

COMSOL LEP tutorial for Nonisothermal plug flow reactor with Heat exchange

Step 1: Open chapter 12 and click on **COMSOL** tab present in the bottom of the page

The screenshot shows the website interface for 'Elements of Chemical Reaction Engineering, 5th Edition'. The page is for Chapter 12: Steady-State Nonisothermal Reactor Design: Flow Reactors with Heat Exchange. The left sidebar contains navigation options like 'BY CHAPTER', 'BY CONCEPT', and 'U OF M'. The main content area includes 'Objectives' and a list of learning outcomes. At the bottom, there are several tabs: 'Learning Resources', 'Living Example Problems', 'Expanded Material', 'Youtube Videos', 'Professional Reference Shelf', 'Additional Homework Problems', 'Web Modules', 'COMSOL', and 'Learn ChemE Videos'. The 'COMSOL' tab is circled in red.

Step 2: The following page will open. Click on “How to access COMSOL”

The screenshot shows the 'How to access COMSOL' page. The left sidebar is the same as in the previous screenshot. The main content area has a red circle around the link 'How to access COMSOL' and a blue box around the link 'COMSOL LEP tutorial'.

Step 3: The following page will open. Click “Here”

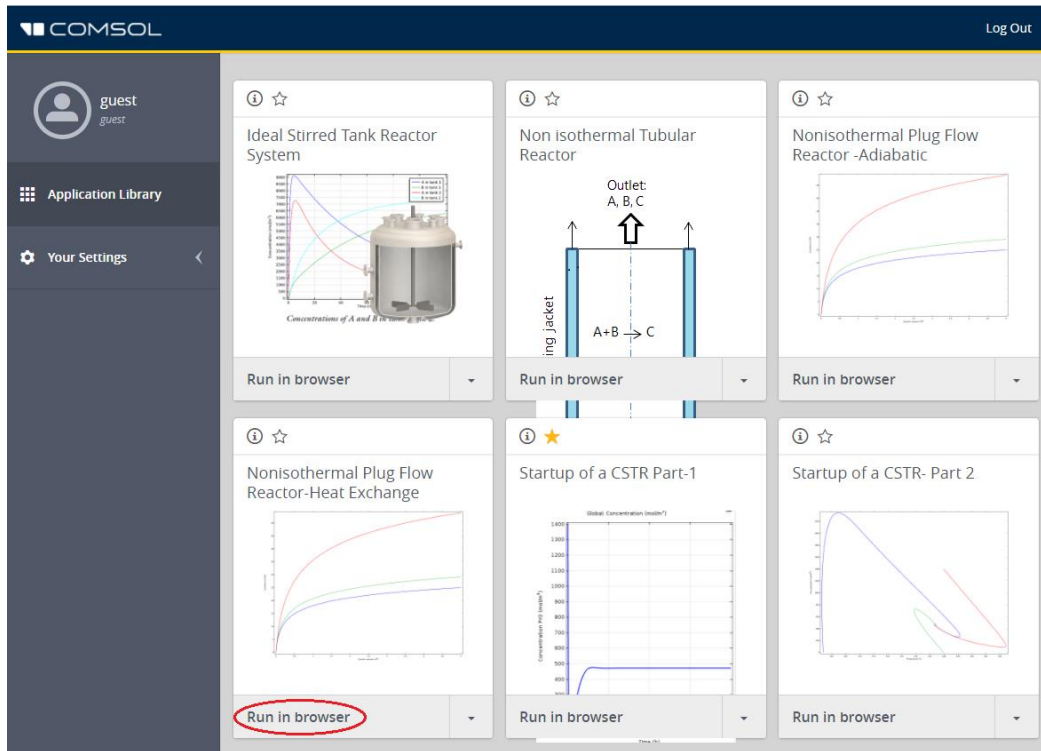
The screenshot shows the top navigation bar of a website. On the left, it says "Elements of Chemical Reaction Engineering 5th Edition". In the center, there are two book cover images and a link that says "Home Problem Solving Updates and FAQs". On the right, it says "Essentials of Chemical Reaction Engineering". Below the navigation bar is a table of contents (TOC) with chapters 1 through 18 and Appendices. On the left side, there is a sidebar menu titled "BY CHAPTER" with options like "Objectives", "Learning Resources", "Summary Notes", "Living Example Problems", "Professional Reference Shelf", "Additional HW Problems", "FAQs", and "Expanded Material". The main content area contains the text: "Please visit [HERE](#) to access COMSOL." followed by two bullet points: "If you are a student at the University of Michigan, please use your unique-name and password." and "If you are not a University of Michigan student, use". Below the bullet points, it lists "username: guest" and "password: guest".

Step 4: This will take you to COMSOL Server. If you are a student at the University of Michigan, please use your Uniqname and password. If you are not a University of Michigan student, use

username: guest
password : guest

The screenshot shows the COMSOL Server login page. At the top, the text "COMSOL SERVER™" is displayed in a large, pink font. Below this, there is a horizontal line. Underneath the line, there are two input fields: "Username" and "Password". The "Username" field contains the text "guest". The "Password" field contains six dots. At the bottom of the page, there is a large pink button with the text "Log in to COMSOL Server" inside it, which is circled in black.

Step 5: This will open up COMSOL library where you see many COMSOL files to solve chemical reaction engineering problems. Find “**Nonisothermal Plug Flow Reactor-Heat exchange**”. Click on “Run in browser” to start the application



You will see that following window opens which has input parameters, description, graphical features and a few buttons. You can see the conversion profile on the right side of the page

File

Input and Description

Compute

Input

Inlet volumetric flow: m³/s

Inlet mole fraction, A: mol/mol

Inlet concentration, A: mol/m³

Activation energy, E_1 : J/mol

Inlet temperature: K

Volumetric heat transfer coefficient: W/m³K

Heating fluid temperature: K

Process Reaction

Gas-phase production of acetic anhydride (ketene) from acetone:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4$$

(A) (K) (M)

Acetone Ketene Methane

Reaction rate expression:

$$r_1 = k_1 C_A$$

Rate constant from Arrhenius equation:

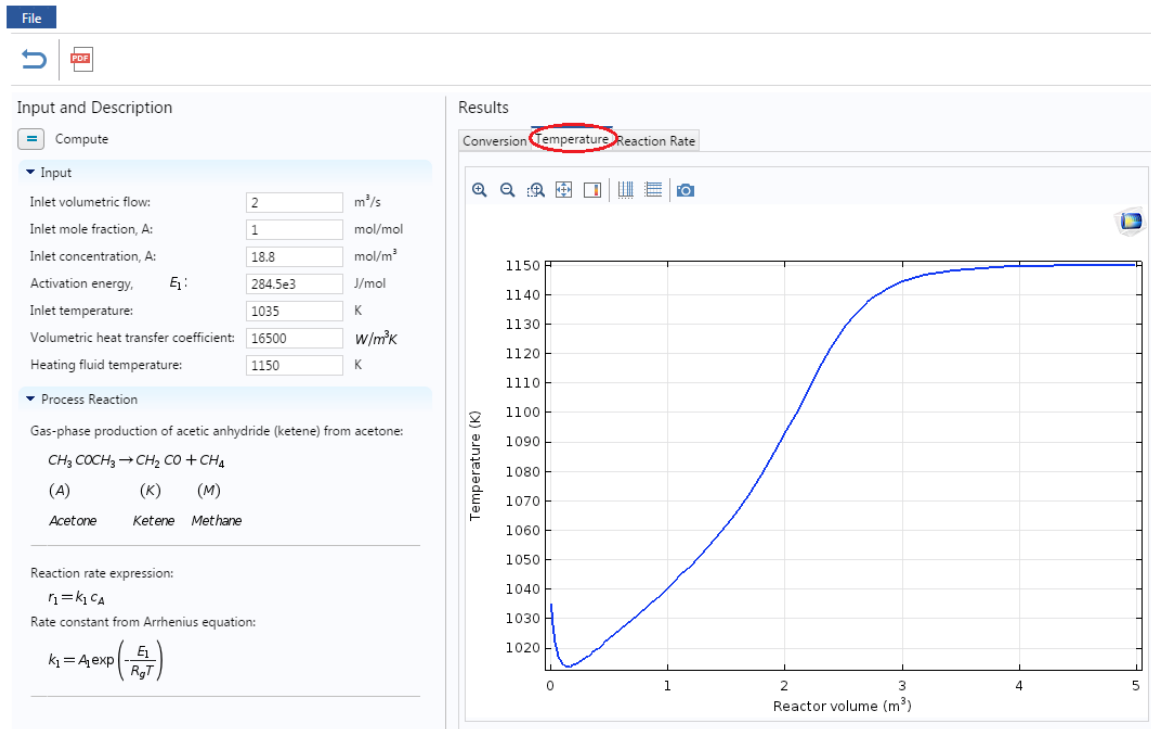
$$k_1 = A_1 \exp\left(-\frac{E_1}{R_g T}\right)$$

Results

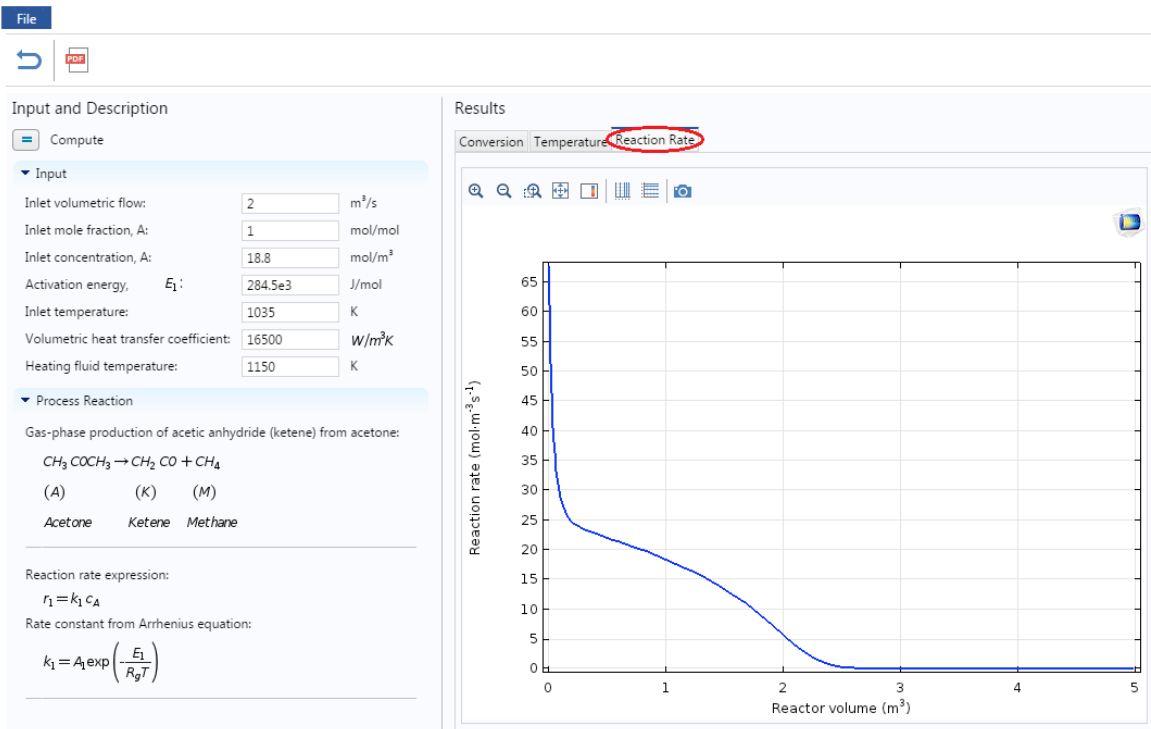
Conversion Temperature Reaction Rate

Reactor volume (m³)	Conversion A (%)
0	0
0.5	35
1.0	65
1.5	85
2.0	95
2.5	100
3.0	100
4.0	100
5.0	100

Step 6: Click on Temperature tab to view Temperature graph

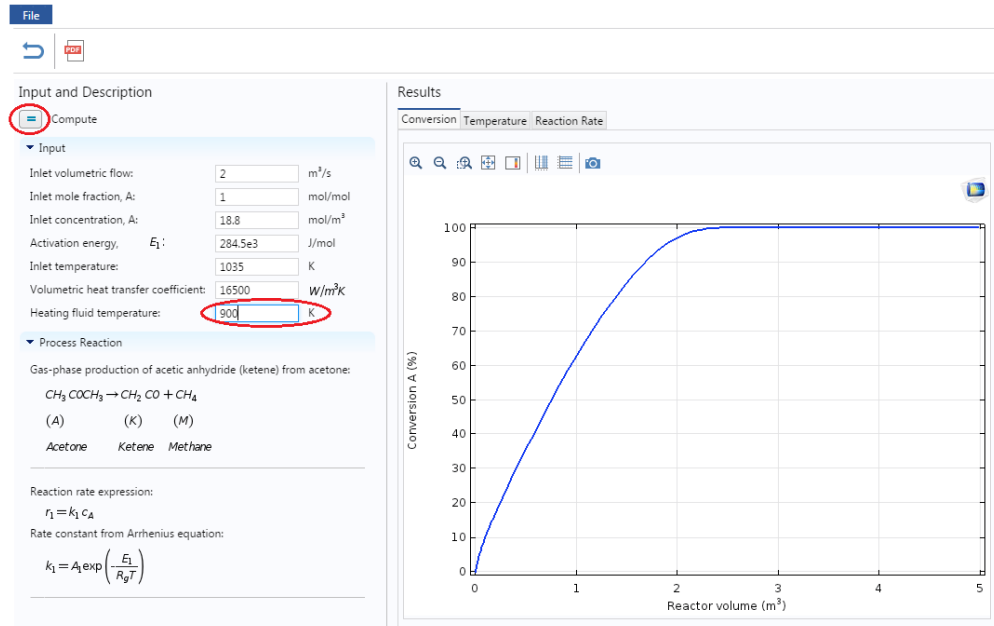


Click on Reaction Rate tab to view graph of reaction rate

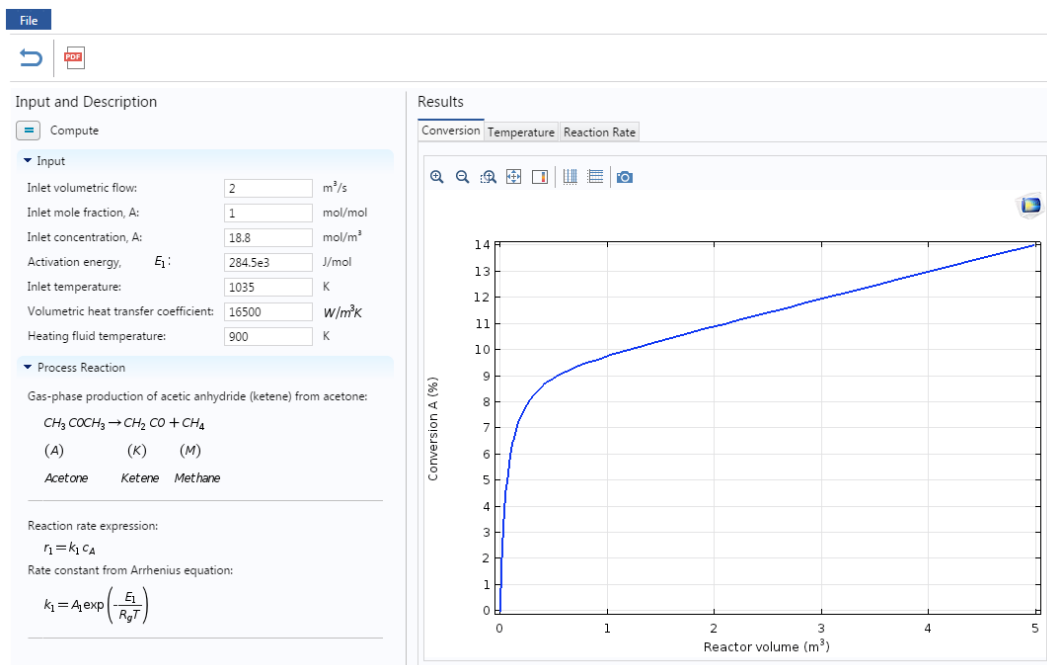


Step 7: Under Input section on the left hand side, you can view and change any parameter values. Let's change a parameter and see the effect on the profile. Change the Temperature of heat exchanger medium from 1150 K to 900 K. After you are done, click on Compute button (=) present above the Input parameters

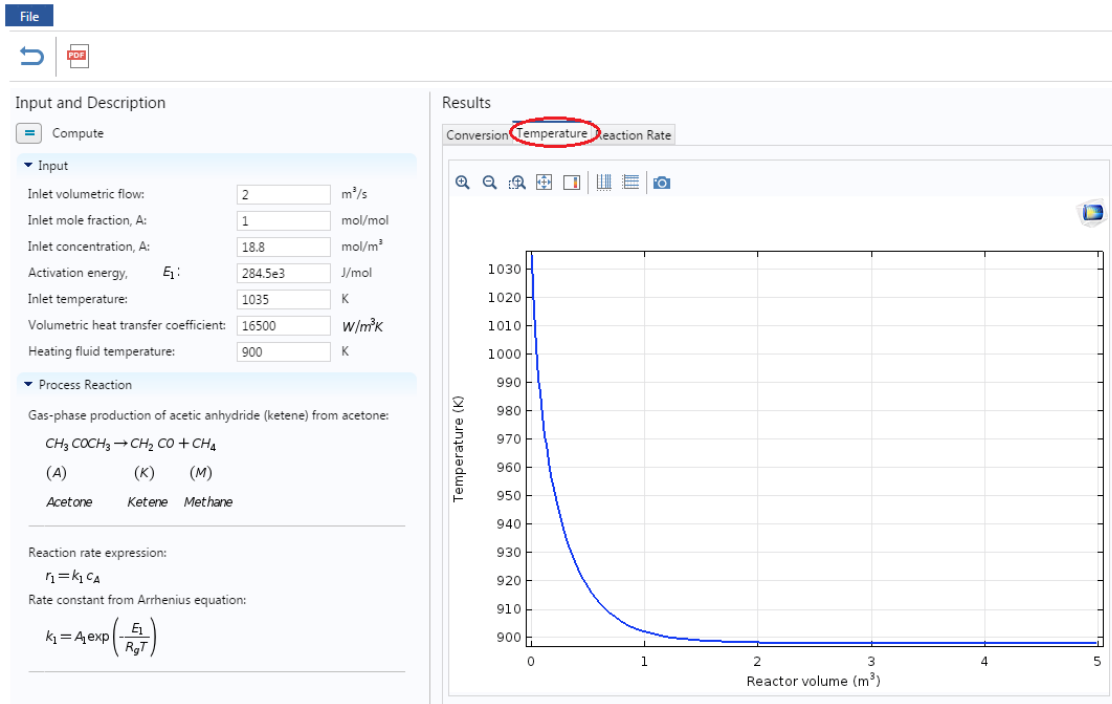
Caution: The y axis is dynamic and scale changes with respect to the values. Make sure to look at both scale and graph



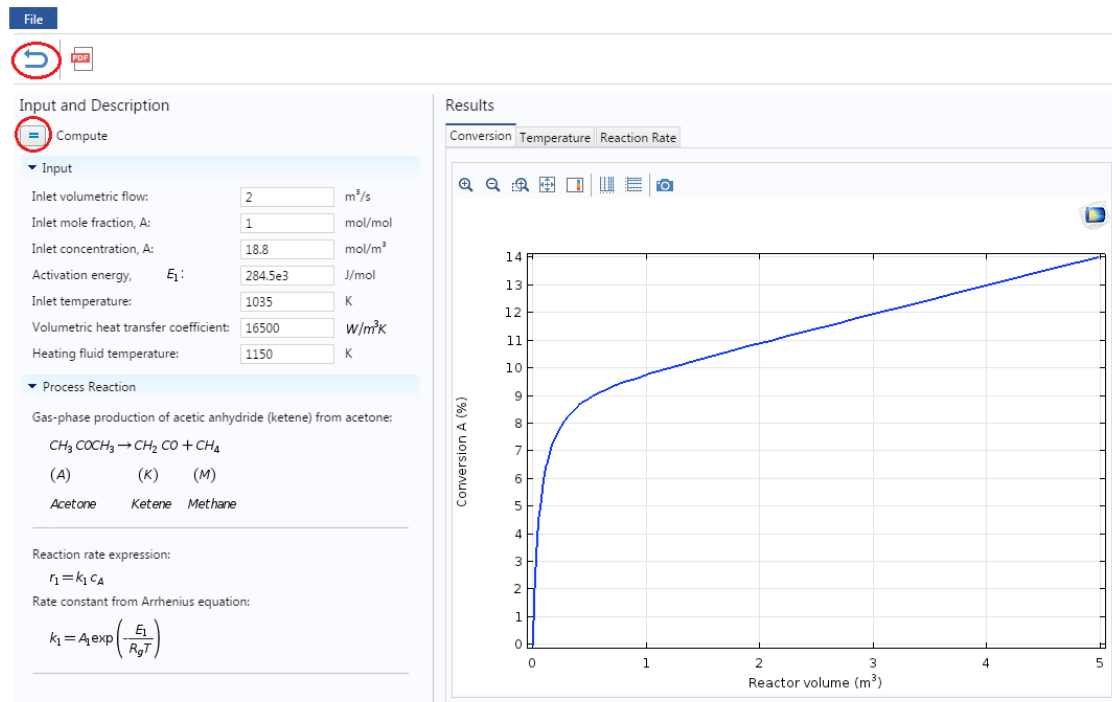
Step 8: Now check the Conversion and Temperature profiles. The following graph is obtained for Conversion. You can see that conversion has decreased at lower heating fluid temperature



The following graph is obtained for Temperature profile which shows that temperature has also decreased

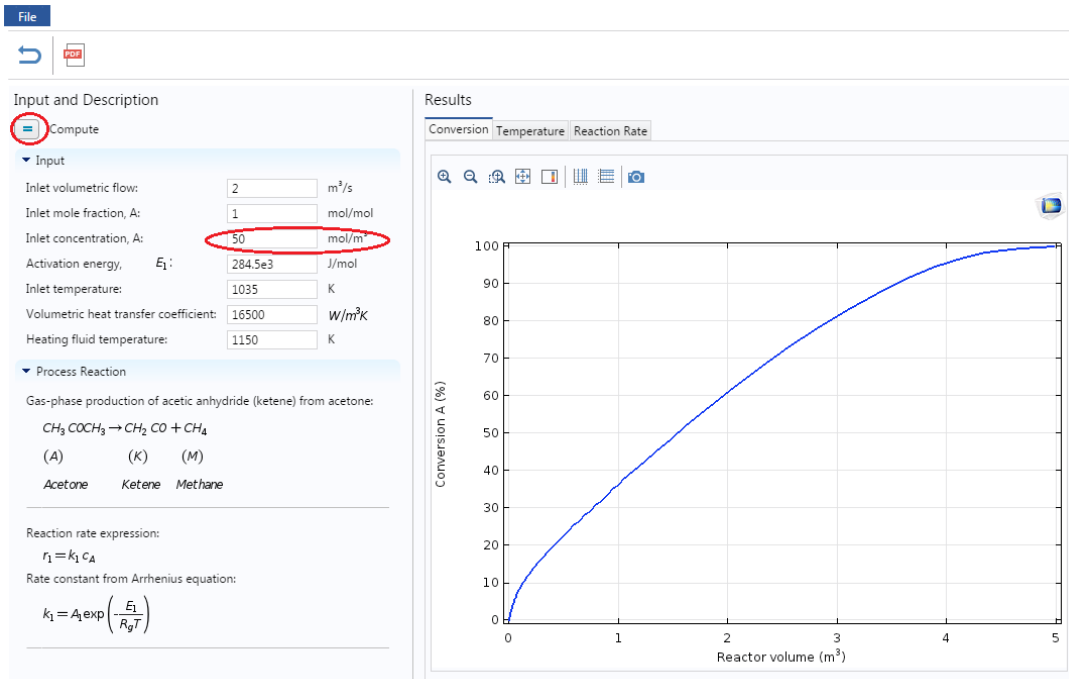


Step 9: Now if you want to re-set all the parameter values to its initial values, click on “reset to default button(↶). Click on this button and you will find that it resets the value of Temperature. To update the graph, click on Compute button. Each time you change a variable, click Compute

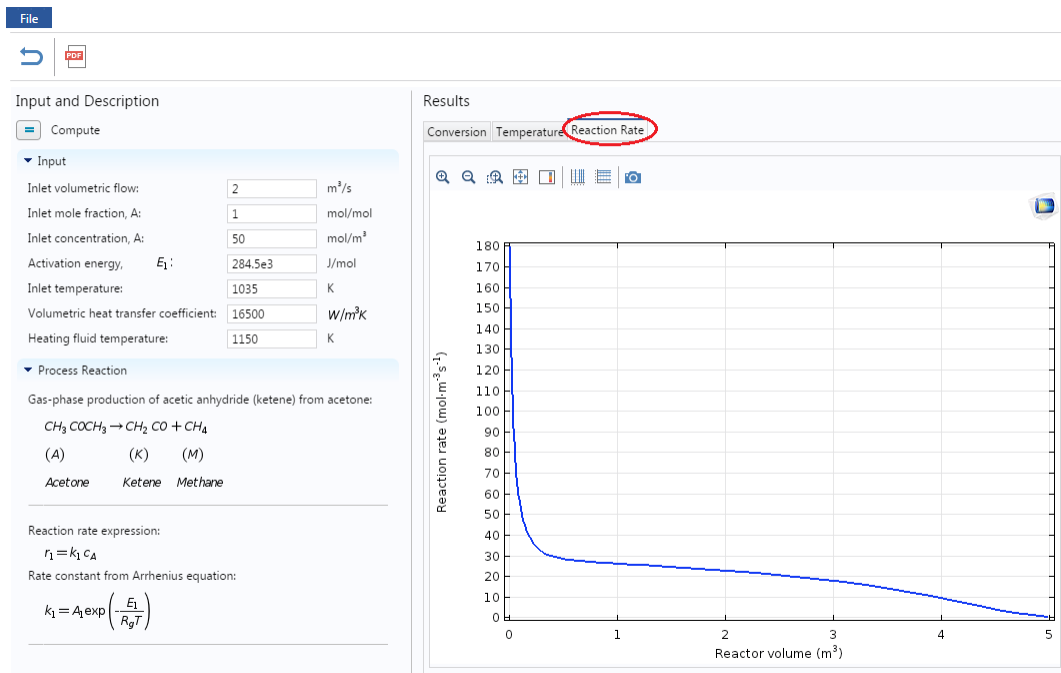


Step 10: Now let's consider a case where you want to maintain the Inlet concentration such that 100 % conversion is achieved at the end of the reactor. Enter the inlet concentration of A as 50 mol/m³ and click compute to see its effect on profile.

The following graph will be obtained for conversion. You can see that as inlet concentration is increased, 100% conversion is shifted towards the end of the reactor



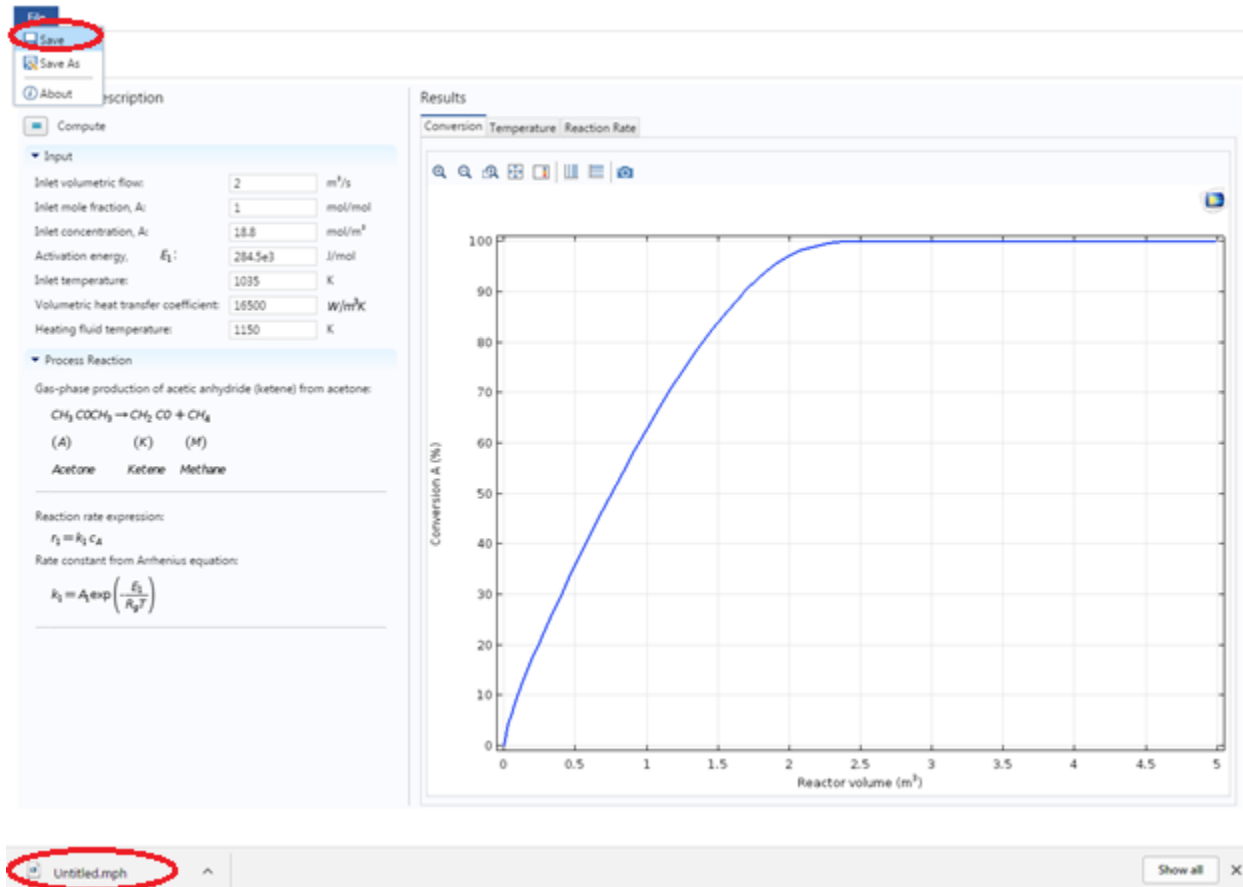
The following graph will be obtained for reaction rate which shows reaction rate now decreases slowly



Step 11: Now, you can change any listed parameter value and check its effect on profiles. Make sure to click Compute button after you change a variable.

Step 12: If you have COMSOL installed on your computer, then you can also download the complete COMSOL file (with user interface)

- Go to file on toolbar and click on Save button. This will download the file at the bottom of the browser(if you are using Chrome)
- Click on the downloaded file to open the application



Step 13: You can also open a pdf documentation which details the reactor model and a step-by-step procedure to create this COMSOL module from scratch. Click on PDF button present on the menu bar

The screenshot displays the COMSOL Multiphysics interface. On the left, the 'Input and Description' panel is active, showing various input parameters for a reactor model. On the right, the 'Results' panel shows a plot of Conversion A (%) versus Reactor volume (m³).

Input and Description

Compute

Input

Inlet volumetric flow:	2	m³/s
Inlet mole fraction, A:	1	mol/mol
Inlet concentration, A:	18.8	mol/m³
Activation energy, E_1 :	284.5e3	J/mol
Inlet temperature:	1035	K
Volumetric heat transfer coefficient:	16500	W/m²K
Heating fluid temperature:	1150	K

Process Reaction

Gas-phase production of acetic anhydride (ketene) from acetone:

$$CH_3COCH_3 \rightarrow CH_2CO + CH_4$$

(A) (K) (M)
Acetone Ketene Methane

Reaction rate expression:
 $r_1 = k_1 C_A$

Rate constant from Arrhenius equation:
 $k_1 = A_1 \exp\left(-\frac{E_1}{R_g T}\right)$

Results

Conversion | Temperature | Reaction Rate

Reactor volume (m³)	Conversion A (%)
0	0
0.5	35
1.0	65
1.5	85
2.0	95
2.5	100
3.0	100
4.0	100
5.0	100

This will open up a new tab with PDF file which you can also download

The screenshot shows a PDF document viewer displaying a document titled "Plug flow.pdf". The document content includes the text "Created in COMSOL Multiphysics 5.2a" and a large heading "Non-Isothermal Plug Flow Reactor" with a small COMSOL logo above it.

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Created in COMSOL Multiphysics 5.2a

Non-Isothermal Plug Flow Reactor