

COMSOL LEP tutorial for Nonisothermal Tubular reactor with radial and axial variation (Chapter 12, Example W12-8)

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 browser address bar displays "umich.edu/~elements/5e/12chap/obj.html". The page title is "Chapter 12: Steady-State Nonisothermal Reactor Design: Flow Reactors with Heat Exchange". Under the "Objectives" section, it lists several goals for the chapter, including describing algorithms for CSTRs, PFRs, and PBRs, and analyzing multiple reactions. A navigation menu on the left lists various resources like "Learning Resources", "Living Example Problems", and "Professional Reference Shelf". At the bottom of the page, there are several buttons for additional resources, with the "COMSOL" button circled in red.

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
 - Adiabatic
 - Constant ambient exchange temperature
 - Co-current heat exchange
 - 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”

This screenshot shows the same website interface as the previous one, but with the "How to access COMSOL" link in the left-hand navigation menu circled in red. Below this link, 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”

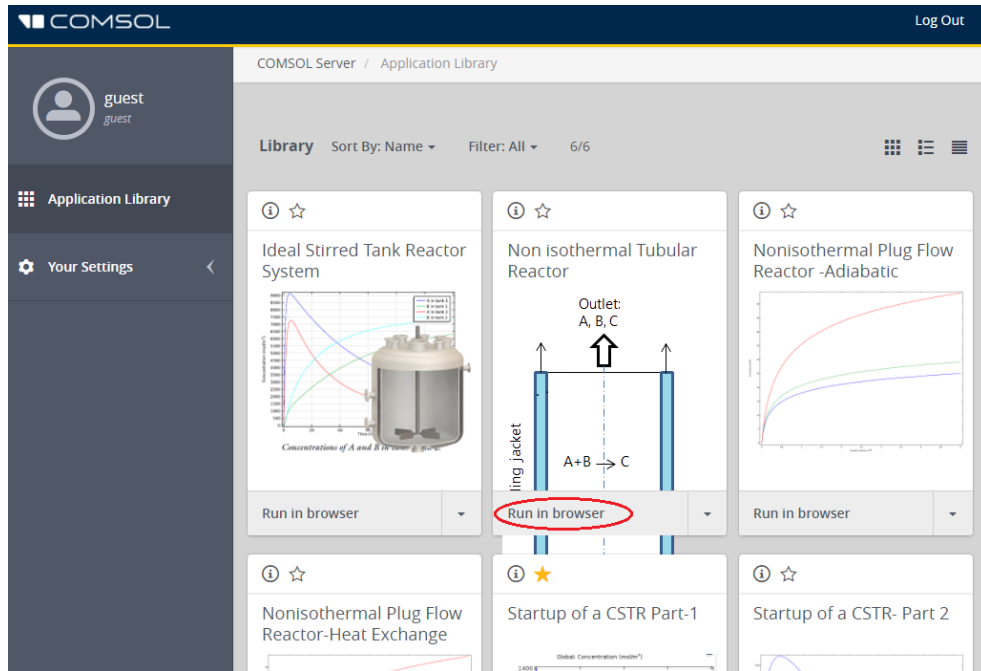
The screenshot shows the top navigation bar of a website. On the left, it says "Elements of Chemical Reaction Engineering 5th Edition". In the center, there are two book covers and a link that says "Home Problem Solving Updates and FAQs". On the right, it says "Essentials of Chemical Reaction Engineering". 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 these are the fields "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

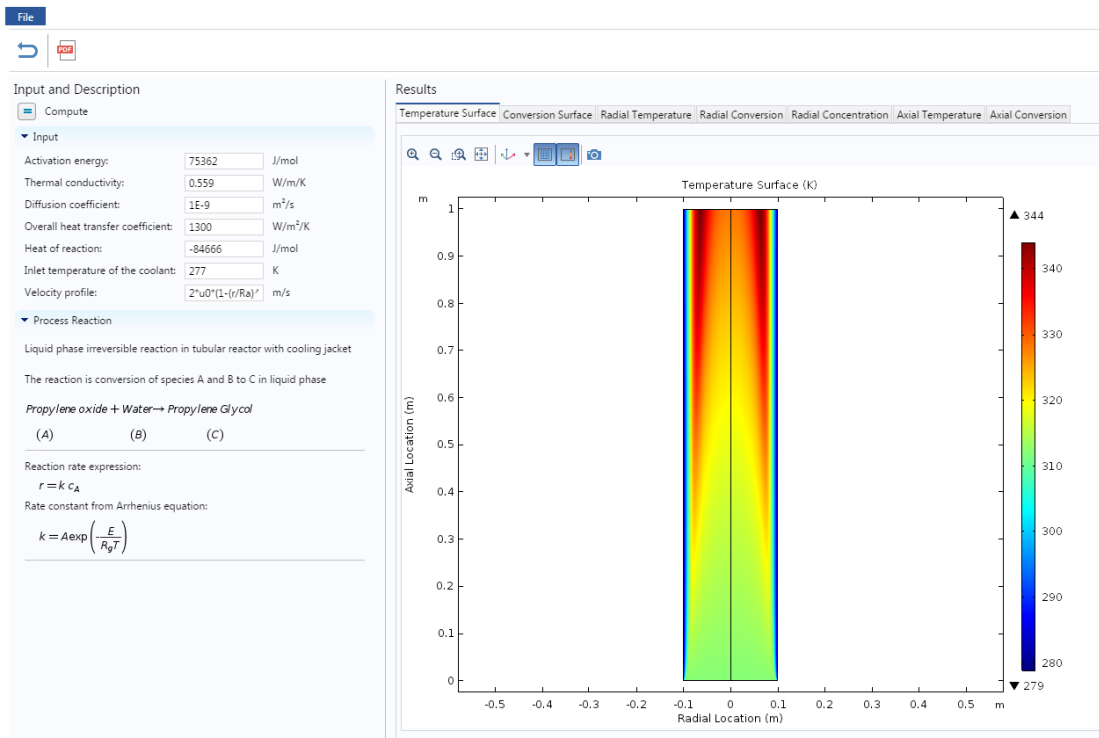
username: guest
password : guest

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.

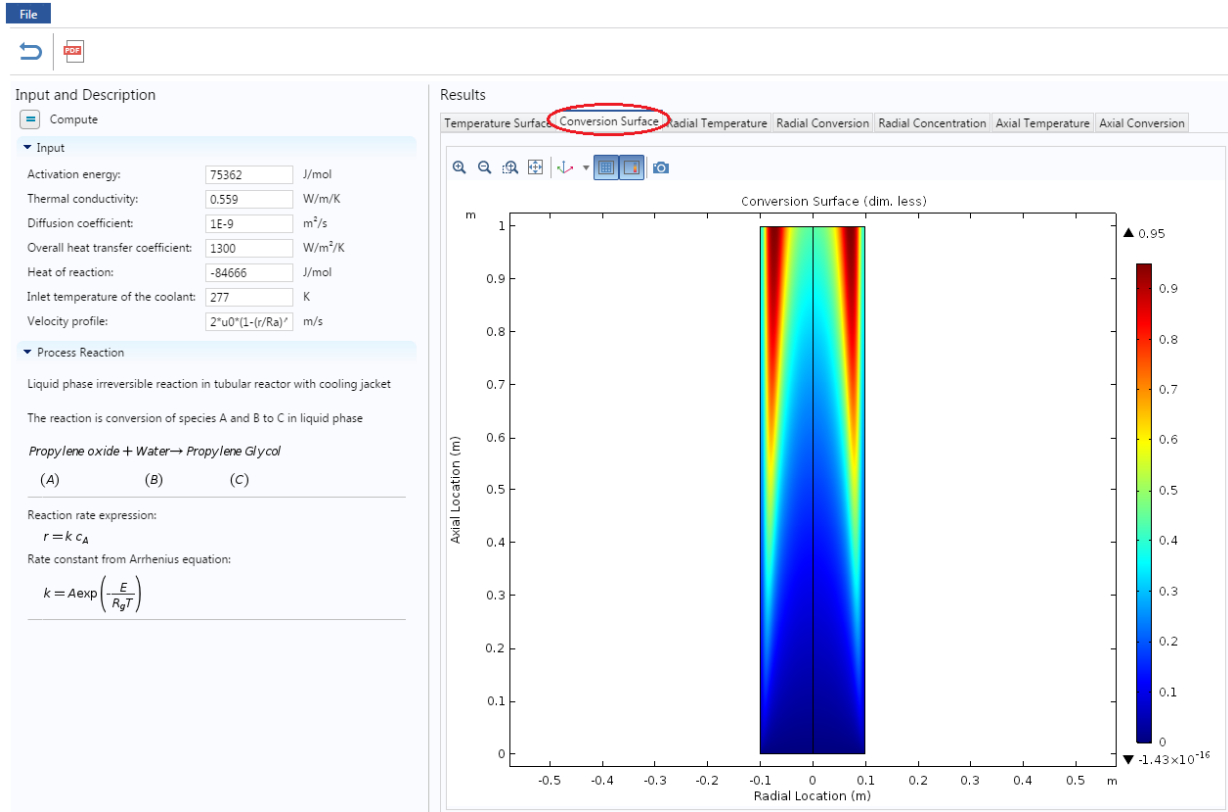
Step 5: This will open up COMSOL library where you see many COMSOL files to solve chemical reaction engineering problems. Find “**Non isothermal Tubular Reactor**”. Click on “Run in browser” to start the application



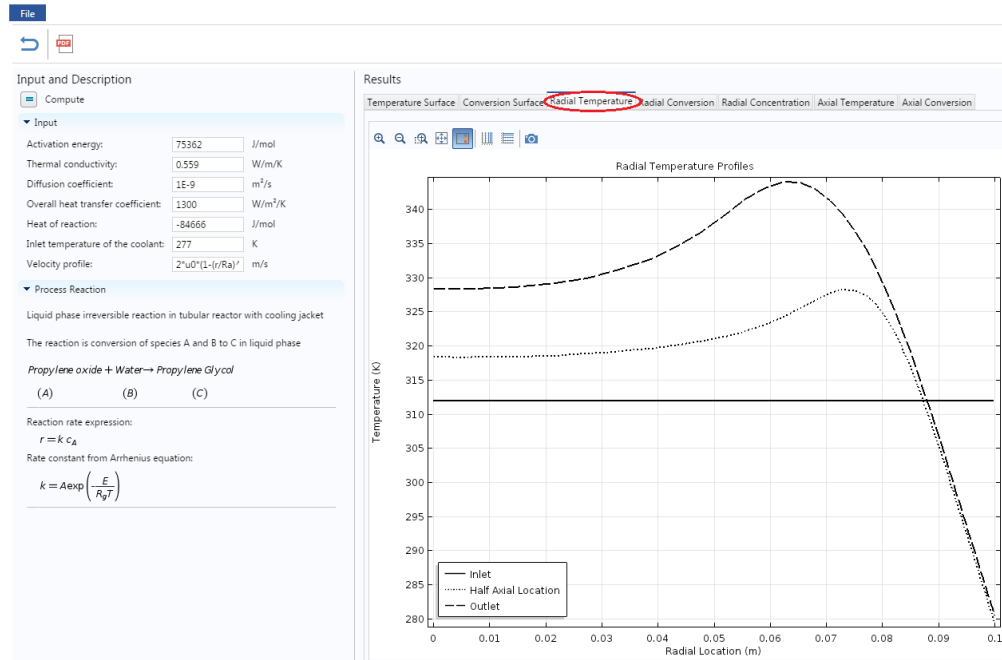
You will see that the following window opens which has input parameters, description, graphical features and a few buttons. You can see the Temperature distribution (Surface graph) on the right side of the page



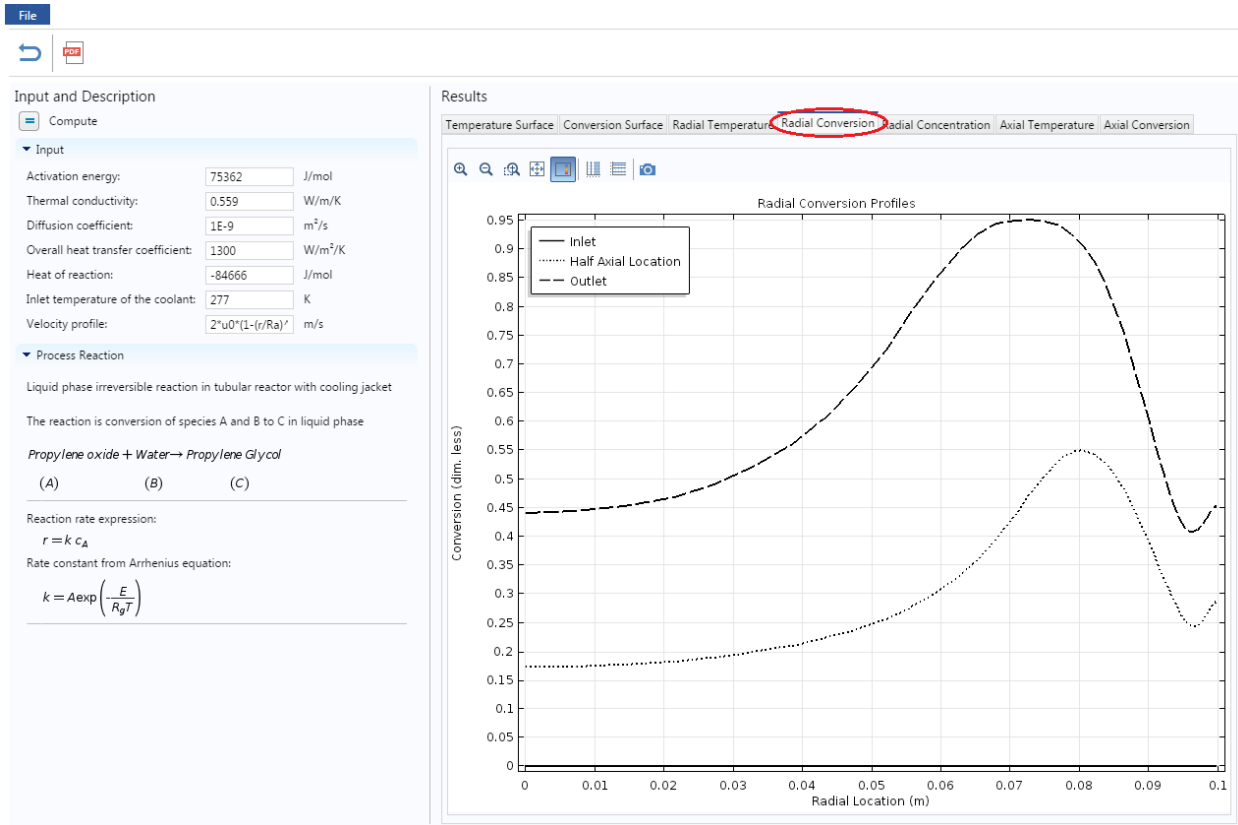
Step 6: Click on Conversion surface to view Conversion surface (2 D graph) plot



Click on Radial Temperature to view Radial Temperature profiles



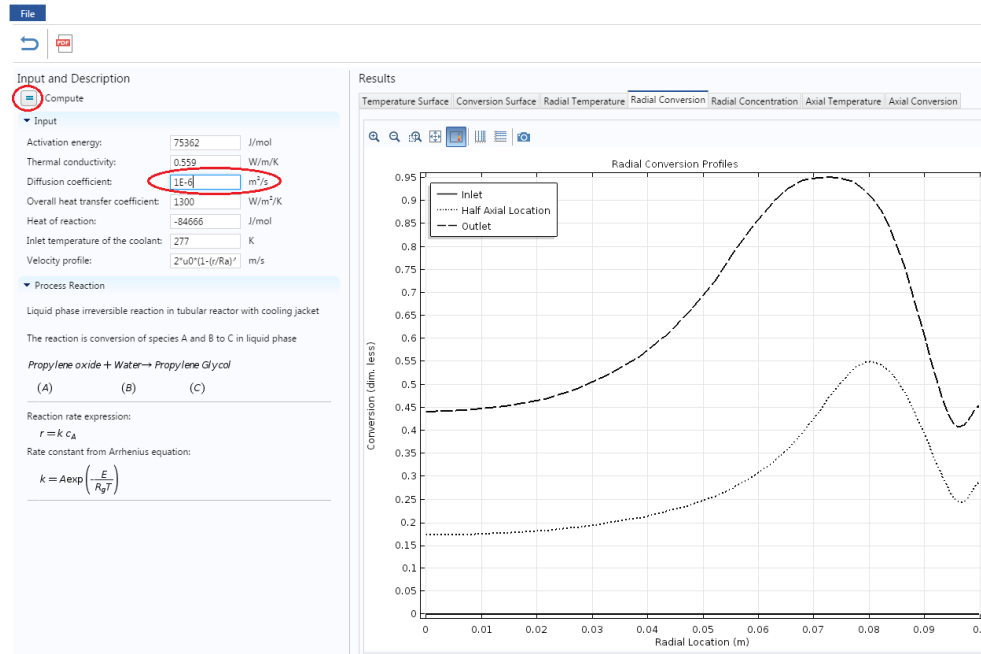
Click on Conversion profiles tab to view Conversion 1D graph



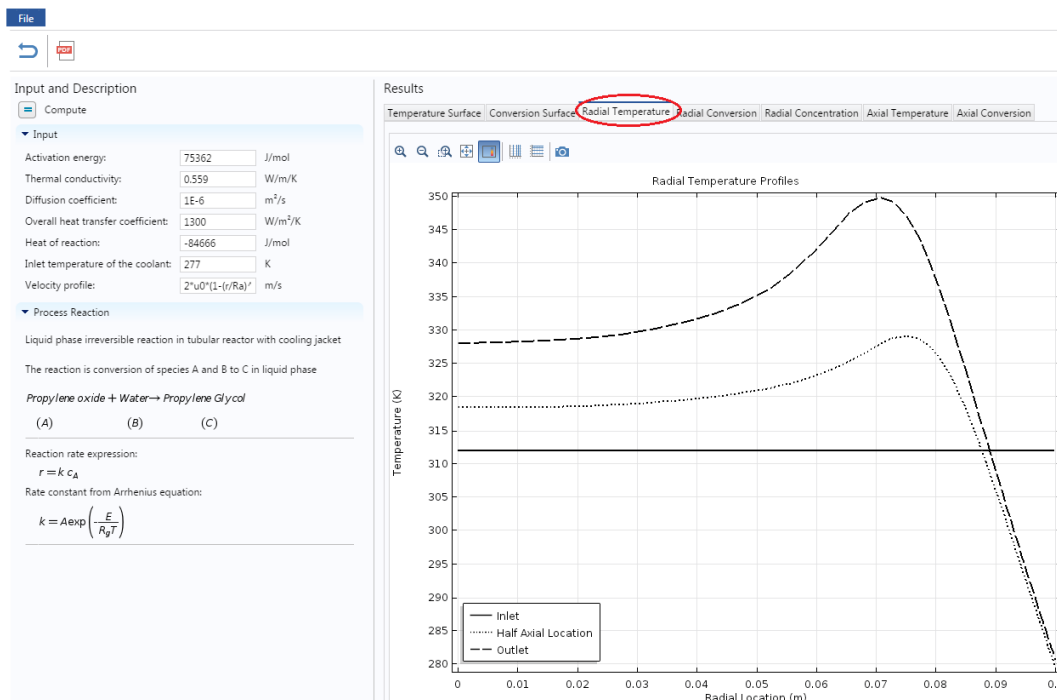
Similarly click on other tabs to view Radial Conversion, Axial Temperature and Axial Conversion profiles

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. Increase the Diffusivity value from its initial value of $1\text{e-}9$ to $1\text{e-}6$. After you are done, click on Compute button (=) present above the Input parameters

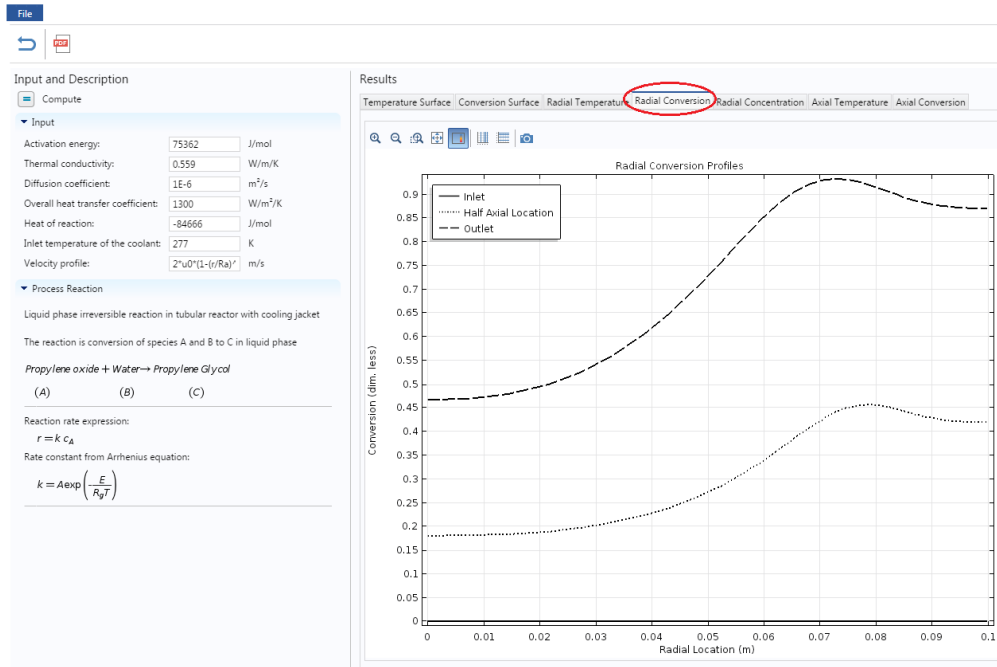
Caution: The y axis is dynamic and scale changes with respect to the values. Make sure to look at both scale and graph



Step 8: Now check the Temperature and Conversion profiles. The following graph will be obtained for Temperature profile. You can see that temperature has increased in the radial direction

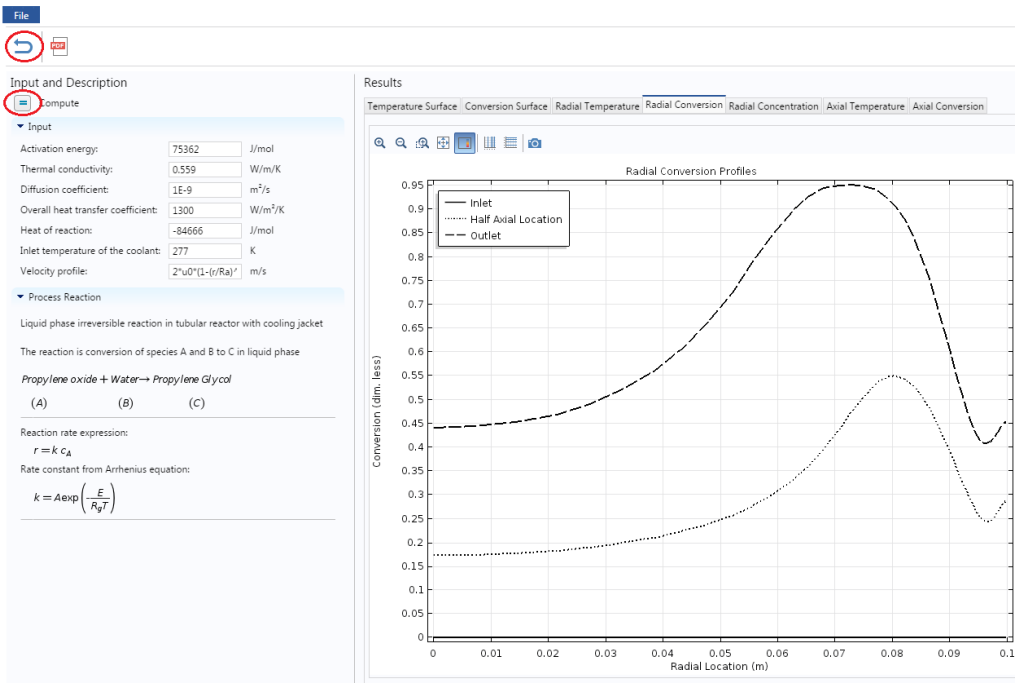


The following graph is obtained for conversion profile. With the increase in diffusivity, higher conversion will be achieved near to the wall of the reactor

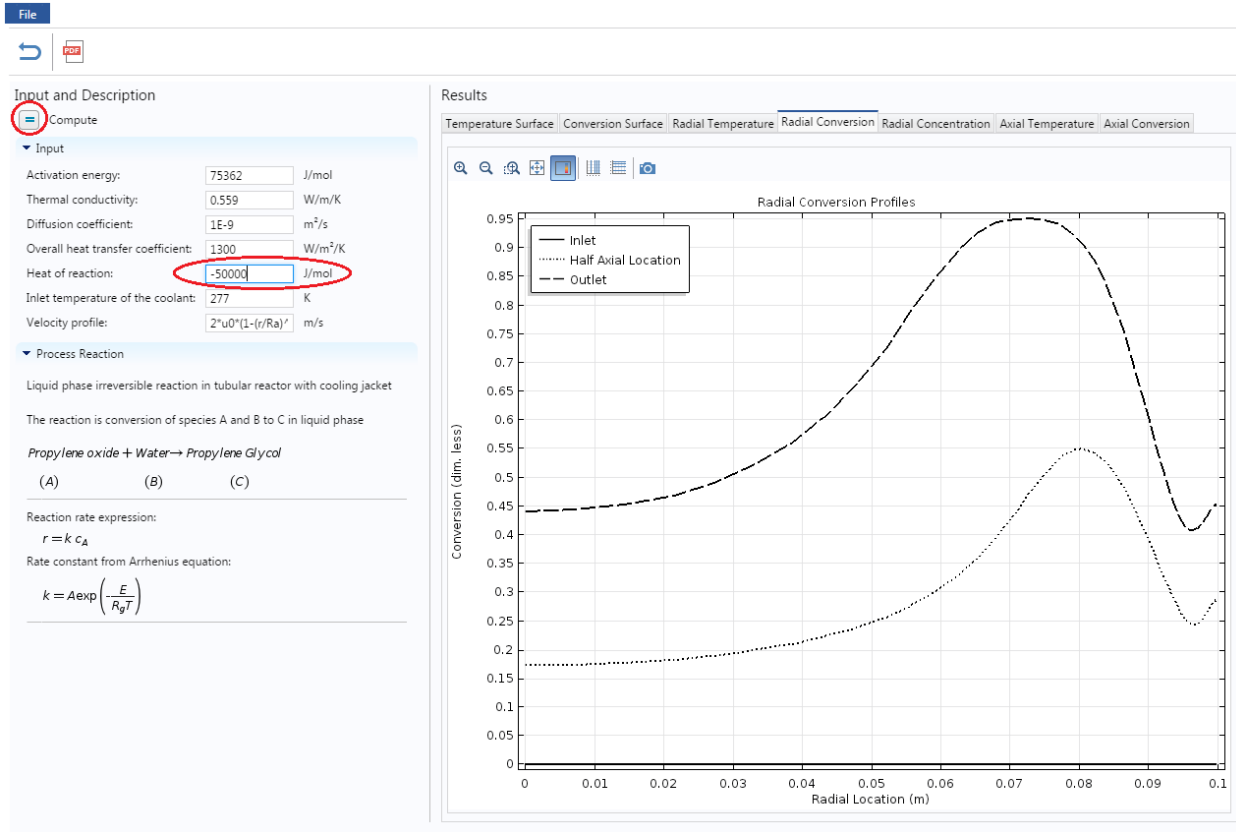


Step 9: Now if you want to re-set all the parameter values to its initial values, click on “reset to default button(↶). Click on this button to reset the value of diffusivity. To update the graph, you will have to click on Compute button each time you change a variable.

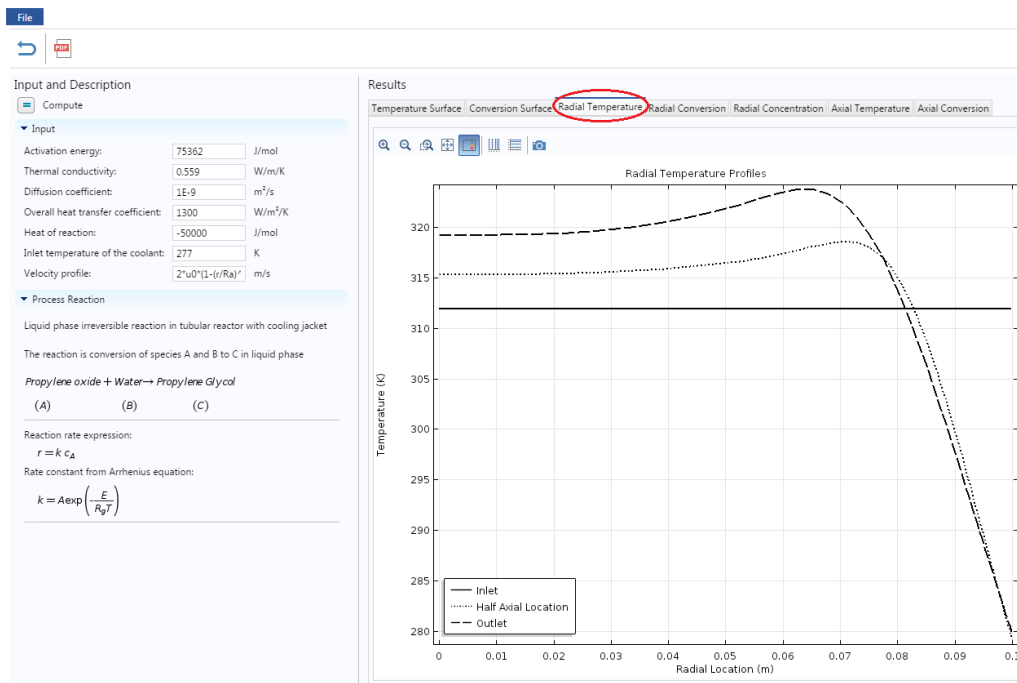
Please note that reset to default button doesn't reset the expression for Velocity profile. If you change the velocity profile, then you need to reset it manually

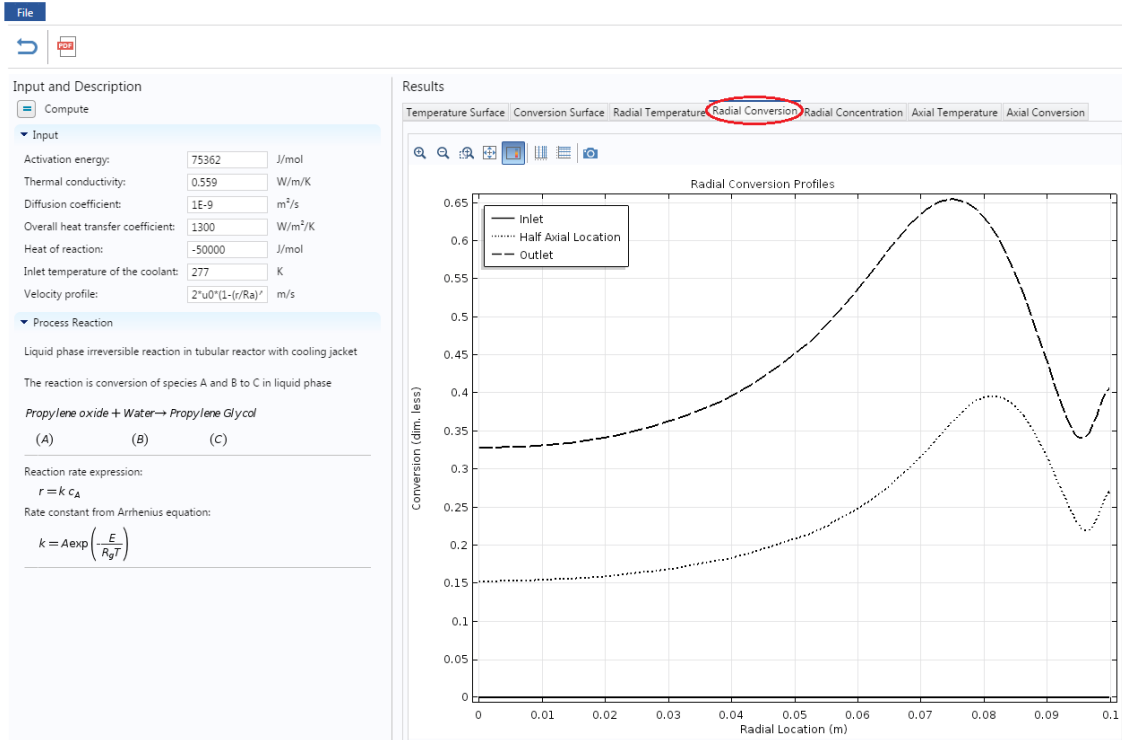


Step 10: Now let's change the heat of reaction and see its effect on profile. Enter the Heat of reaction to be -50000 and click compute to update the results

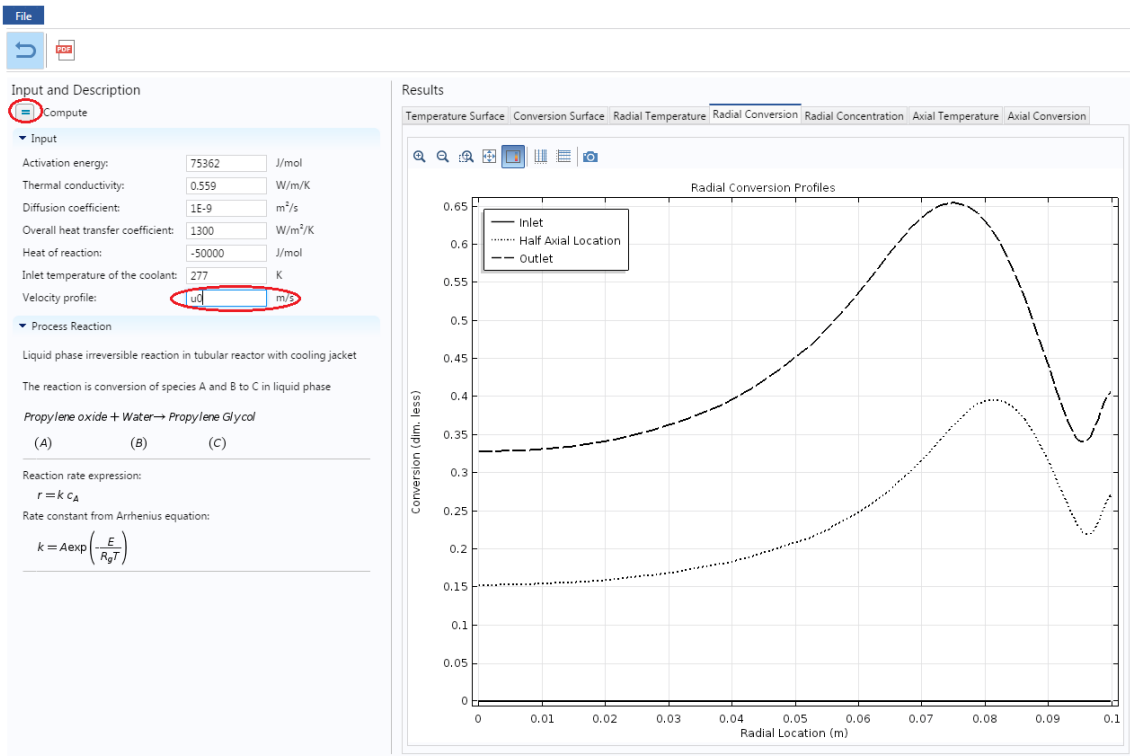


The following graph will be obtained for Temperature and Conversion profiles

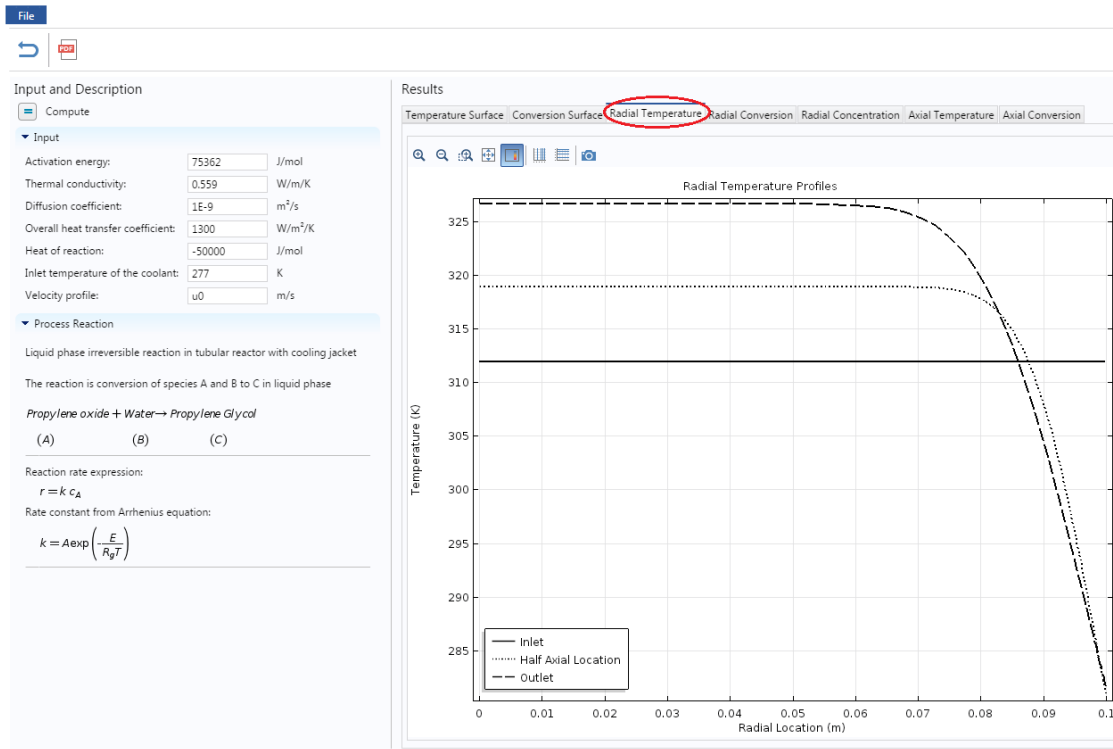




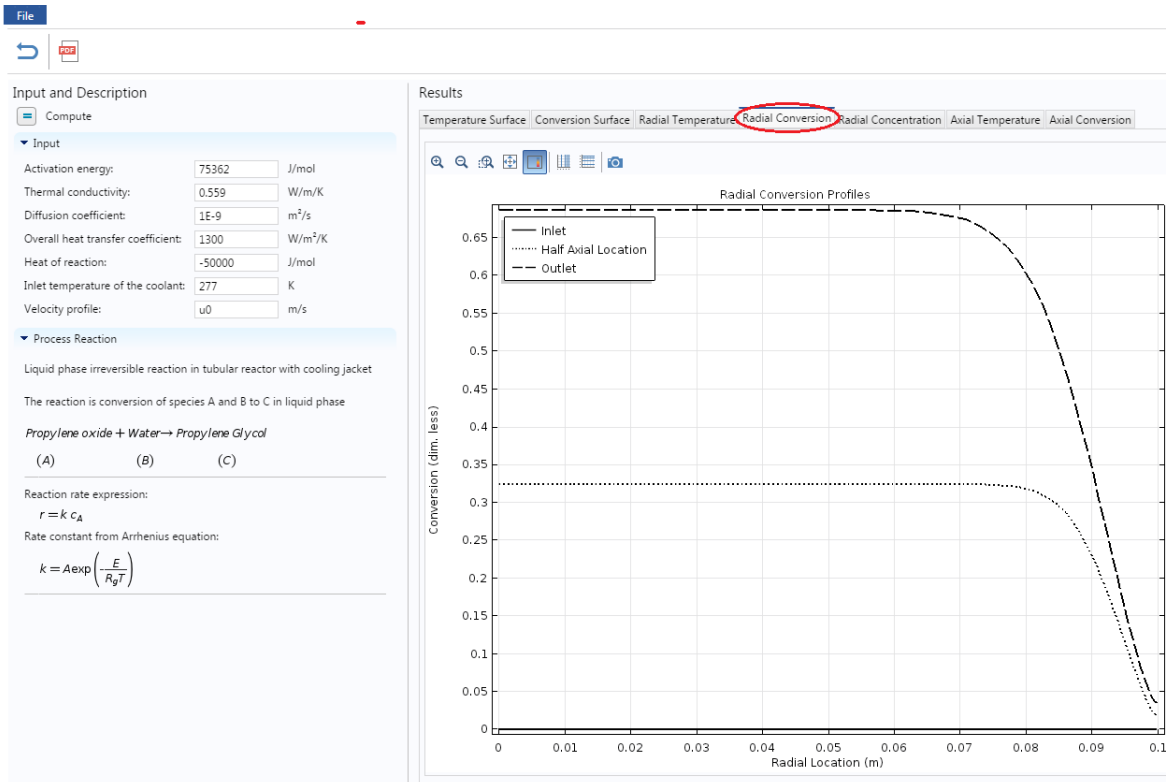
Step 11: To change the flow conditions from laminar to plug flow or turbulent flow, enter the corresponding equation for Velocity profile in the text field. For plug flow, enter the velocity profile as u_0 . Click compute



The following graph is obtained for radial temperature under plug flow conditions



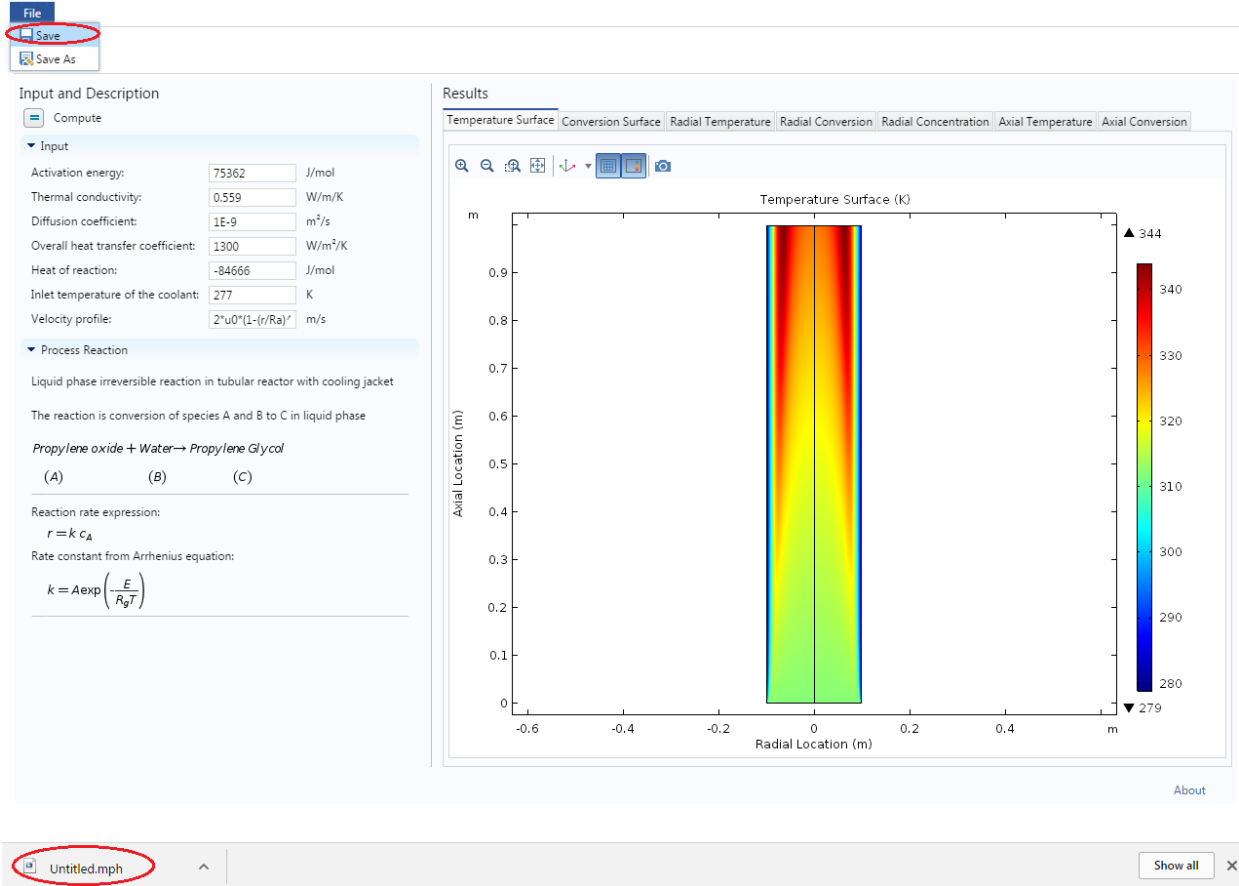
The following graph is obtained for radial conversion under plug flow conditions



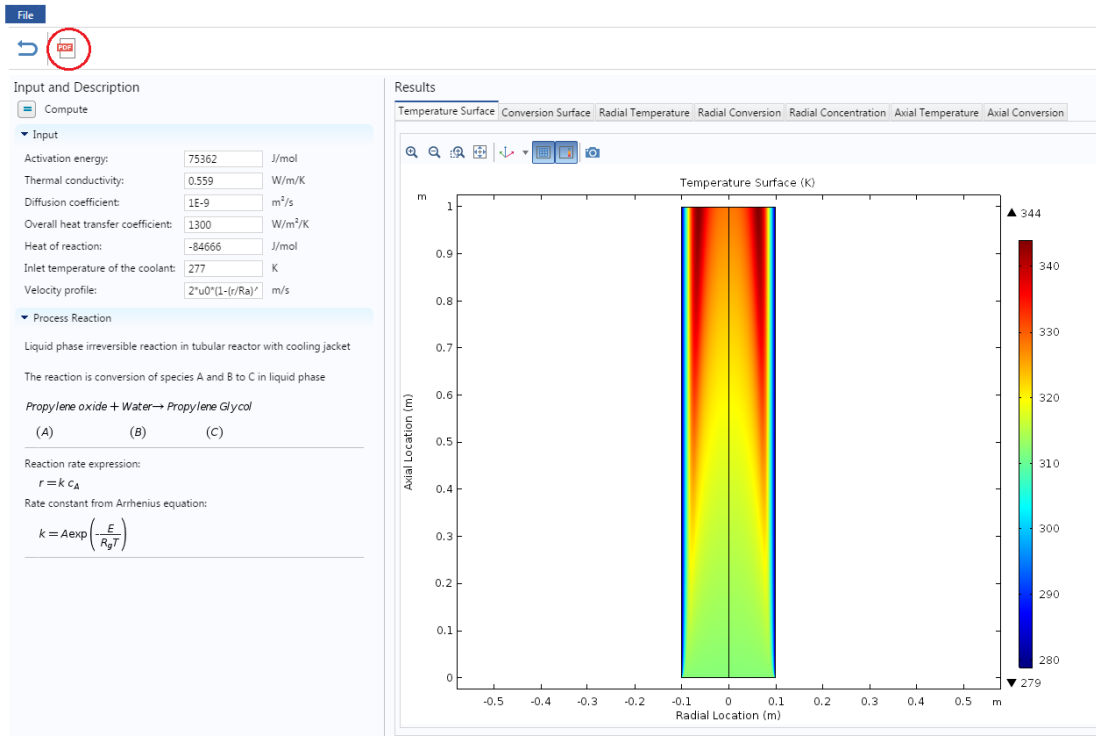
Step 12: Now, you can change any listed parameter value and check its effect on profiles. Make sure to click Compute button after you change a variable.

Step 13: If you have COMSOL installed on your computer, then you can also download the complete COMSOL file (with user interface)

- a) 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)
- b) Click on the downloaded file to open the application



Step 14: You can also open a pdf documentation which details the reactor model by clicking on PDF button



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

