

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

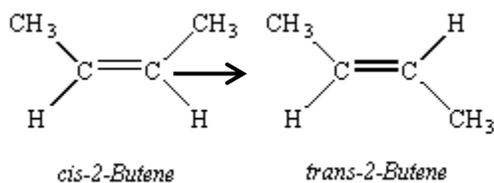
2. Prerequisites

- 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

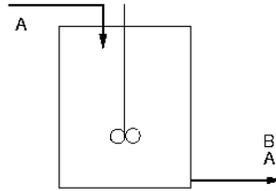


1st order reaction kinetics $r_A = kC_A, k = 0.23\text{min}^{-1} = 0.003833\text{s}^{-1}$

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

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

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

Conversion (X)

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

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

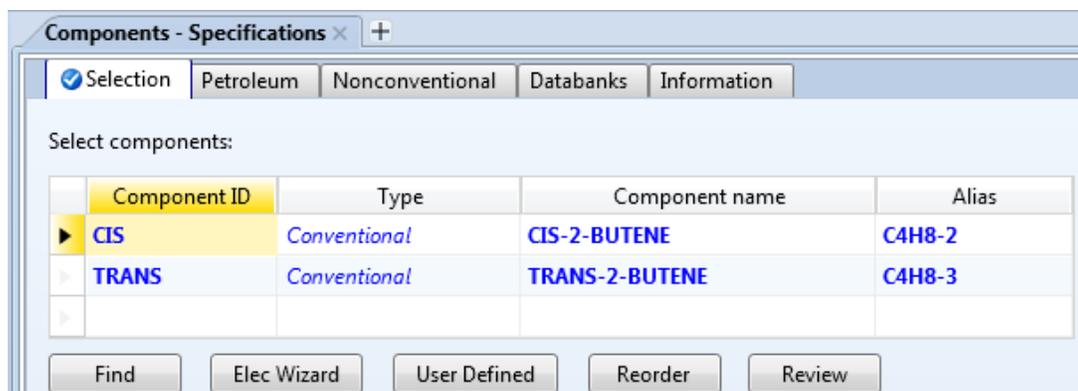
Residence Time (τ)

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

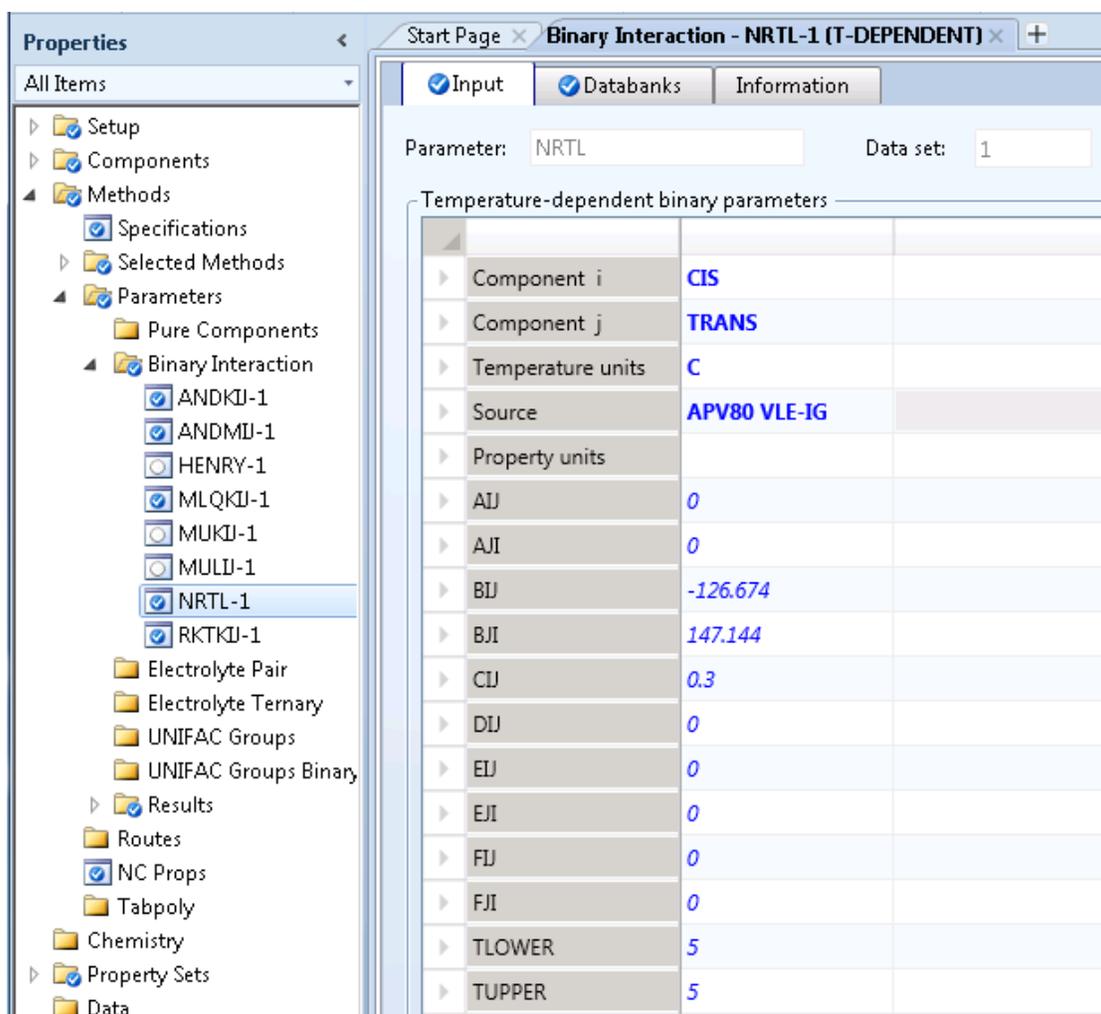
$$\therefore \tau = \frac{X}{k(1-X)} = \frac{0.9}{0.23 \text{ min}^{-1}(1-0.9)} = \mathbf{39.13 \text{ min}}$$

Aspen Plus Solution:

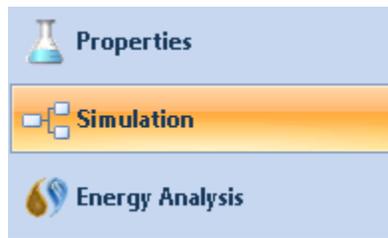
- 4.01. Start **Aspen Plus V8.0**. Select **New | Chemical Processes | Chemicals with Metric Units**. Click **Create**.
- 4.02. Begin by defining the components in the **Components | Specifications | Selection** tab. Enter **CIS-2-BUTENE** and **TRANS-2-BUTENE** for **Component name**. Enter **CIS**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



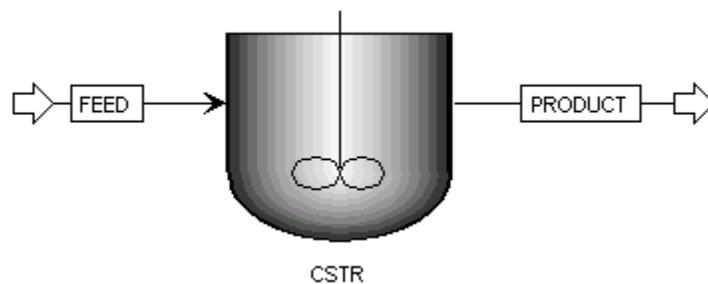
- 4.03. Populate the binary interaction parameters by going to **Methods | Parameters | Binary Interaction | NRTL-1**. The parameters will be automatically generated.



- 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: Reaction class:

Name: Status:

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 software interface with the **Kinetic** tab selected. The reaction is **1) CIS(MIXED) --> TRANS(MIXED)**. The **Reaction class** is **POWERLAW**. The **Powerlaw kinetic expression** is $r = [\text{Kinetic factor}][\text{Driving force}]$. The **Kinetic factor** is defined as $k(T/T_0)^n e^{-(E/R)(1/T-1/T_0)}$ if T_0 is specified, and $kT^n e^{-E/RT}$ if T_0 is not specified. The **k** value is **0.003833**, **n** is **0**, **E** is **0 kcal/mol**, and **To** is **C**. The **Driving Force Expression** dialog box is open, showing the **Driving Force** button highlighted with a red arrow. The **Driving Force Expression** dialog box has the **Reaction is reversible** checkbox unchecked. The **Reverse rate calculation option** is set to **Compute reverse rate using microscopic reversibility**. The **Concentration exponents** table is as follows:

Reactants		Exponent	Products		Exponent
CIS		1	TRANS		

The **Coefficients for driving force constant** are 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.

Variable Definition

Select a variable category and reference

Variable name: **MOLEFRAC**

Category

All

Blocks

Streams

Model Utility

Physical Property Parameters

Reactions

Reference

Type: **Mole-Frac**

Stream: **PRODUCT**

Substream: **MIXED**

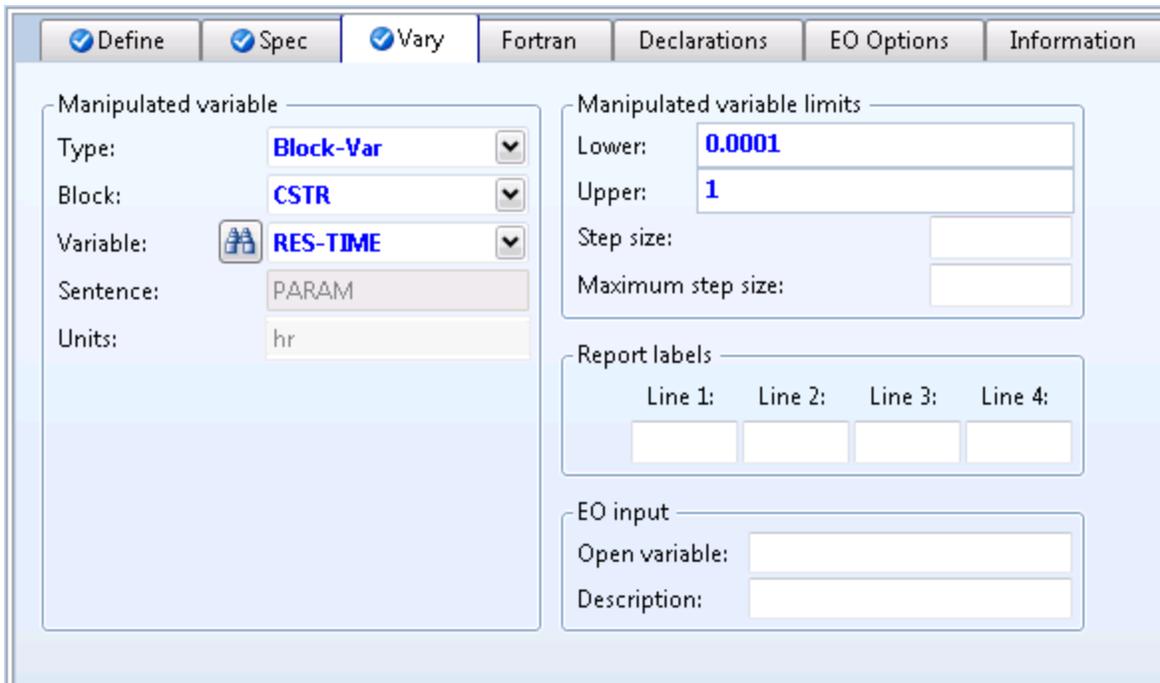
Component: **TRANS**

EO input

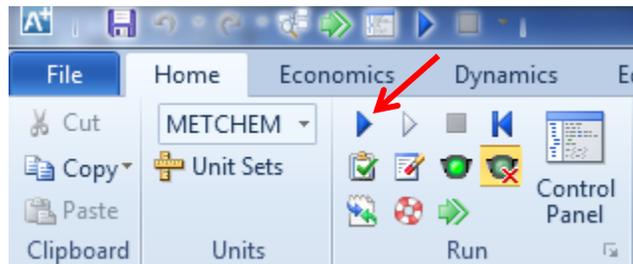
Open variable:

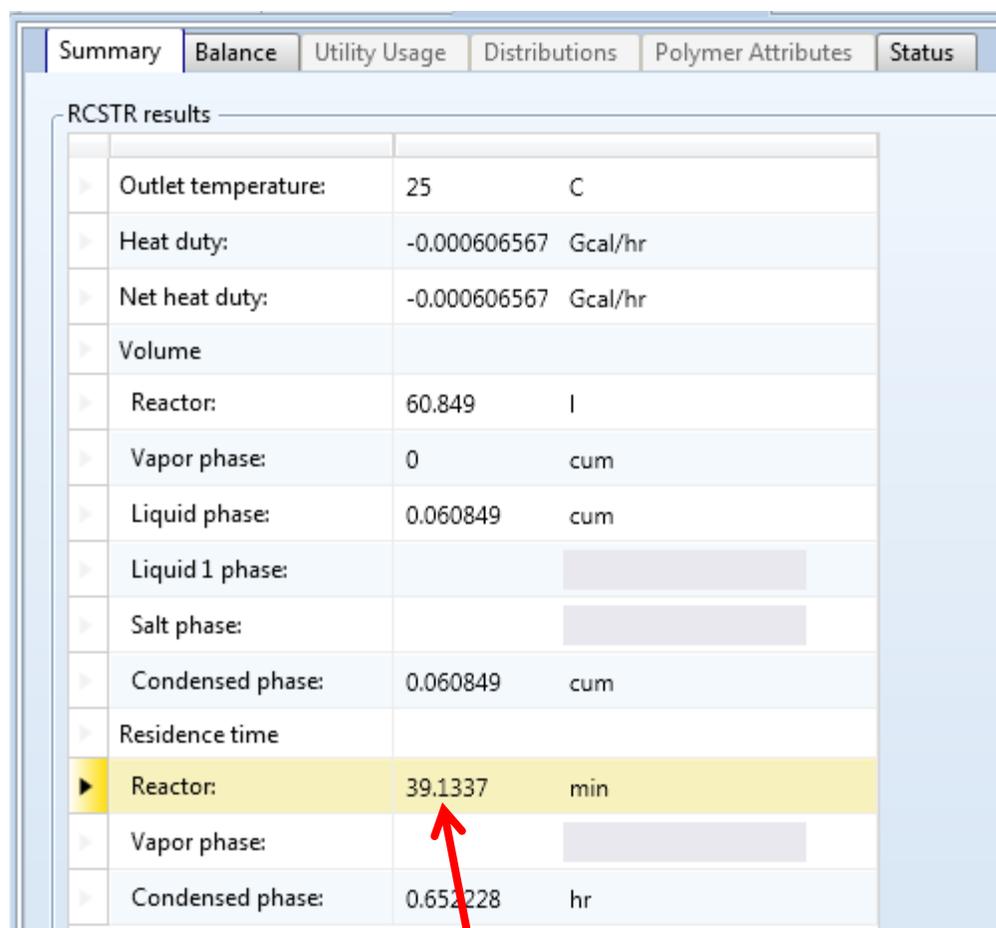
Description:

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.





The screenshot displays the 'RCSTR results' window in Aspen Plus. The window has tabs for 'Summary', 'Balance', 'Utility Usage', 'Distributions', 'Polymer Attributes', and 'Status'. The 'Summary' tab is active, showing a table of results. A red arrow points to the 'Reactor' residence time value of 39.1337 min.

Parameter	Value	Unit
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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