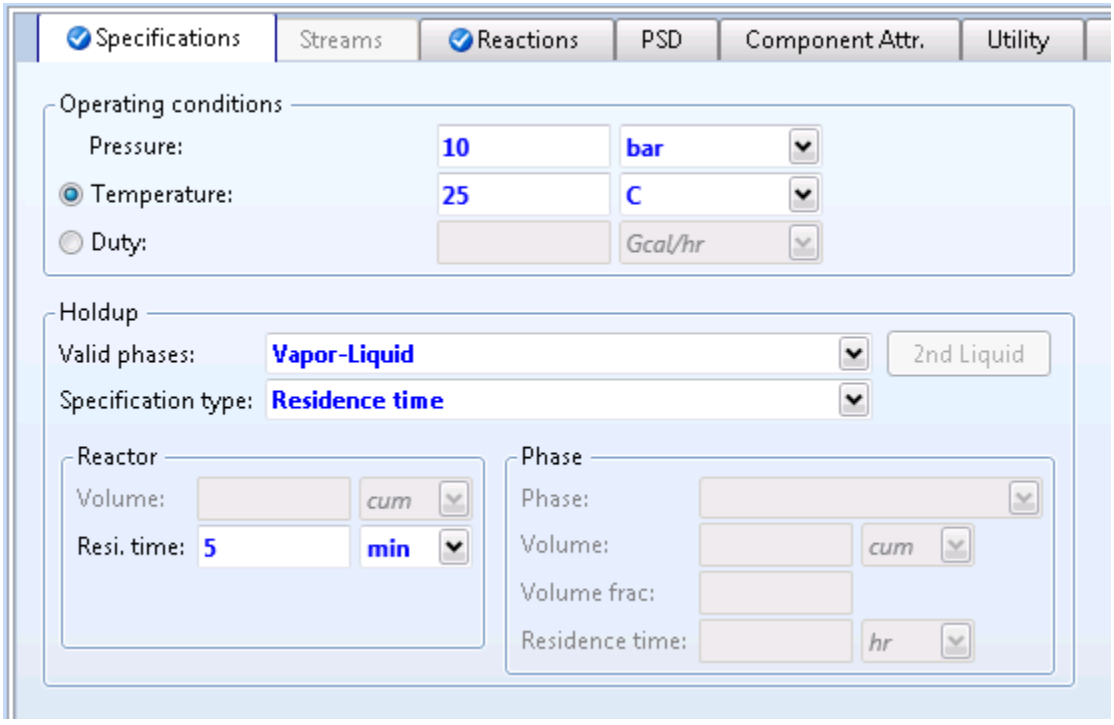
4.07. Click the **Kinetic** tab and enter **k = 0.003833** and **E = 0** since this reactor will be isothermal. Note the units of k here are inverse seconds. Next click **Driving Force** and enter **1** for the CIS reactant exponent.




4.08. Specify the feed stream. Click **Streams | FEED | Input**. Under **Composition** select **Mole-Flow** and enter a value of **1 kmol/hr** for **CIS** and **0** for **TRANS**. Under **State variables** enter **T = 25°C**, and **P = 10 bar**. Note that the specified flowrate will not affect the calculated residence time. It will only change the required reactor volume.

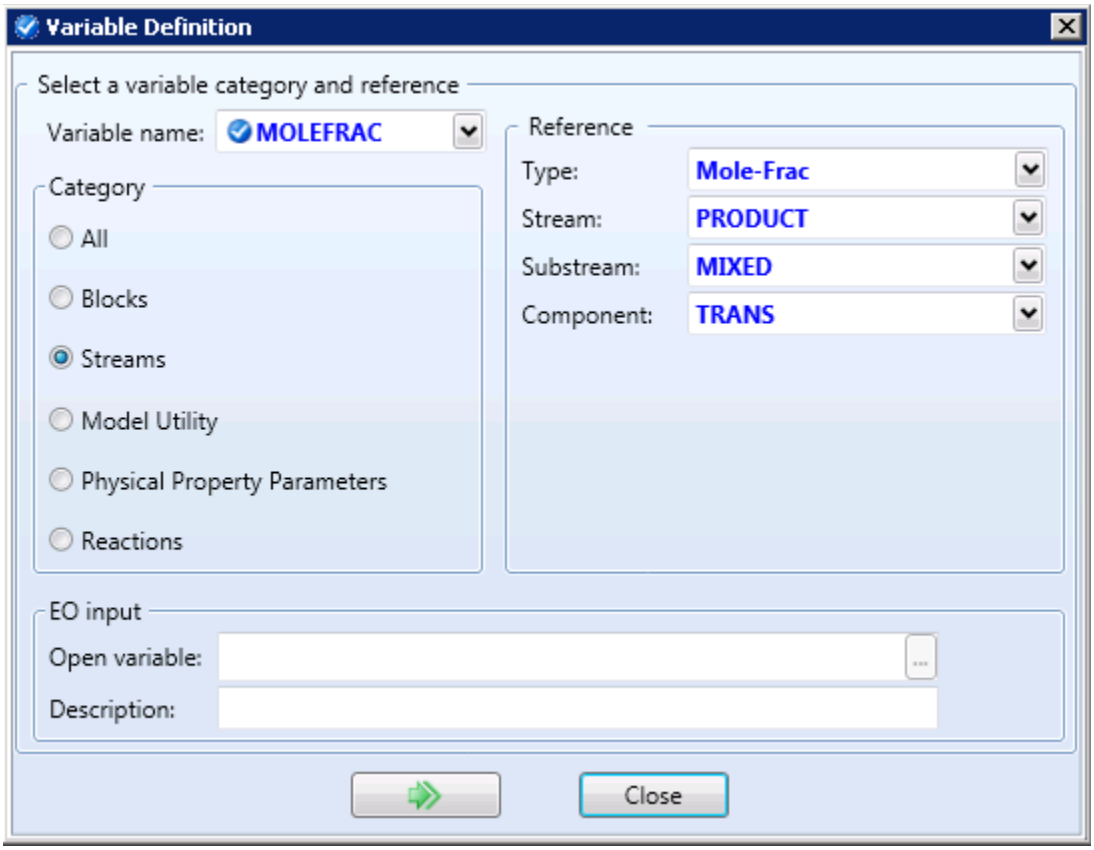



4.09. Specify the CSTR operating conditions by clicking **Blocks | CSTR | Setup**. Enter **P = 10 bar** and **T = 25°C**. Select **Vapor-Liquid** for **Valid phases**, and **Residence time** for **Specification type**. Enter an initial guess for residence time of **5 minutes**. Click on the **Reactions** tab and move **R-1** into the **Selected reaction sets** area.

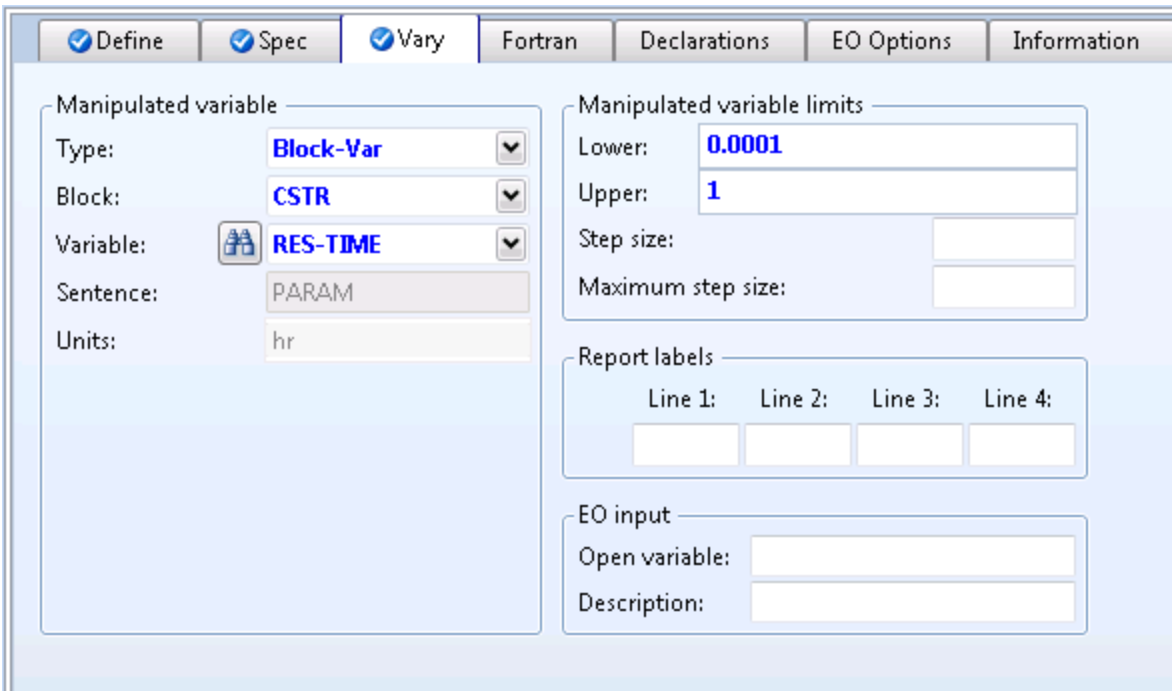



4.10. Create a design specification to determine the residence time required to achieve 90% reactor conversion. Design specifications allow you to manipulate an input variable in order to reach a specified condition. In this case we would like to vary the reactor residence time until we reach a desired mole fraction of trans-2-butene in the product stream. In the navigation pane, click **Flowsheeting Options | Design Spec | New**. A design spec with the default name **DS-1** will be created. In **DS-1** under the **Define**

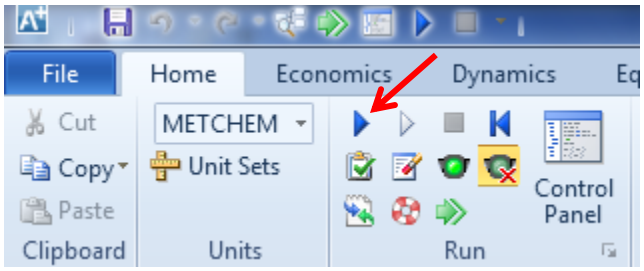
tab click on **New** and create the variable named **MOLEFRAC**. This variable will be defined as the mole fraction of trans-2-butene in the product stream, as shown below.

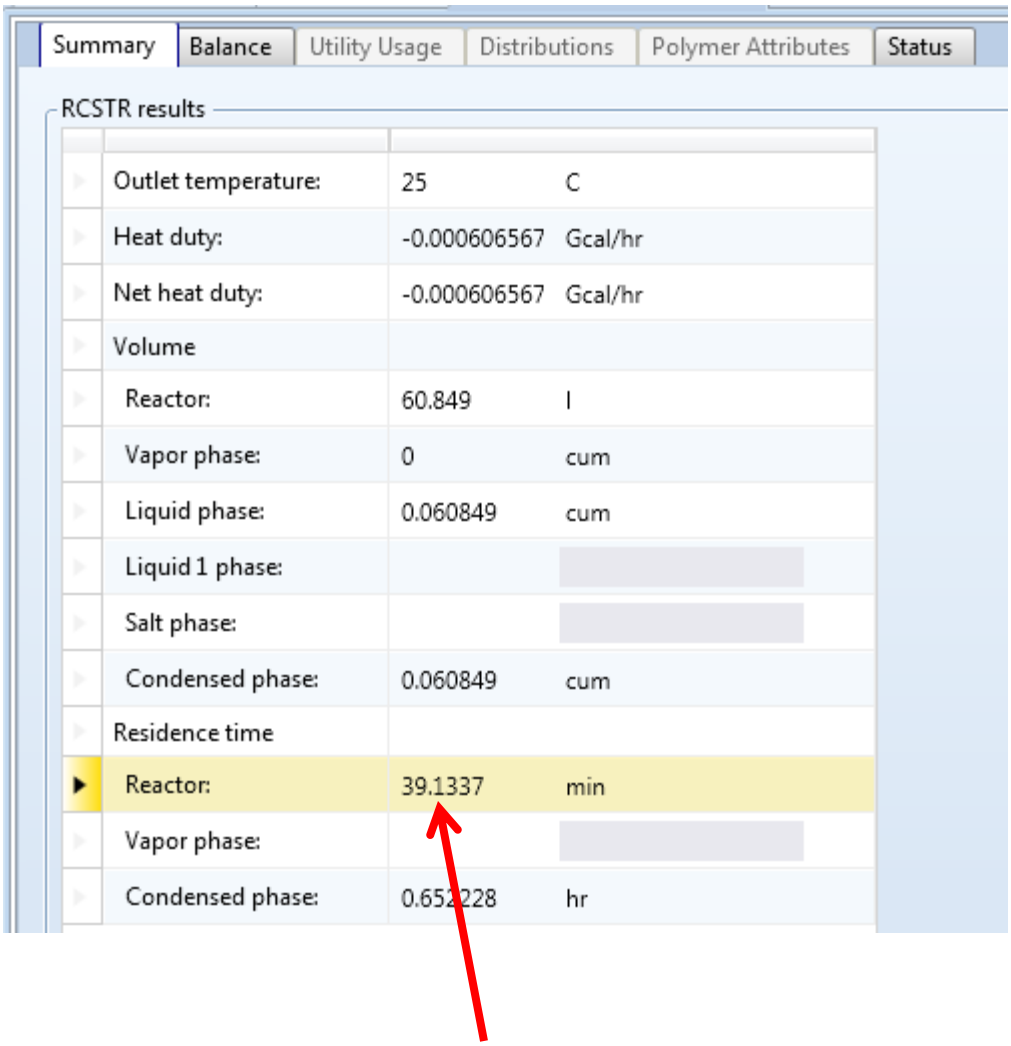



Next, click on the **Spec** tab in **DS-1**. Enter **Spec = MOLEFRAC**, **Target = 0.90**, **Tolerance = 0.0001**. Click on the **Vary** tab and specify the **Residence time** to be the manipulated variable. This is shown below.




4.11. Open the **Control Panel** and run the simulation (**F5**). Click **Blocks | CSTR | Results** to check results. Residence time = **39.13 min**. Note that this solution is the same as the analytic solution.






Required reactor residence time to reach 90% conversion of cis-2-butene to trans-2-butene.

## 5. Conclusion

Both the analytical solution and design spec in Aspen Plus produced the same required residence time of 39.13 min. to achieve 90% reaction conversion in a CSTR. The residence time for a CSTR is longer than for a batch reactor or PFR because of the back-mixing: product is mixed in with the feed, slowing the reaction. Additionally, using RCSTR allows for more advanced calculations. It will model complex reaction systems including parallel and series reactions which lead to coupled systems of ODEs which would be difficult to calculate by hand.

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