

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

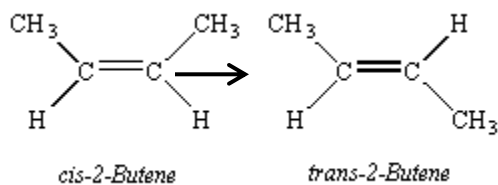
2. Prerequisites

- 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

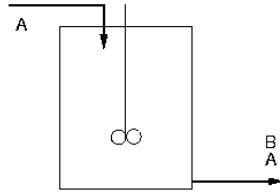


1st order reaction kinetics $r_A = kC_A, k = 0.23\text{min}^{-1} = 0.003833\text{s}^{-1}$

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)

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

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

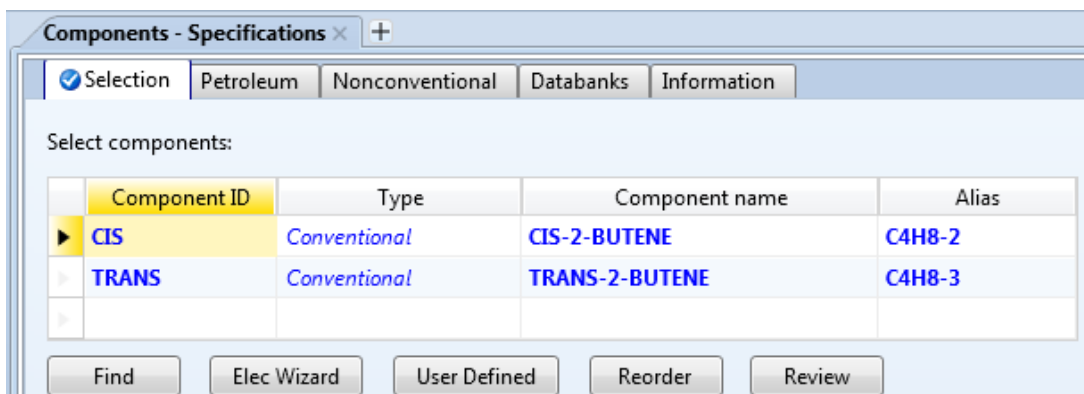
Residence Time (τ)

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

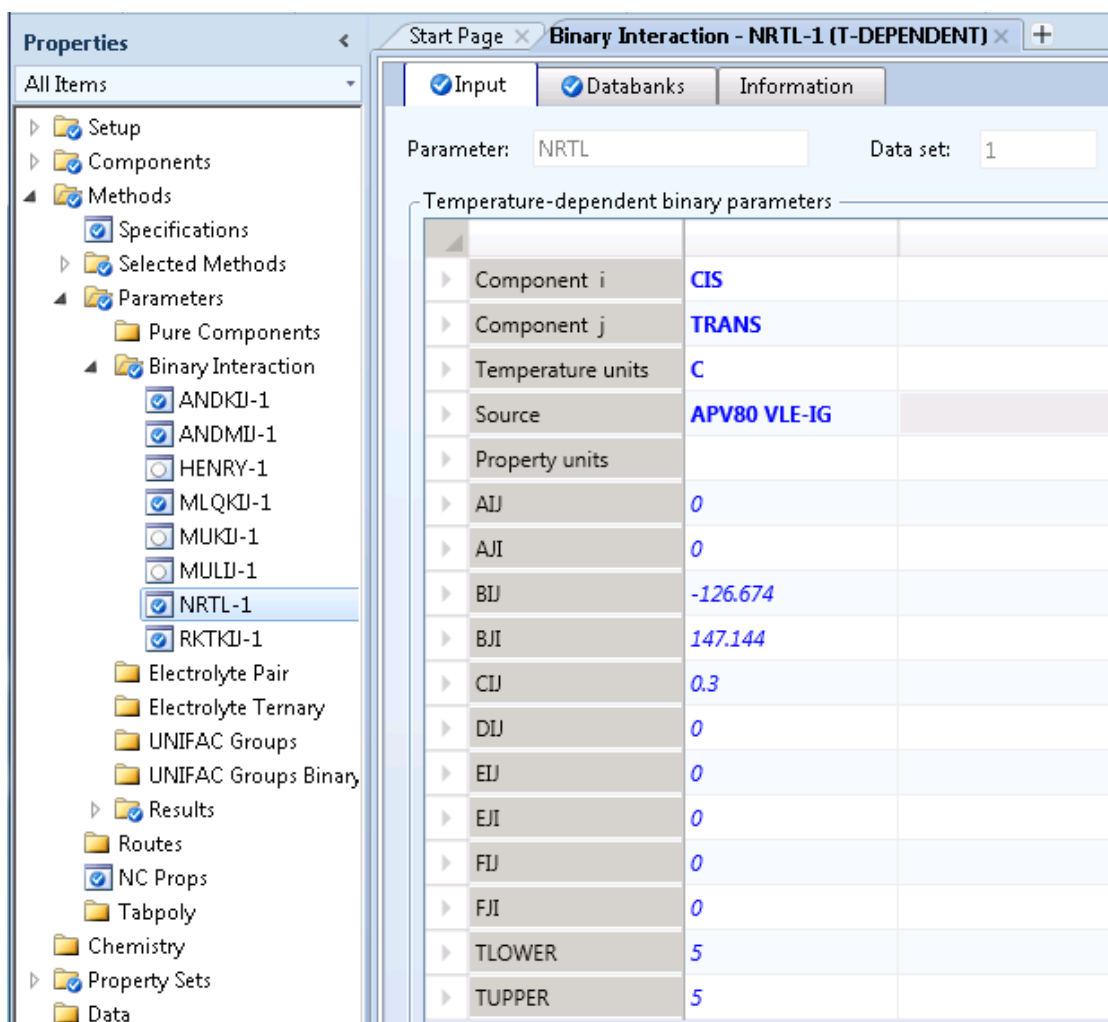
$$\therefore \tau = \frac{X}{k(1-X)} = \frac{0.9}{0.23 \text{ min}^{-1}(1-0.9)} = \mathbf{39.13 \text{ min}}$$

Aspen Plus Solution:

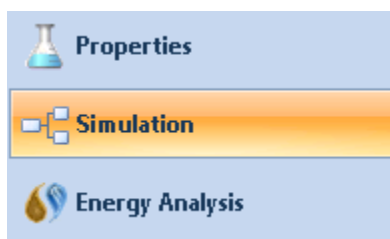
- 4.01. Start **Aspen Plus V8.0**. Select **New | Chemical Processes | Chemicals with Metric Units**. Click **Create**.
- 4.02. Begin by defining the components in the **Components | Specifications | Selection** tab. Enter **CIS-2-BUTENE** and **TRANS-2-BUTENE** for **Component name**. Enter **CIS** and **TRANS** as the **Component ID's**. If a dialogue box appears informing you that parameters will be updated, click **Yes**.



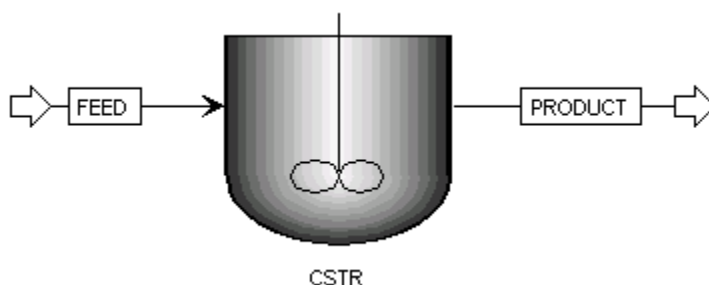
- 4.03. Populate the binary interaction parameters by going to **Methods | Parameters | Binary Interaction | NRTL-1**. The parameters will be automatically generated.



- 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.

Edit Stoichiometry

No: ☒ 1 Reaction class: **POWERLAW**

Name: **RXN1** Status: **On**

☐ Reaction is reversible

Reactants		
	Component	Coefficient
▶	CIS	-1
▶		

Products		
	Component	Coefficient
▶	TRANS	1
▶		

- 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.

The screenshot shows the 'Kinetic' tab of a software interface. The reaction is '1) CIS(MIXED) --> TRANS(MIXED)'. The reaction class is 'POWERLAW'. The reacting phase is 'Liquid'. The [Ci] basis is 'Molarity'. The [Ci] units are 'kmol/cum'. The rate basis is 'Reac (vol)'. The rate units are 'kmol/cum-s'. The kinetic factor is defined as $r = [\text{Kinetic factor}][\text{Driving force}]$. The kinetic factor is defined as $\text{Kinetic factor} = k(T/T_o)^n e^{-(E/R)(1/T-1/T_o)}$ if T_o is specified, and $\text{Kinetic factor} = kT^n e^{-E/RT}$ if T_o is not specified. The kinetic factor parameters are: $k = 0.003833$, $n = 0$, $E = 0$ kcal/mol, and $T_o = C$. The 'Driving Force' button is highlighted with a red arrow.

The 'Driving Force Expression' dialog box is open. It shows the reaction '1) CIS(MIXED) --> TRANS(MIXED)' and the reacting phase 'Liquid'. The [Ci] basis is 'Molarity'. The 'Reverse rate calculation option' is set to 'Compute reverse rate using microscopic reversibility'. The 'Concentration exponents' section shows the following table:

Reactants		Exponent	Products		Exponent
CIS		1	TRANS		

The 'Coefficients for driving force constant' section shows: A: , B: , C: , D: . The 'Close' button is highlighted with a red arrow.

- 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.

Specifications

Flash Type: **Temperature** **Pressure**

State variables

Temperature: **25** **C**

Pressure: **10** **bar**

Vapor fraction:

Total flow basis: **Mole**

Total flow rate: **kmol/hr**

Solvent:

Composition

Mole-Flow **kmol/hr**

Component	Value
CIS	1
TRANS	0

Total: **1**

- 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.

Specifications Streams **Reactions** PSD Component Attr. Utility

Operating conditions

Pressure: **10** **bar**

☒ Temperature: **25** **C**

☐ Duty: **Gcal/hr**

Holdup

Valid phases: **Vapor-Liquid** **2nd Liquid**

Specification type: **Residence time**

Reactor

Volume: **cum**

Resi. time: **5** **min**

Phase

Phase:

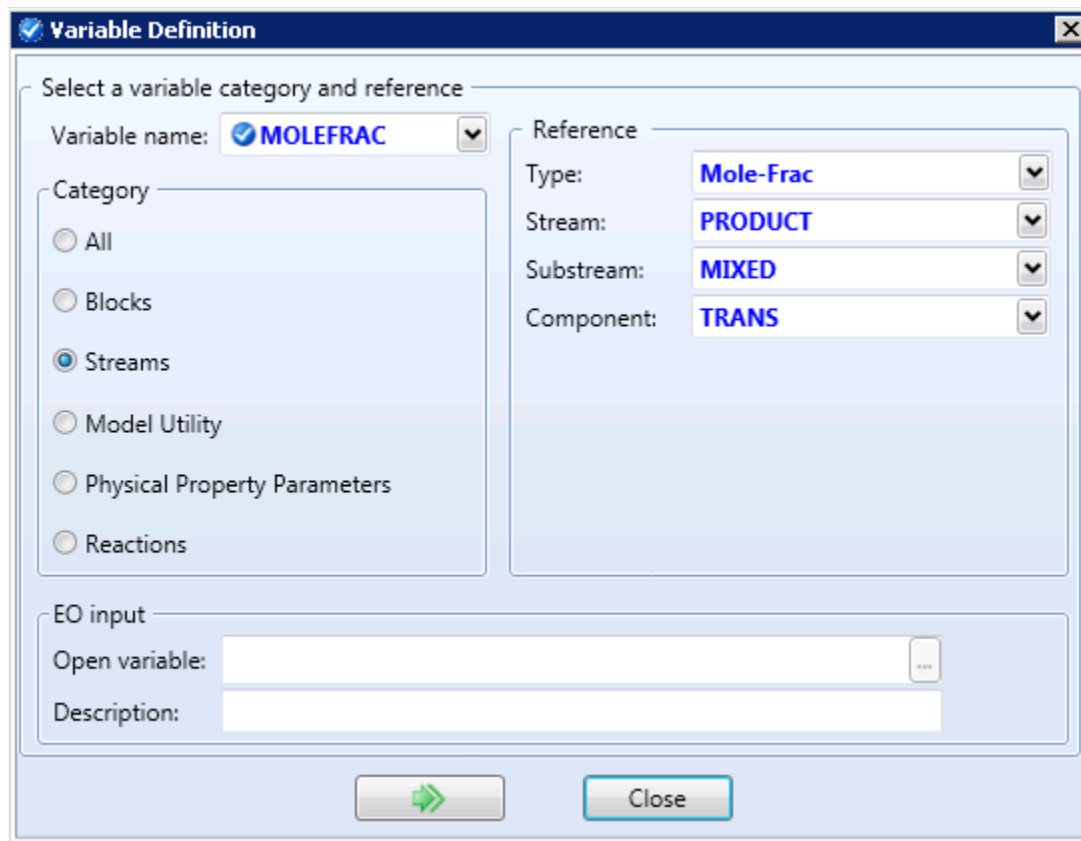
Volume: **cum**

Volume frac:

Residence time: **hr**

- 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.

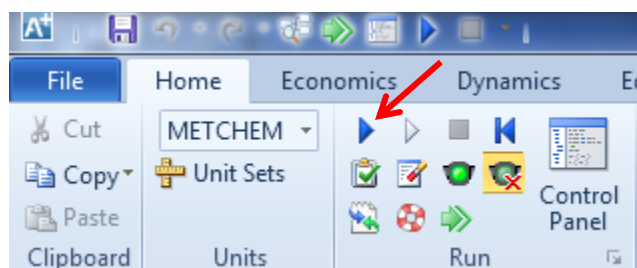


The image shows a 'Variable Definition' dialog box with a blue header bar containing a checkmark icon and the title 'Variable Definition'. The dialog is divided into several sections. The top section, 'Select a variable category and reference', contains a 'Variable name:' dropdown menu with 'MOLEFRAC' selected. Below this is a 'Category' section with radio buttons for 'All', 'Blocks', 'Streams' (which is selected), 'Model Utility', 'Physical Property Parameters', and 'Reactions'. To the right of the category section is a 'Reference' section with four dropdown menus: 'Type:' (Mole-Frac), 'Stream:' (PRODUCT), 'Substream:' (MIXED), and 'Component:' (TRANS). The bottom section, 'EO input', contains two text input fields: 'Open variable:' and 'Description:'. At the bottom of the dialog are two buttons: a green arrow button and a 'Close' button.

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.

The screenshot shows the 'Vary' tab of a software interface. It contains two main sections: 'Manipulated variable' and 'Manipulated variable limits'. The 'Manipulated variable' section has fields for Type (Block-Var), Block (CSTR), Variable (RES-TIME), Sentence (PARAM), and Units (hr). The 'Manipulated variable limits' section has fields for Lower (0.0001), Upper (1), Step size, and Maximum step size. Below these are 'Report labels' with four lines (Line 1 to Line 4) and an 'EO input' section with fields for Open variable and Description.

- 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.



Summary		Balance	Utility Usage	Distributions	Polymer Attributes	Status
RCSTR results						
▶	Outlet temperature:	25	C			
▶	Heat duty:	-0.000606567	Gcal/hr			
▶	Net heat duty:	-0.000606567	Gcal/hr			
▶	Volume					
▶	Reactor:	60.849	l			
▶	Vapor phase:	0	cum			
▶	Liquid phase:	0.060849	cum			
▶	Liquid 1 phase:					
▶	Salt phase:					
▶	Condensed phase:	0.060849	cum			
▶	Residence time					
▶	Reactor:	39.1337	min			
▶	Vapor phase:					
▶	Condensed phase:	0.652228	hr			

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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