

COMSOL LEP tutorial for Nonisothermal plug flow reactor with adiabatic operation

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

The screenshot shows a web browser displaying the 'Elements of Chemical Reaction Engineering' website. The page is for Chapter 12: Steady-State Nonisothermal Reactor Design: Flow Reactors with Heat Exchange. The navigation tabs at the bottom include Learning Resources, Living Example Problems, Expanded Material, Youtube Videos, Professional Reference Shelf, Additional Homework Problems, Web Modules, and COMSOL (circled in red). The COMSOL tab is highlighted with a red circle.

Elements of Chemical Reaction Engineering 5th Edition

Chapter 12: Steady-State Nonisothermal Reactor Design: Flow Reactors with Heat Exchange

Objectives

After completing **Chapter 12** of the text and associated website material, the reader will be able to:

- Describe the algorithm for CSTRs, PFRs, and PBRs that are not operated isothermally.
- Size nonadiabatic CSTRs, PFRs, and PBRs.
- Describe and compare the different traits for PFRs with the following different heat exchange taking place
 1. Adiabatic
 2. Constant ambient exchange temperature
 3. Co-current heat exchange
 4. Counter current heat exchange
- Carry out an analysis to determine the Multiple Steady States (MSS) in a CSTR along with the ignition and extinction temperatures.
- Analyze multiple reactions carried out in CSTRs, PFRs, and PBRs which are not operated isothermally in order to determine the concentrations and temperature as a function of position (PFR/PBR) and operating variables.

[Learning Resources](#) [Living Example Problems](#) [Expanded Material](#) [Youtube Videos](#)
[Professional Reference Shelf](#) [Additional Homework Problems](#) [Web Modules](#) [COMSOL](#)
[Learn ChemE Videos](#)

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

The screenshot shows the same website as in Step 1, but with the 'How to access COMSOL' link highlighted in a red circle. Below it, the 'COMSOL LEP tutorial' link is also visible.

Elements of Chemical Reaction Engineering 5th Edition

How to access COMSOL

[COMSOL LEP tutorial](#)

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

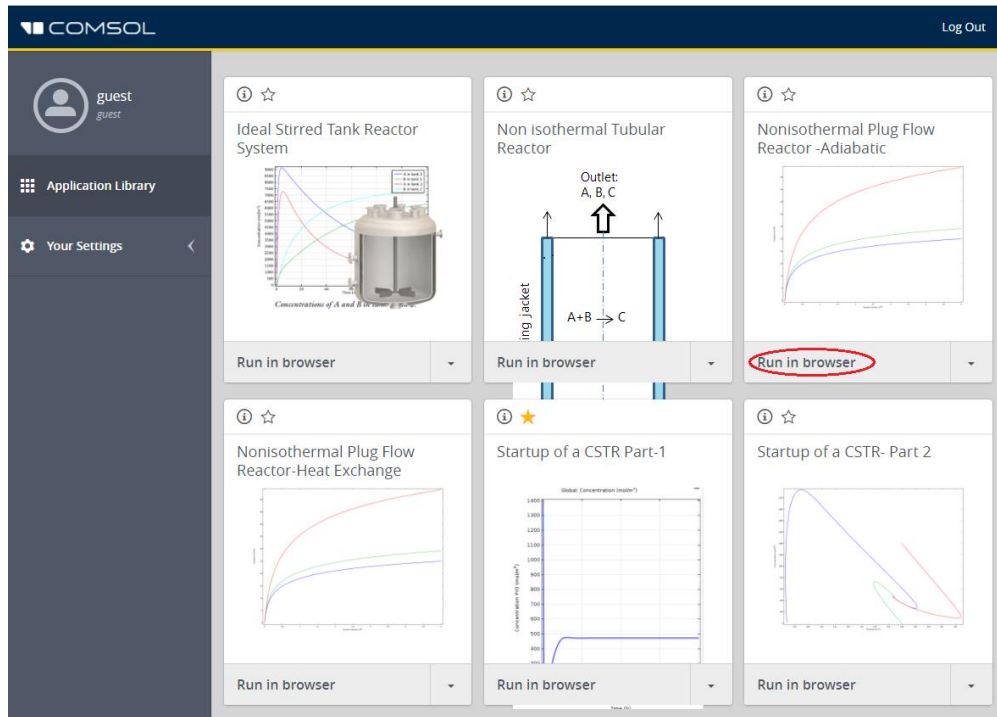
The screenshot shows the top navigation bar of a website. On the left, it says "Elements of Chemical Reaction Engineering 5th Edition". In the center, there are two book covers and a link that says "Home Problem Solving Updates and FAQs". On the right, it says "Essentials of Chemical Reaction Engineering". 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 says "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 five dots. At the bottom of the page, there is a pink button with the text "Log in to COMSOL Server" 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-Adiabatic”. 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

↶
PDF

Input and Description

Compute

Input

Inlet volumetric flow: m³/s

Inlet mole fraction, A: mol/mol

Inlet concentration, A: mol/m³

Activation energy, E₁: J/mol

Inlet 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:

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

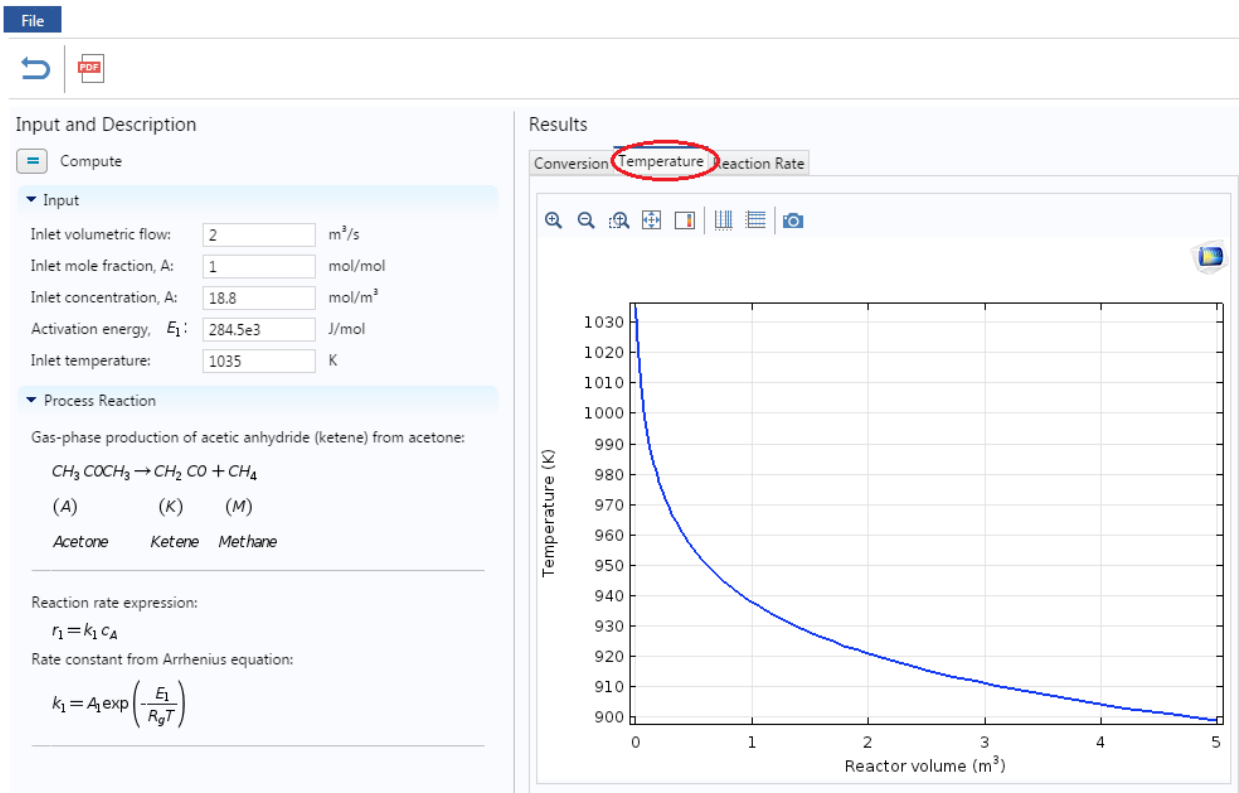
Results

Conversion Temperature Reaction Rate

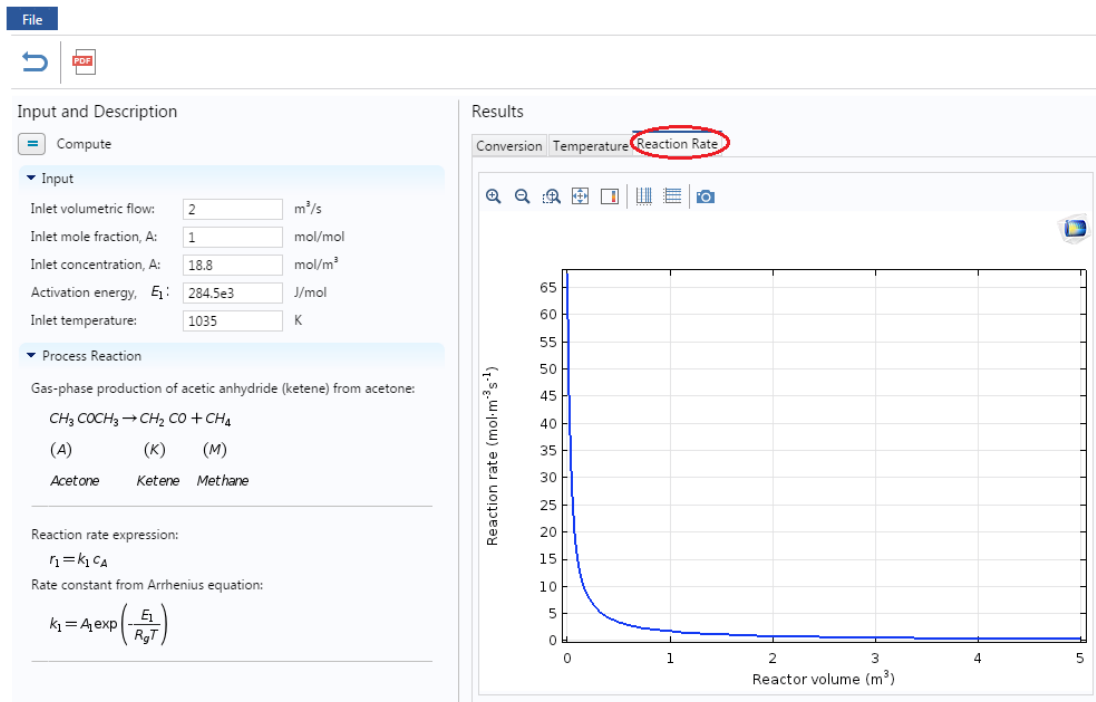
Conversion A (%)

Reactor volume (m³)

Step 6: Click on Temperature tab to view Temperature graph

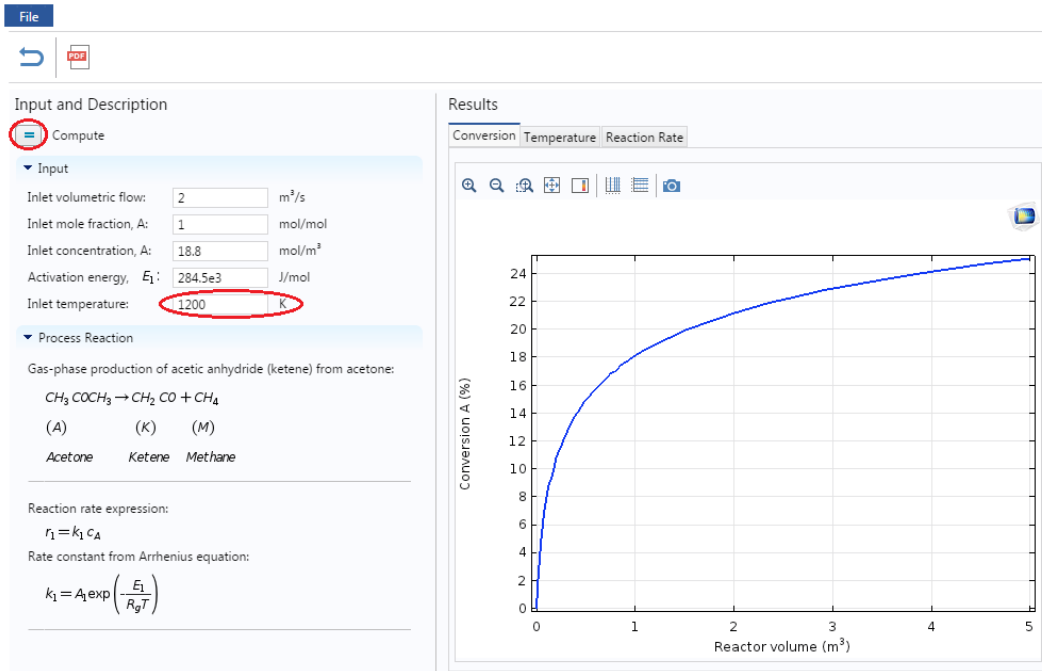


Click on Reaction Rate tab to view graph of reaction rate

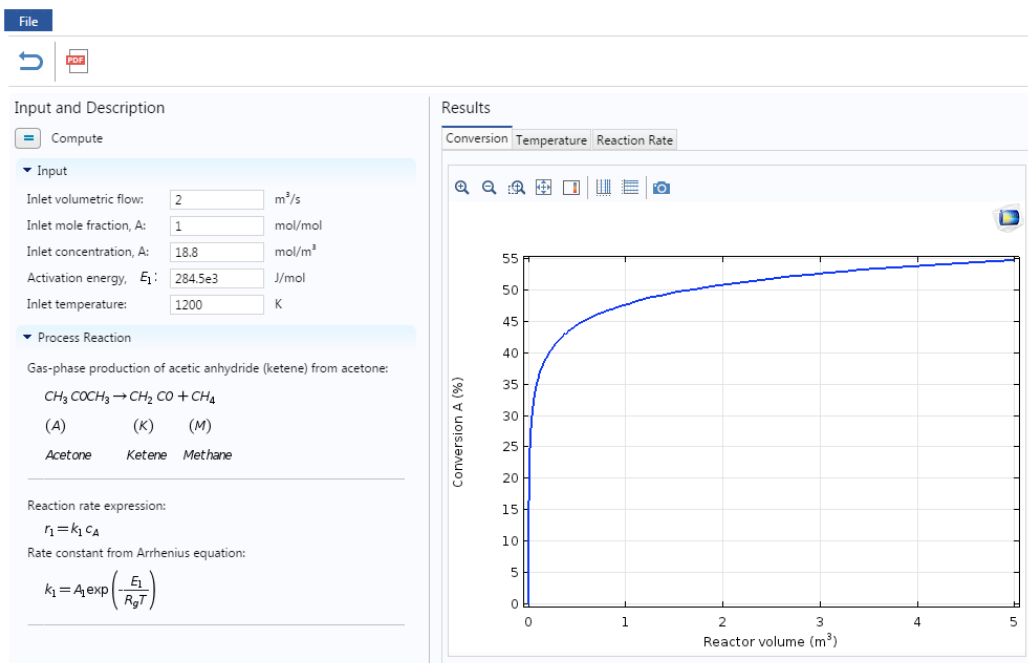


Step 7: Under Input section on the left hand side, you can view and change any parameter values. Let's change a parameter and see the effect on the profile. Change the Inlet temperature to 1200 K from 1035 K. After you are done, click on Compute button (=) present above the Input parameters

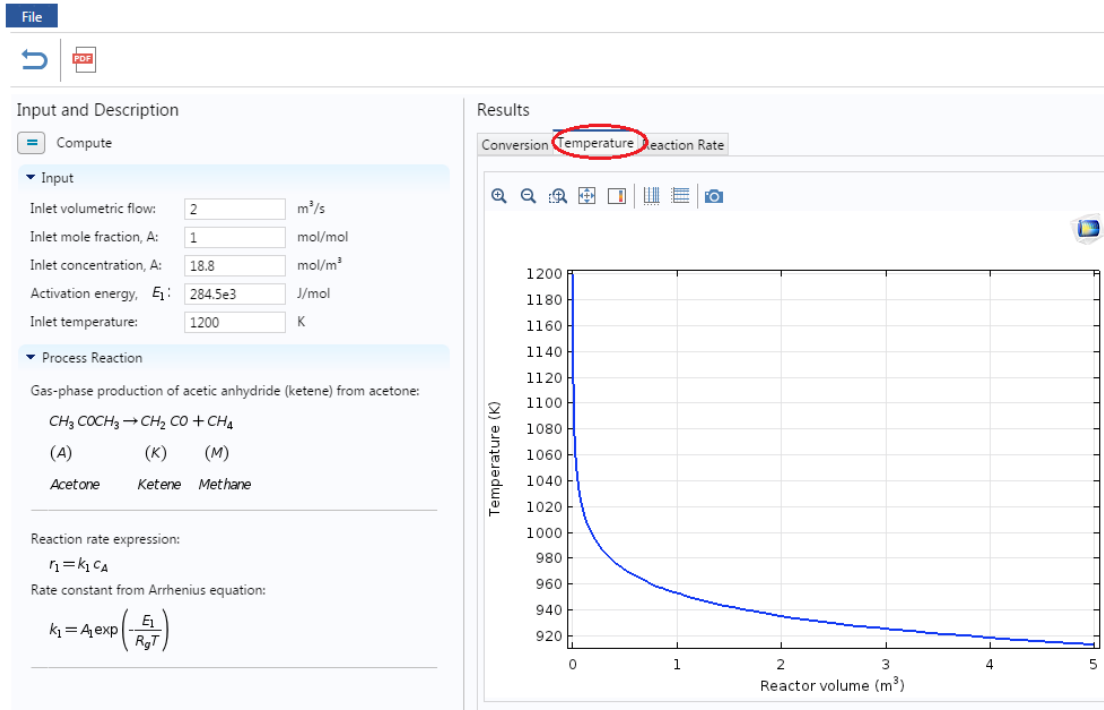
Caution: The y axis is dynamic and scale changes with respect to the values. Make sure to look at both scale and graph



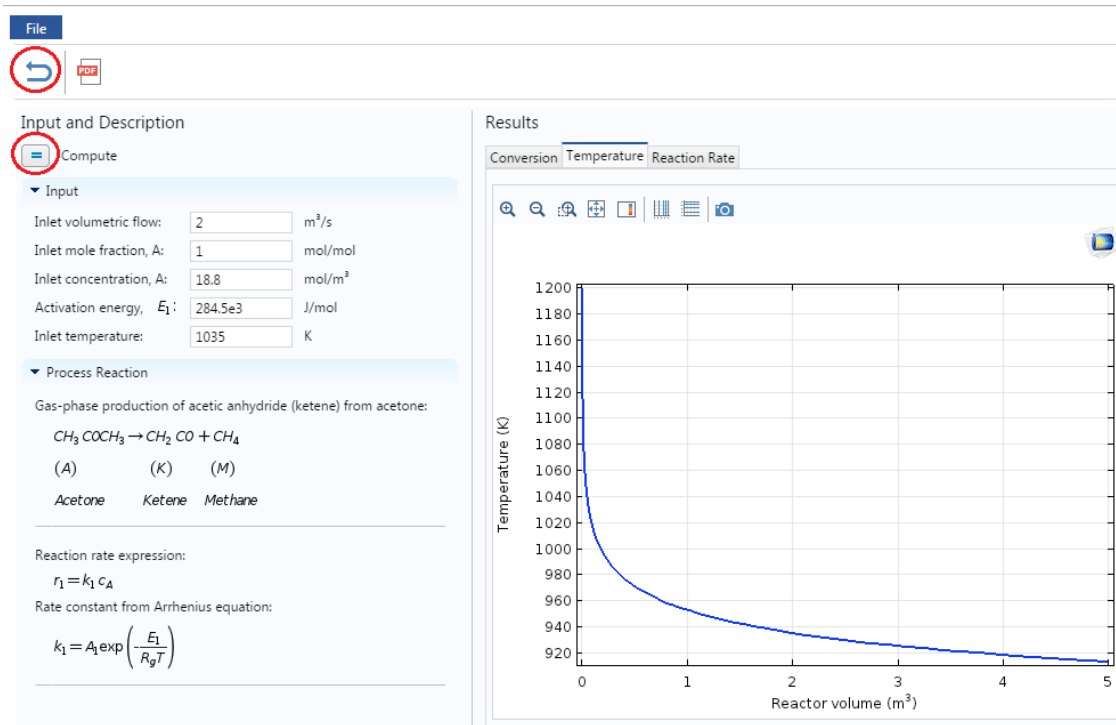
Step 8: Now check the Conversion and Temperature profiles. The following graph is obtained for conversion. You can see that conversion has increased at higher temperature



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

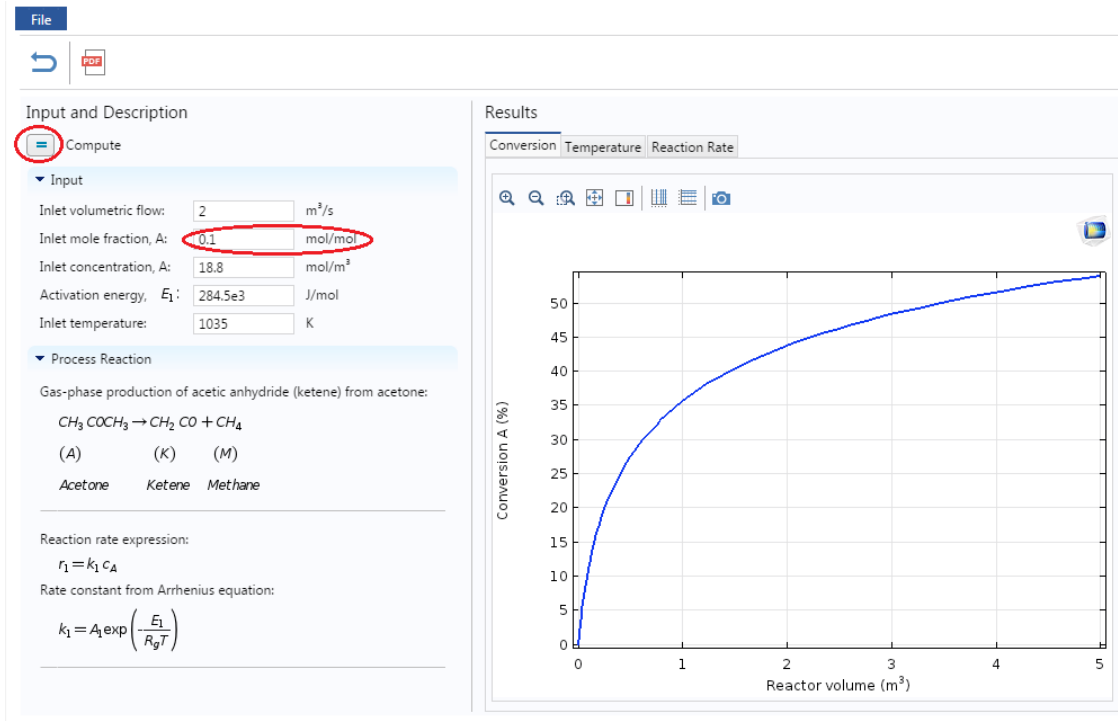


Step 9: Now if you want to re-set all the parameter values to its initial values, click on “reset to default button(↶). Click on this button and you will find that it resets the value of Temperature. To update the graph, click on Compute button. Each time you change a variable, click Compute

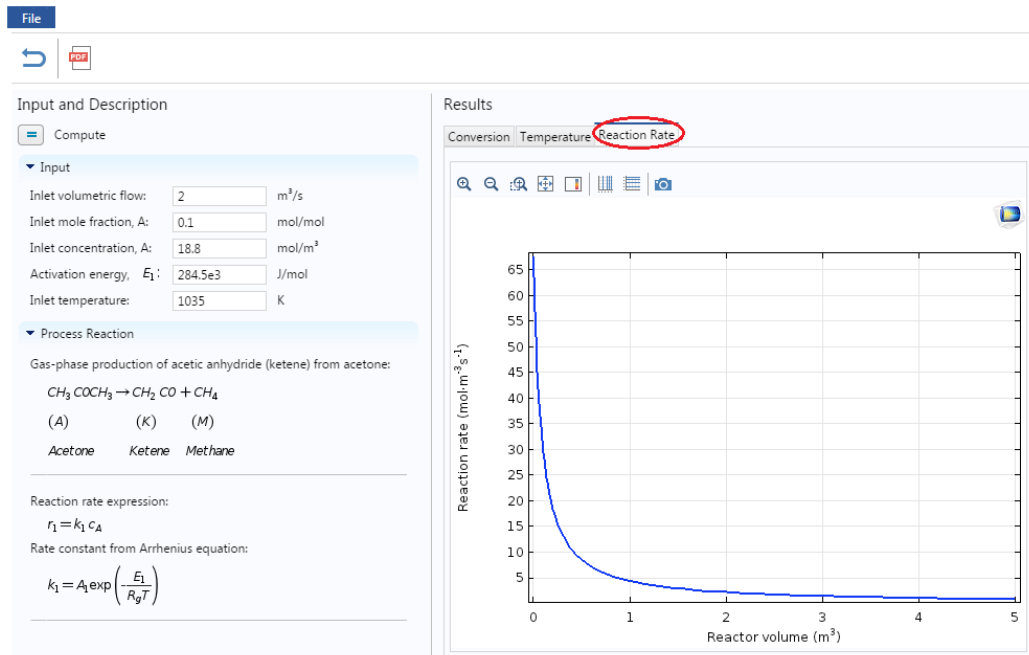


Step 10: Now let's consider a case where inert is present in the inlet. Change the inlet mole fraction of A to 0.1 instead of 1 and click compute to see its effect on profile.

The following graph will be obtained for conversion. You can see that with the presence of Inert, conversion has increased to more than 50%



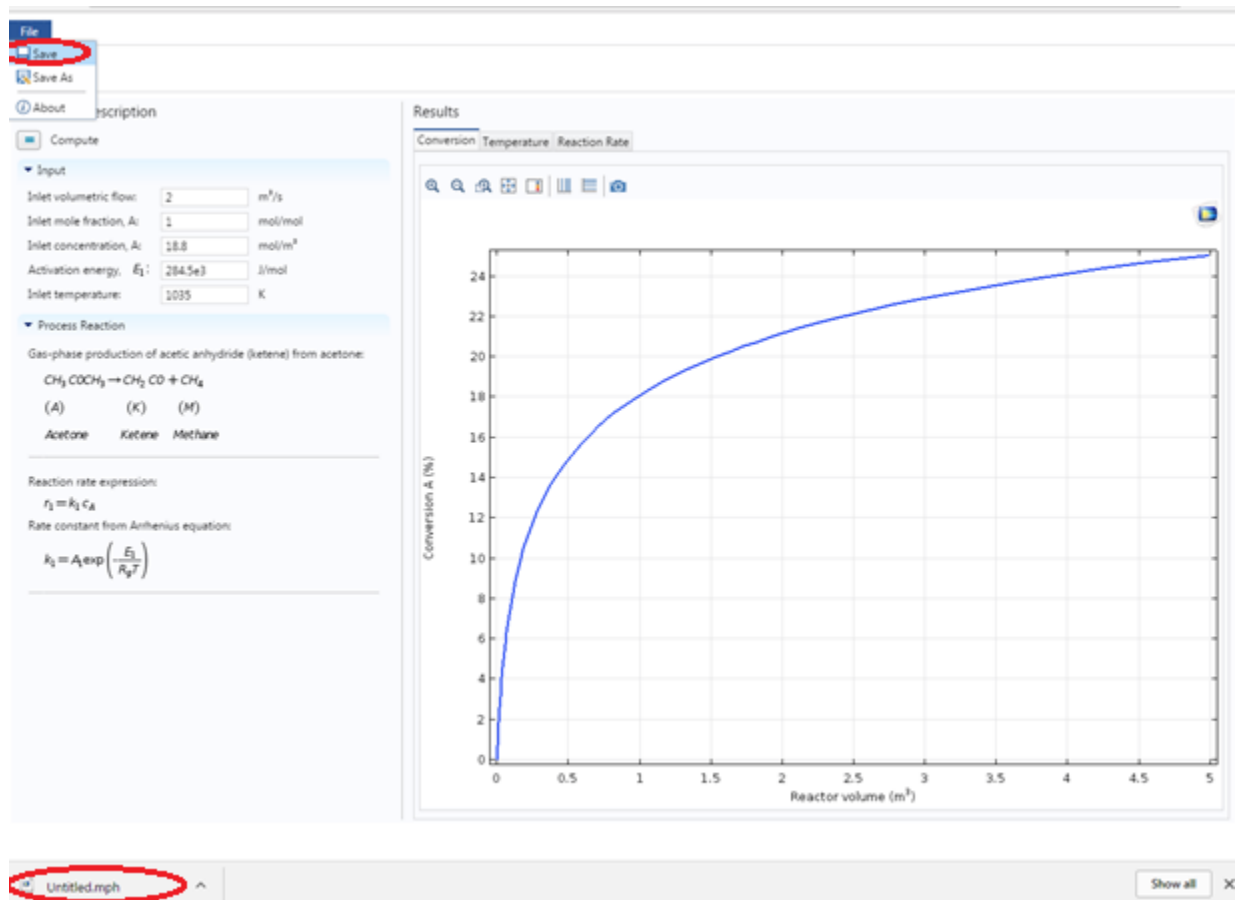
Click on Reaction rate graph. The following graph will be obtained for reaction rate which shows reaction rate has increased



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

File

PDF

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

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 (m ³)	Conversion A (%)
0	0
0.5	10
1.0	16
1.5	19
2.0	21
3.0	23
4.0	24
5.0	24

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

Plug flow.pdf 1 / 20

Created in COMSOL Multiphysics 5.2a

Non-Isothermal Plug Flow Reactor