

## COMSOL LEP tutorial for Startup of a CSTR (Chapter-13)

Step 1: Open chapter 13 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 shows 'umich.edu/~elements/5e/13chap/obj.html'. The page title is 'Chapter 13: Unsteady State Nonisothermal Reactor Design'. Under the 'Objectives' section, there are four bullet points: 'Analyze batch reactors and semibatch not operated isothermally.', 'Explain why a reactor exploded when its charge was increased by a factor of three.', 'Analyze perturbations in temperature and presence for CSTRs being operated at steady state and describe under what conditions the reactors can be unsafe (safety).', and 'Analyze multiple reactions in batch and semibatch reactors not operated isothermally.' Below the objectives, there are several resource buttons: 'Learning Resources', 'Living Example Problems', 'Expanded Material', 'Youtube Videos', 'Professional Reference Shelf', 'Additional Homework Problems', 'Web Modules', and 'COMSOL' (circled in red). There is also a 'Learn ChemE Videos' button and a 'Self test' section with 'A. Exercises' and 'B. i-clicker questions' buttons.

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

The screenshot shows the website interface for 'Elements of Chemical Reaction Engineering, 5th Edition'. The page title is 'How to access COMSOL'. There are two buttons: 'How to access COMSOL' (circled in red) and 'COMSOL LEP tutorial'.

**Step 3:** You will see a new page with instruction on how to access COMSOL library. Click “Here”

The screenshot shows a web page for the COMSOL library. At the top, there are two book covers for 'Elements of Chemical Reaction Engineering 5th Edition'. Between them is a link: 'Home Problem Solving Updates and FAQs'. To the right is another book cover for 'Essentials of Chemical Reaction Engineering'. Below the covers is a table of contents (TOC) with chapters 1 through 18 and Appendices. On the left side, there is a sidebar menu with options: 'BY CHAPTER', 'Objectives', 'Learning Resources - Summary Notes', 'Living Example Problems', 'Professional Reference Shelf', 'Additional HW Problems', 'FAQs', and 'Expanded Material'. The main content area contains the following text:

Please visit [HERE](#) to access COMSOL.

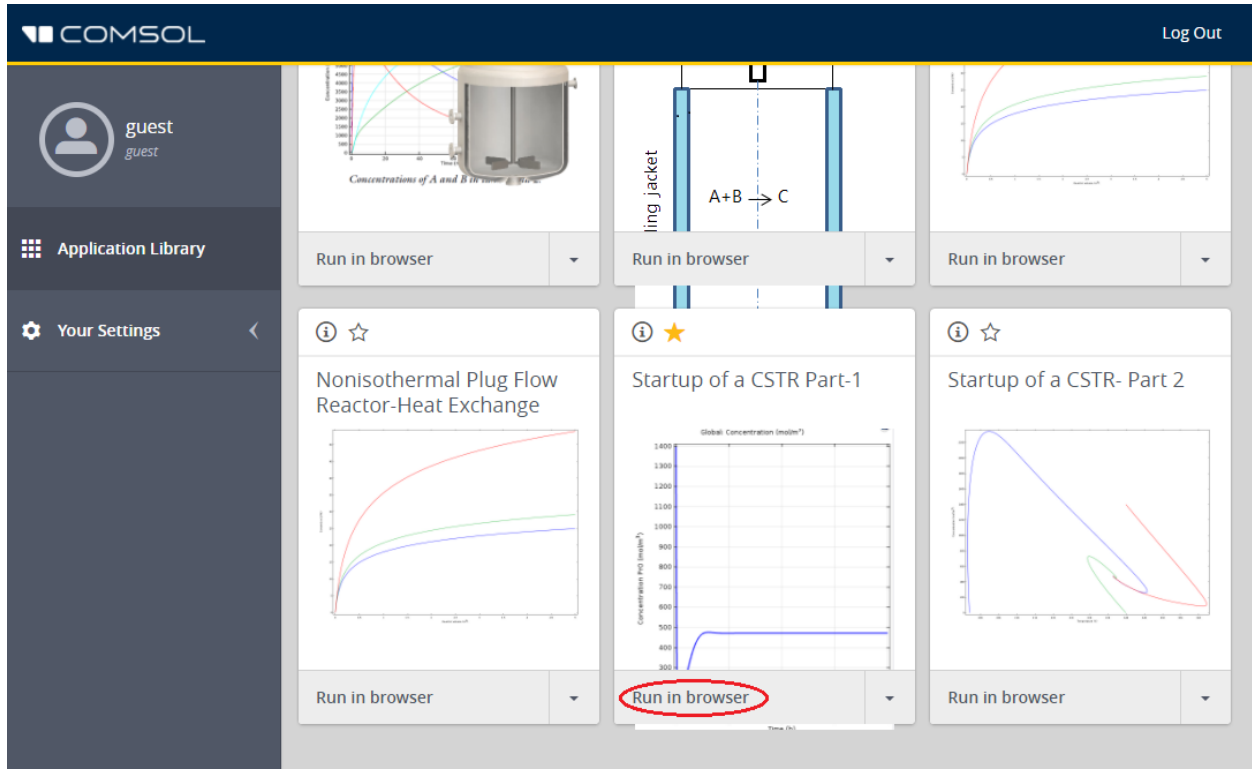
- If you are a student at the University of Michigan, please use your unique-name and password.
- If you are not a University of Michigan student, use  
username: guest  
password: guest

**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

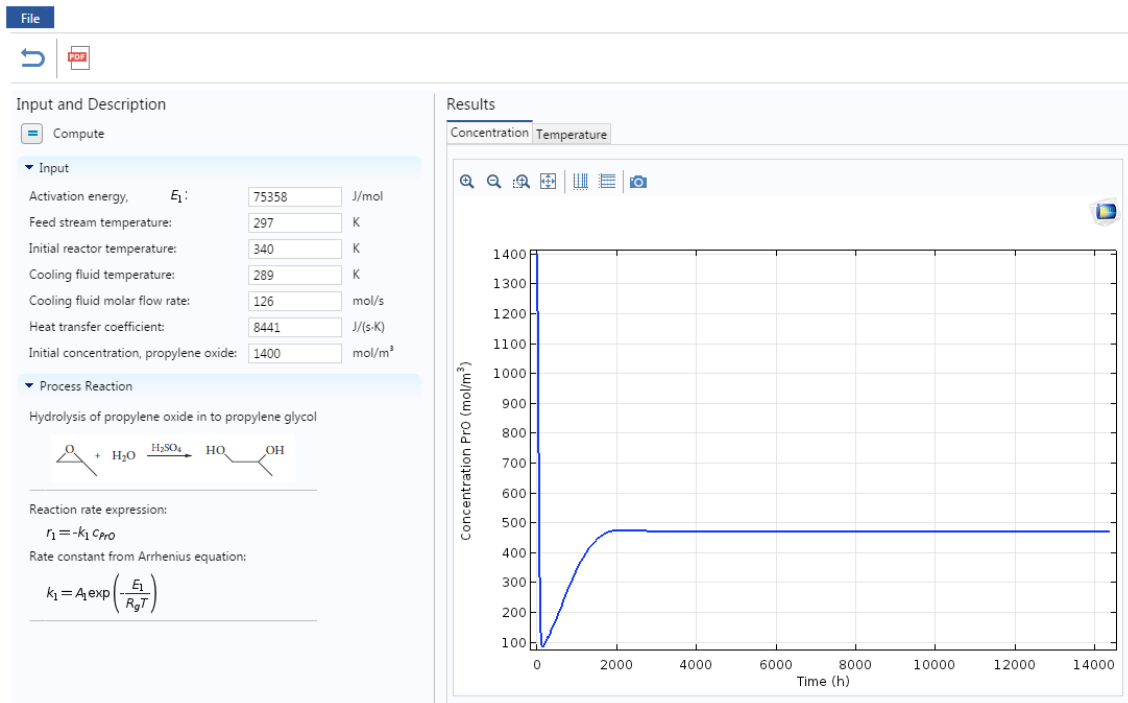
username: guest  
password : guest

The screenshot shows the COMSOL Server login page. The title 'COMSOL SERVER™' is displayed in a large, maroon font. Below the title is a horizontal maroon bar. Underneath the bar, 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 maroon button with the text 'Log in to COMSOL Server' circled in black.

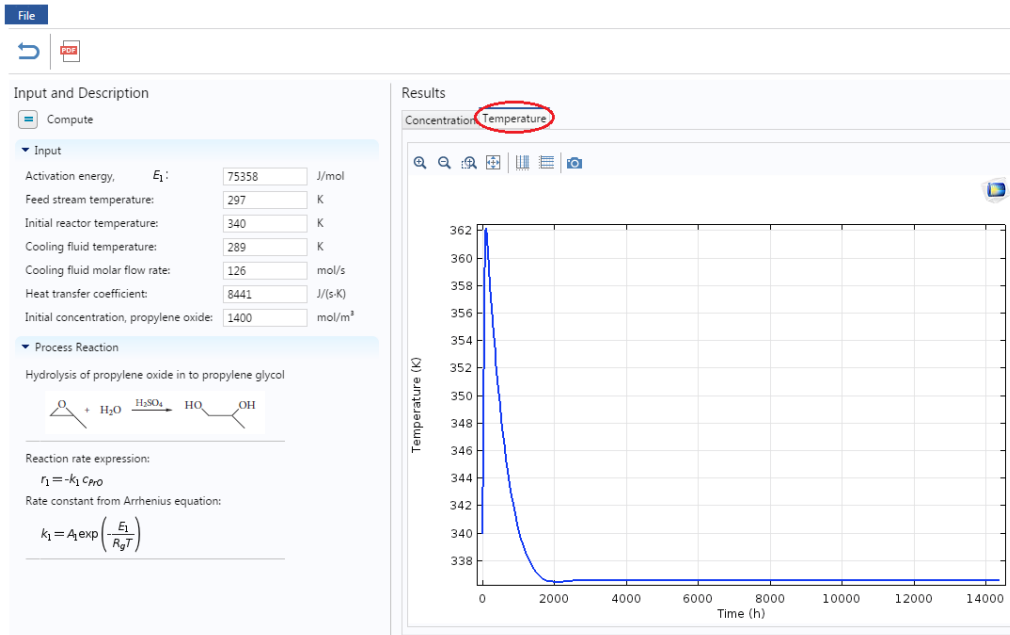
**Step 5:** This will open up COMSOL library where you can see many COMSOL files to solve chemical reaction engineering problems. Find **“Startup of a CSTR Part-1”**. Click on **“Run in browser”** to start the application



You will see that following window opens which has input parameters, description, graphical features (Concentration and Temperature profiles) and a few buttons. Currently Concentration profile is visible.

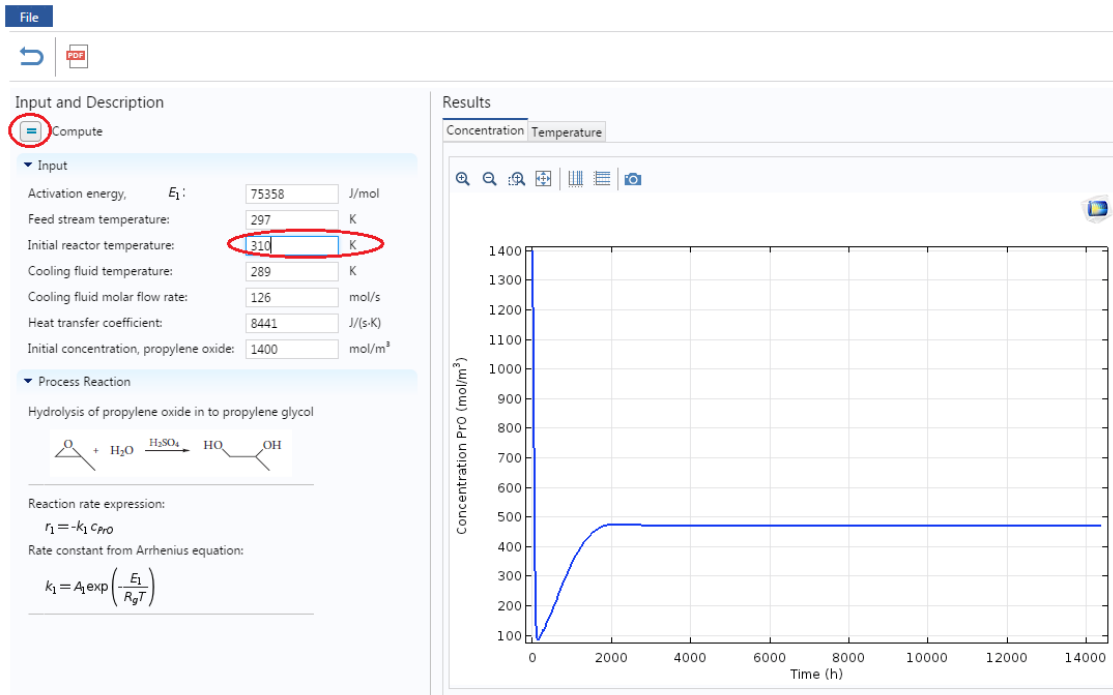


**Step 6:** Click on Temperature tab to view Temperature profile

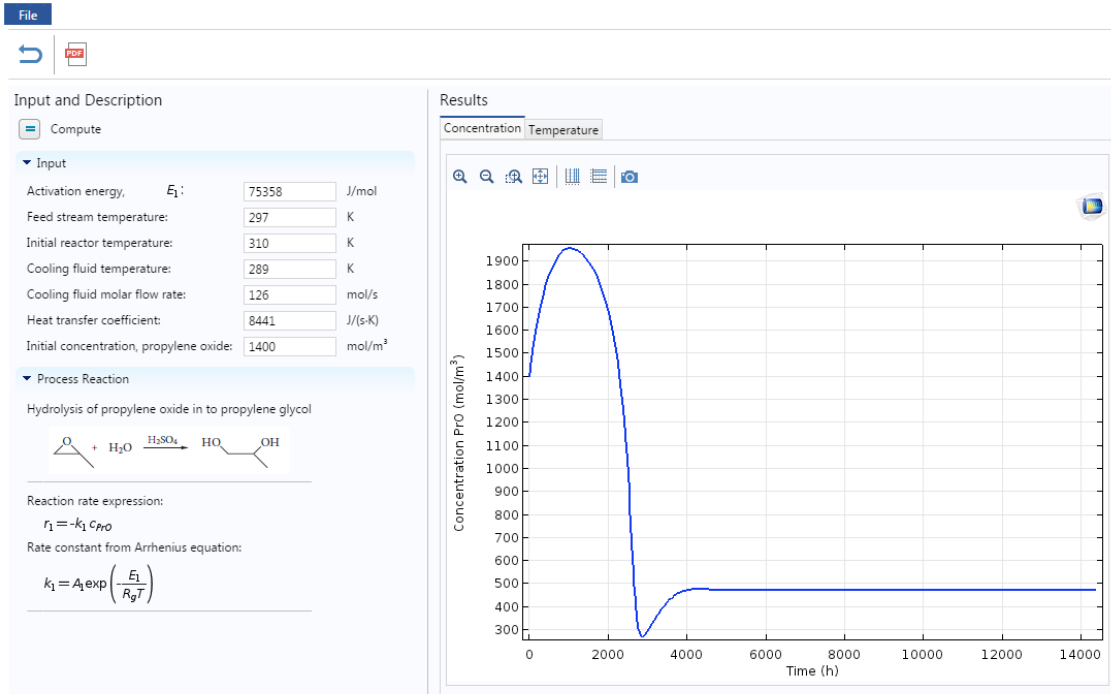


**Step 7:** Under Input section on the left hand side, you can view and change any parameter values. Let's change a parameter and see the effect on the profile. Change the Initial reactor temperature from 340 K to 310 K. After you are done, click on Compute button (=) present above the Input parameters

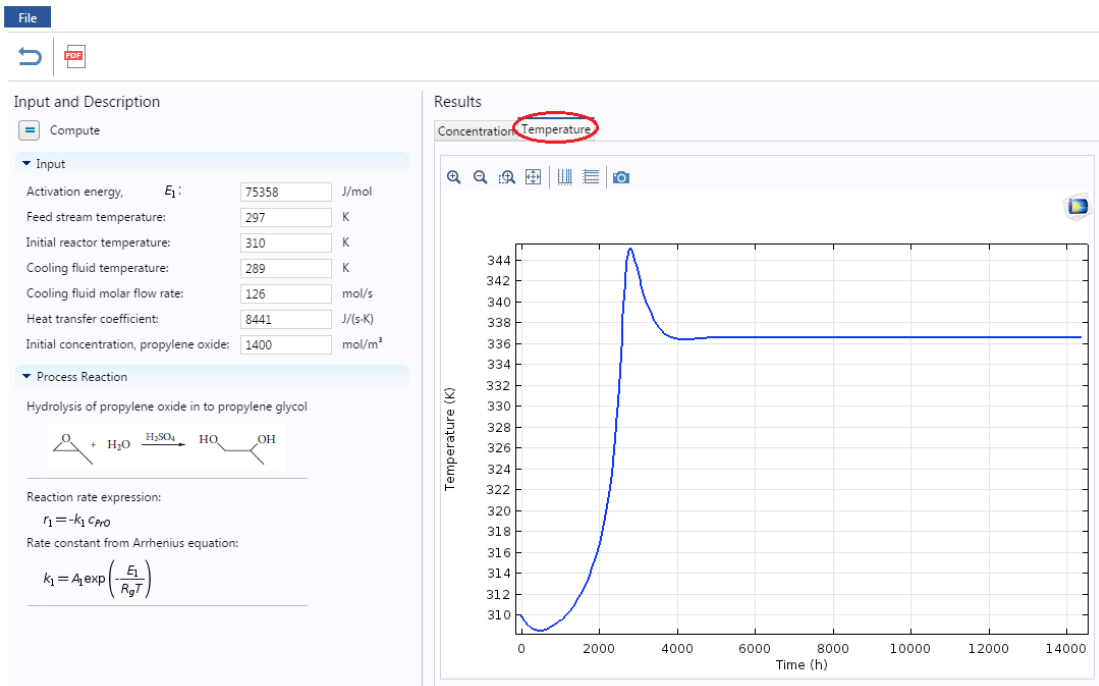
**Caution:** The y axis is dynamic and scale changes with respect to the values. Make sure to look at both scale and graph



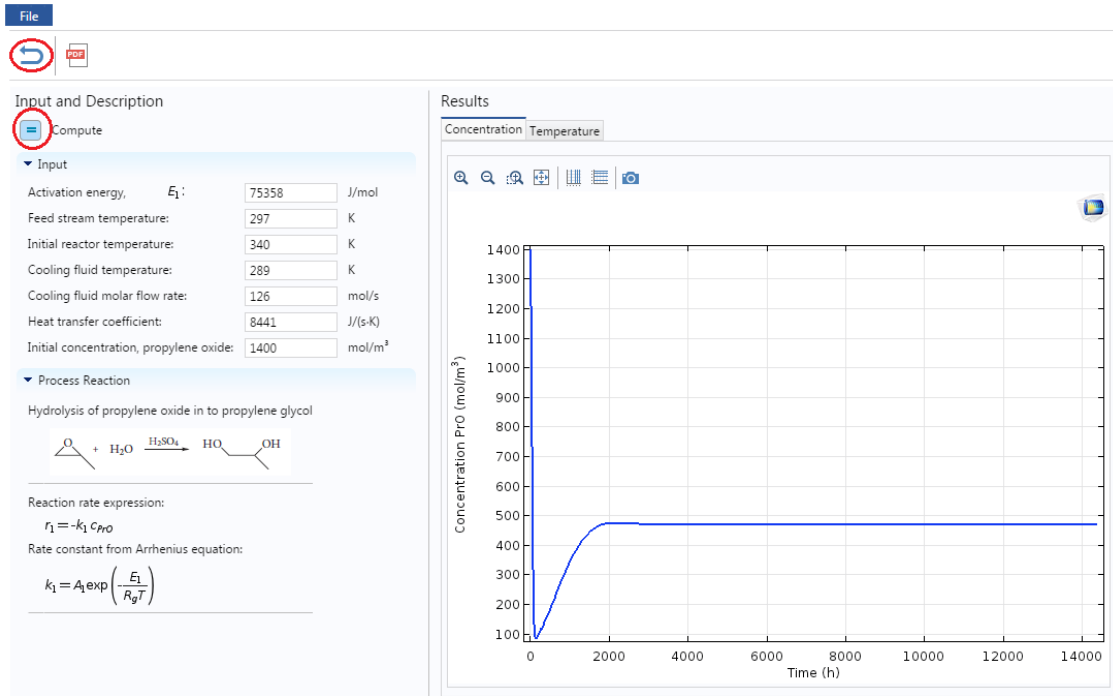
**Step 8:** Now check the Concentration and Temperature profiles. The following graphs will be obtained. You can check that the concentration profile now has more oscillations before reaching steady state



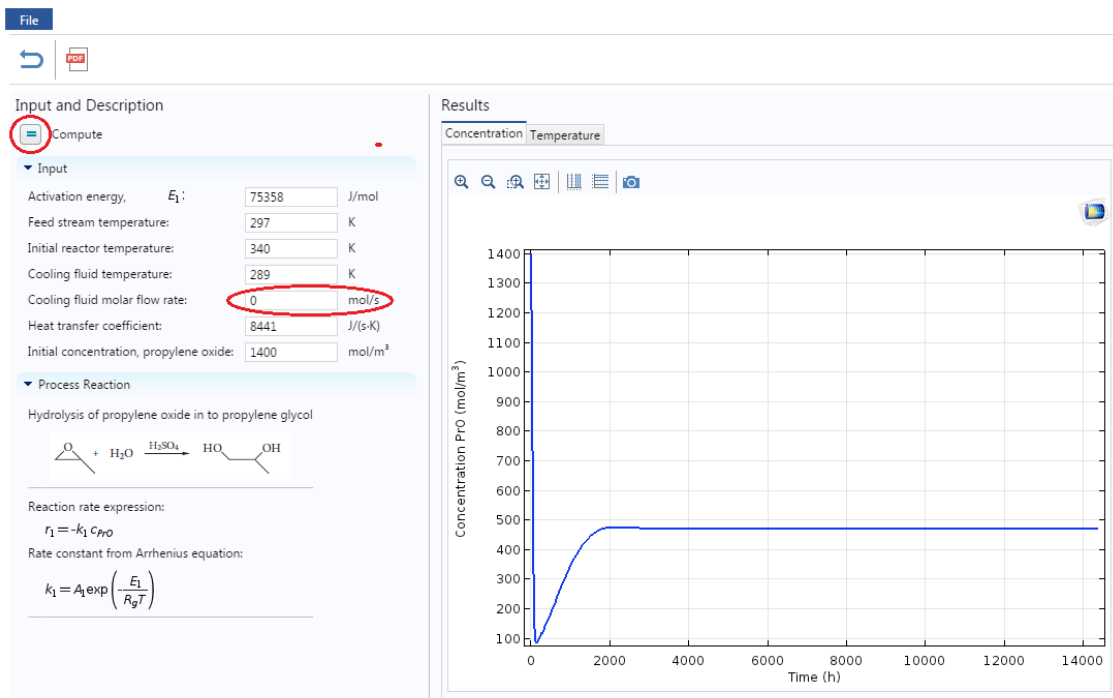
The following is the temperature profile that you will obtain. You can see that at lower temperature, it takes more time to reach the steady state value



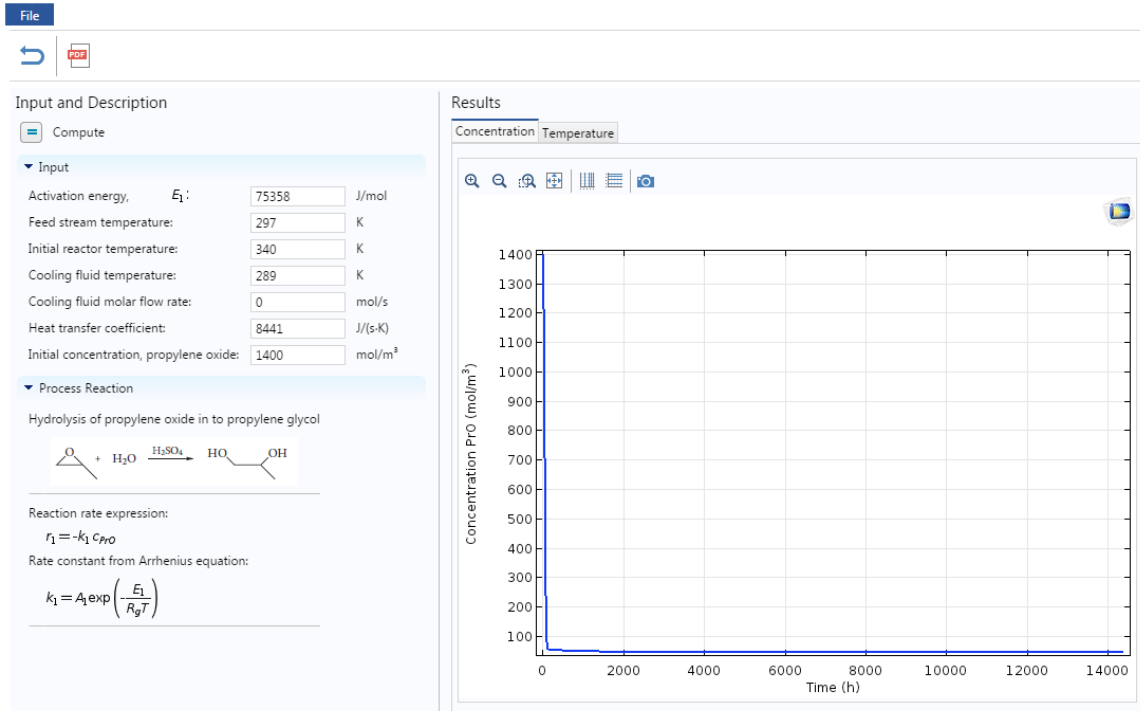
**Step 9:** Now if you want to re-set all the parameter values to its initial values, click on “Reset to Default button( ↶ ) present on the menu bar . Click on this button to reset the value of Temperature. To update the graph, click on Compute button. Each time you change a variable, click Compute



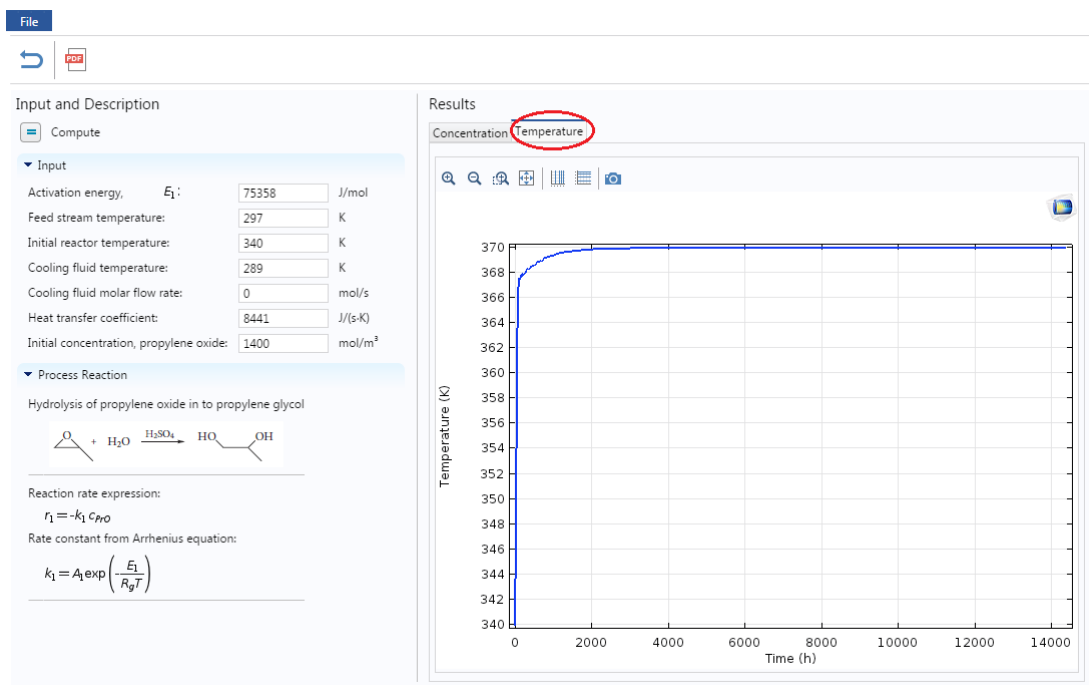
**Step 10:** Now let's consider a case where there is no coolant flow. Enter the Cooling fluid molar flow rate to be 0 mol/s and click compute to see its effect on profile



The following graph will be obtained for Concentration profile. You can see that reactant concentration drops instantaneously without coolant flow



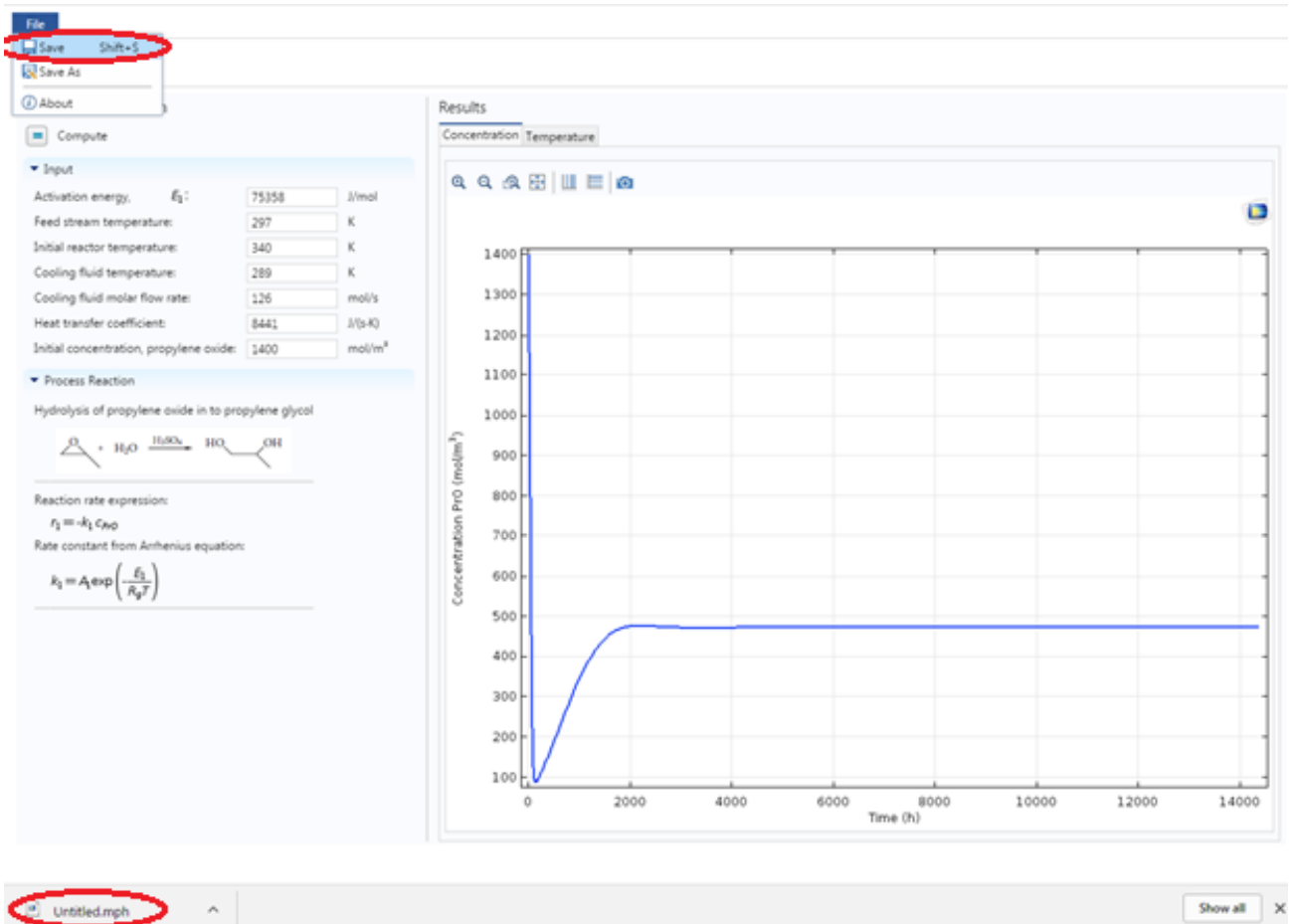
Following is the temperature profile you will obtain. It can be seen that temperature also rises suddenly without coolant flow



**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 shows the COMSOL Multiphysics interface. In the top-left corner, the 'File' menu is open, and the 'PDF' button is circled in red. The main window is divided into two panes: 'Input and Description' on the left and 'Results' on the right.

**Input and Description:**

- Compute:** A button to execute the simulation.
- Input:**
  - Activation energy,  $E_1$ : 75358 J/mol
  - Feed stream temperature: 297 K
  - Initial reactor temperature: 340 K
  - Cooling fluid temperature: 289 K
  - Cooling fluid molar flow rate: 126 mol/s
  - Heat transfer coefficient: 8441 J/(s·K)
  - Initial concentration, propylene oxide: 1400 mol/m<sup>3</sup>
- Process Reaction:**
  - Hydrolysis of propylene oxide in to propylene glycol
  - Chemical reaction: CCOC1OC1 + H2O >>[H2SO4] OCC(O)CO
  - Reaction rate expression:  $r_1 = -k_1 c_{PO}$
  - Rate constant from Arrhenius equation:  $k_1 = A_1 \exp\left(\frac{-E_1}{R_g T}\right)$

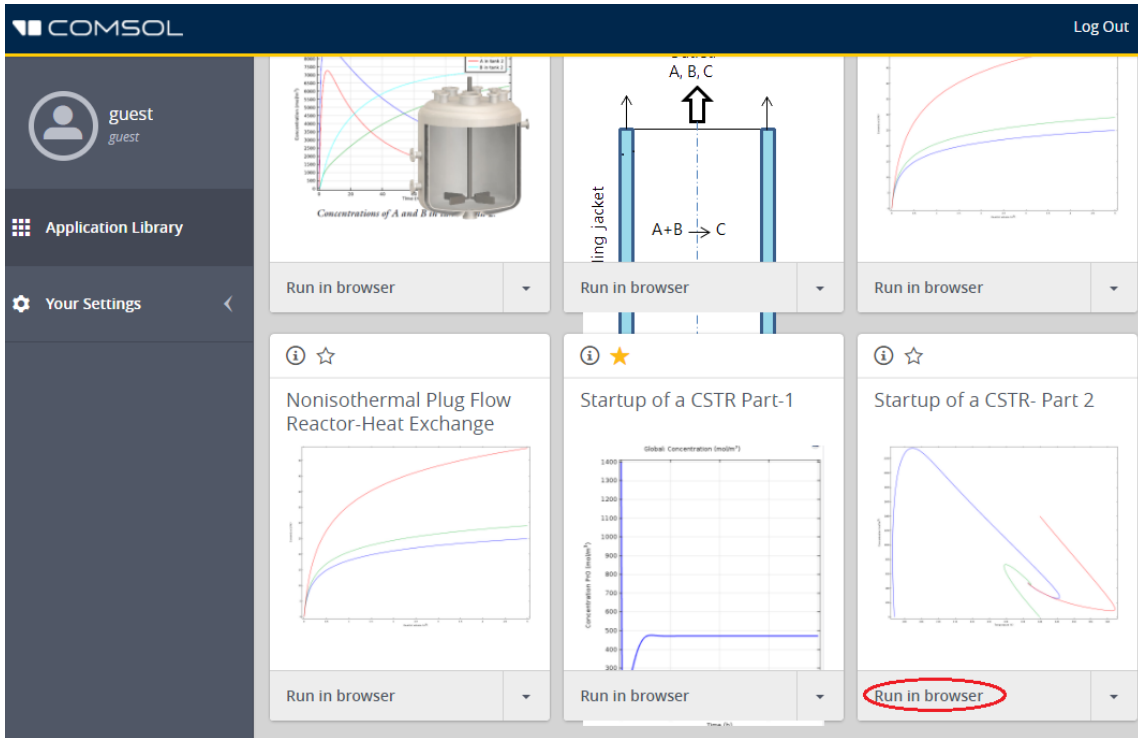
**Results:**

- Concentration:** A plot showing the concentration of propylene oxide (PRO) in mol/m<sup>3</sup> versus time in hours (h). The y-axis ranges from 100 to 1400, and the x-axis ranges from 0 to 14000. The concentration starts at 1400 mol/m<sup>3</sup> at time 0, drops sharply to approximately 100 mol/m<sup>3</sup> by 1000 hours, and then rises to a steady-state value of about 480 mol/m<sup>3</sup> by 2000 hours, remaining constant thereafter.

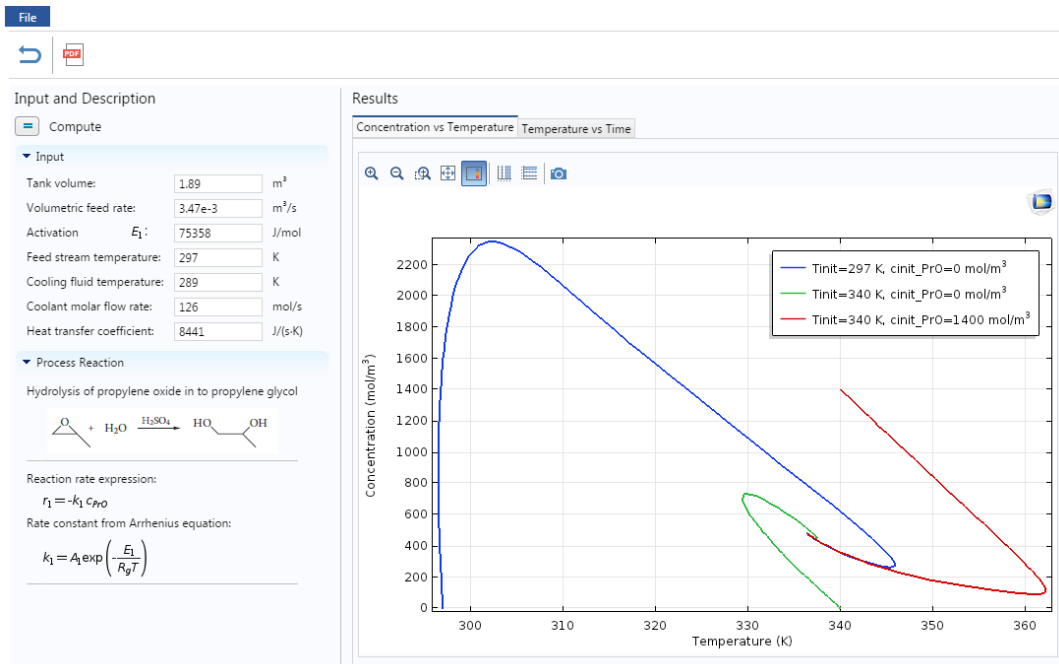
This will open up a new tab with PDF file which you can also download

The screenshot shows a PDF document titled 'CSTR\_startup.pdf' with 16 pages. The document is created in COMSOL Multiphysics 5.3. The main content of the page is the title 'Startup of a Continuous Stirred Tank Reactor' centered on the page, with a small COMSOL logo to the right. The background of the page is white, and the text is in a black serif font.

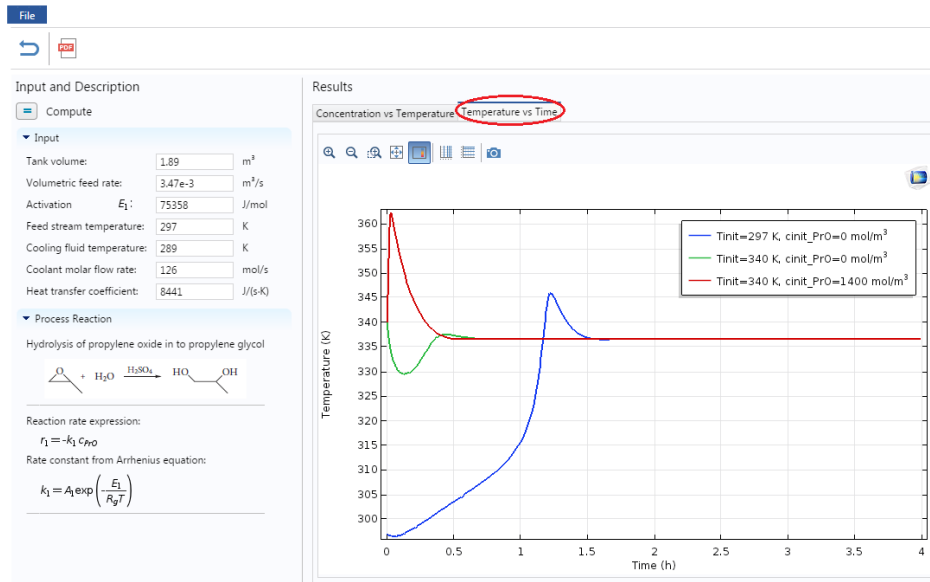
**Step 14:** Now go back to Library and Find “*Startup of a CSTR- Part 2*”. Click on “Run in browser” to start the application. This application contains parametric graph of Concentration vs Temperature



The application will look like this when it opens. Again you can see that there are Input parameters, buttons and graphs. Currently the graph shows parametric plot of Concentration vs Temperature at different initial values of PrO concentration and Reactor temperature

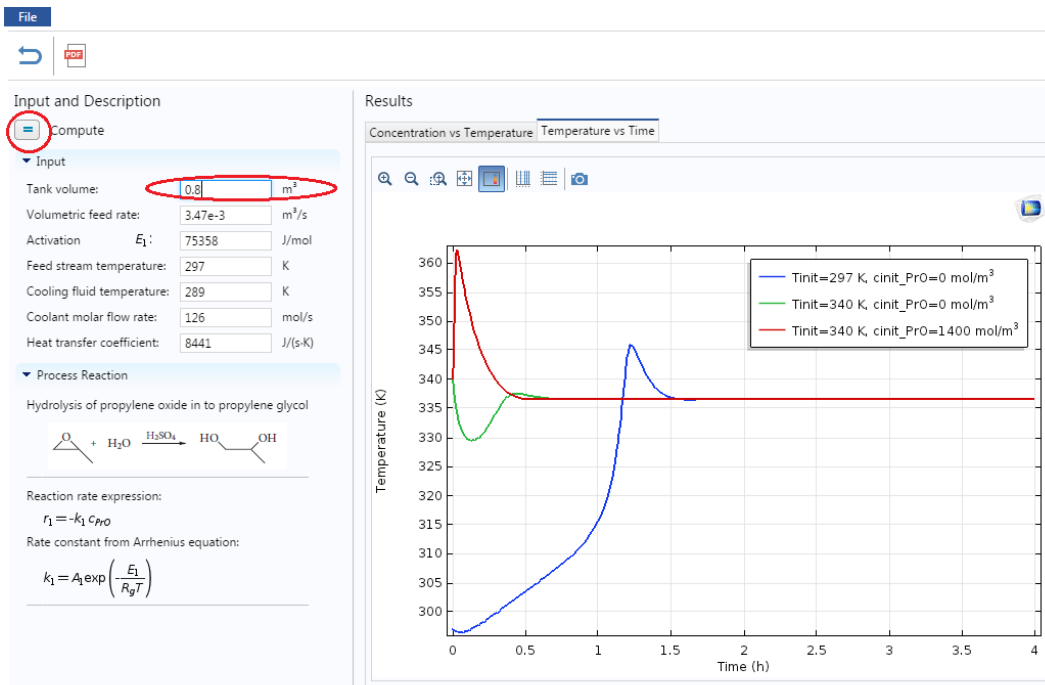


**Step 15:** Click on “Temperature vs Time” tab to obtain Temperature profile at different initial conditions of PrO concentration and Reactor temperature

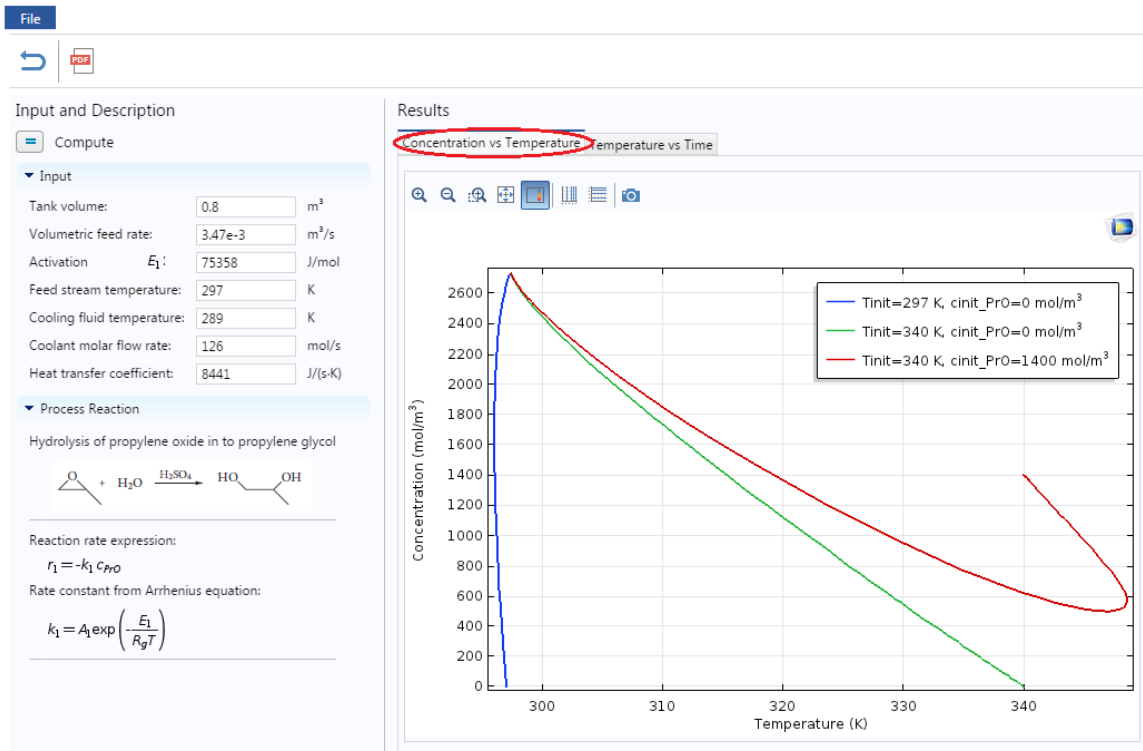


**Step 16:** Let's change a parameter and see the effect on the profile. Suppose Practical stability limit is 350 K and you want to size the reactor so that maximum reactor temperature is below this limit. Change the Tank volume to 0.8 m<sup>3</sup> from 1.89 m<sup>3</sup>. After you are done, click on Compute button ( = ) present above the Input parameters

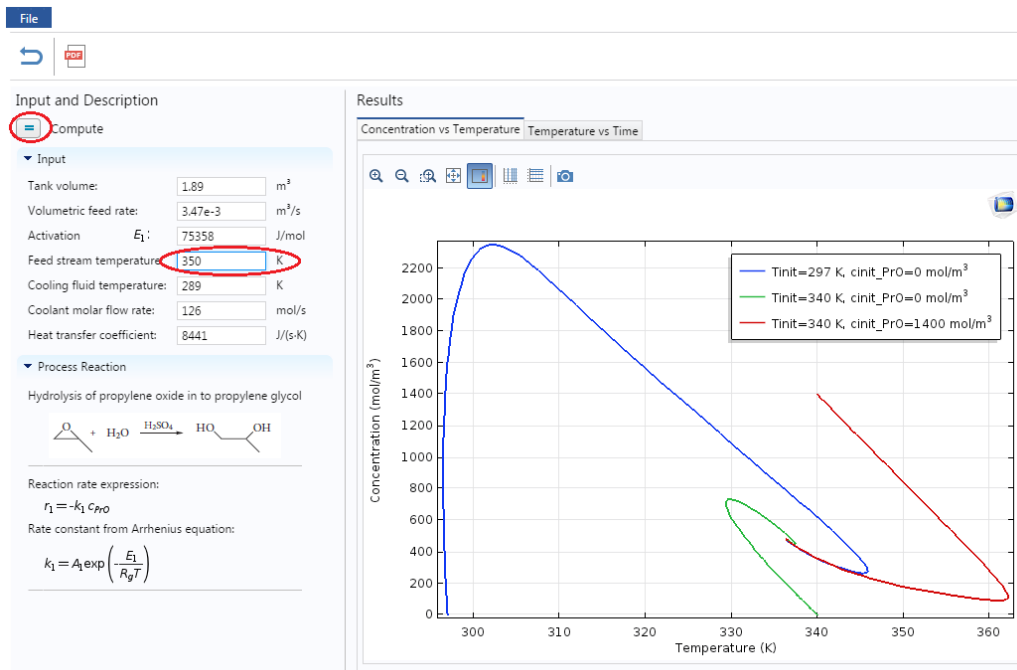
**Caution:** The y axis is dynamic and scale changes with respect to the values. Make sure to look at both scale and graph



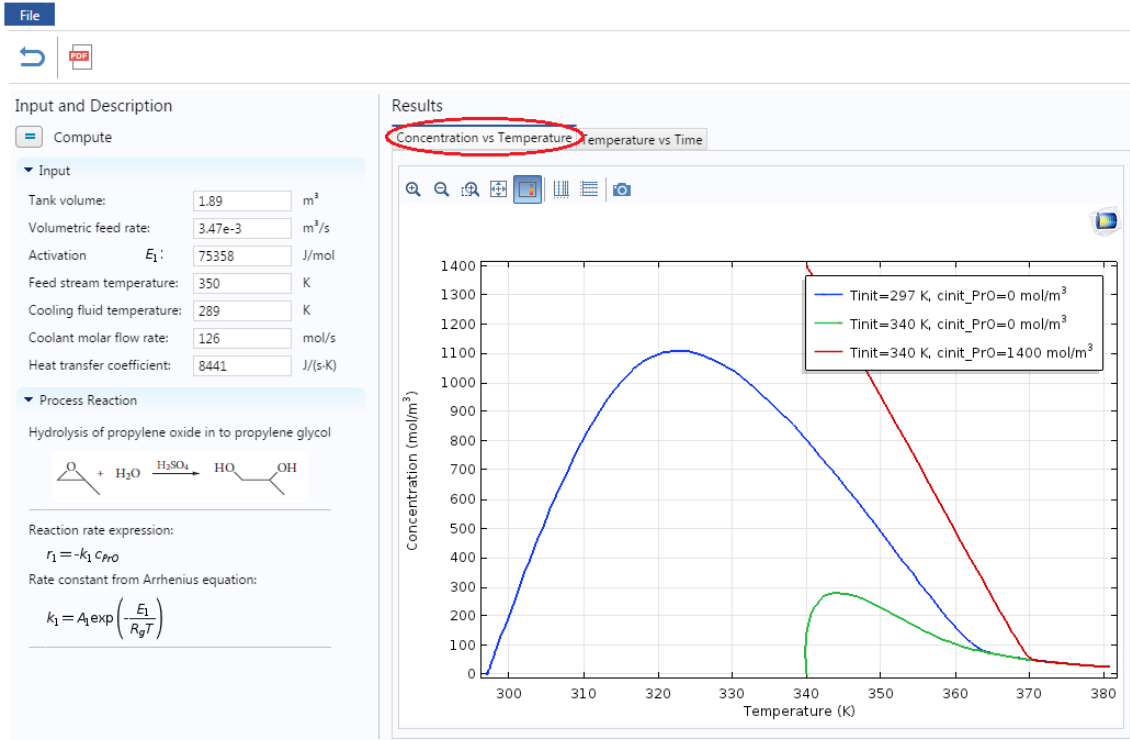
The following graph will be obtained for “Concentration vs Temperature”. It can be seen that reactor temperature doesn’t cross the Practical stability limit at Tank volume=0.8 m3



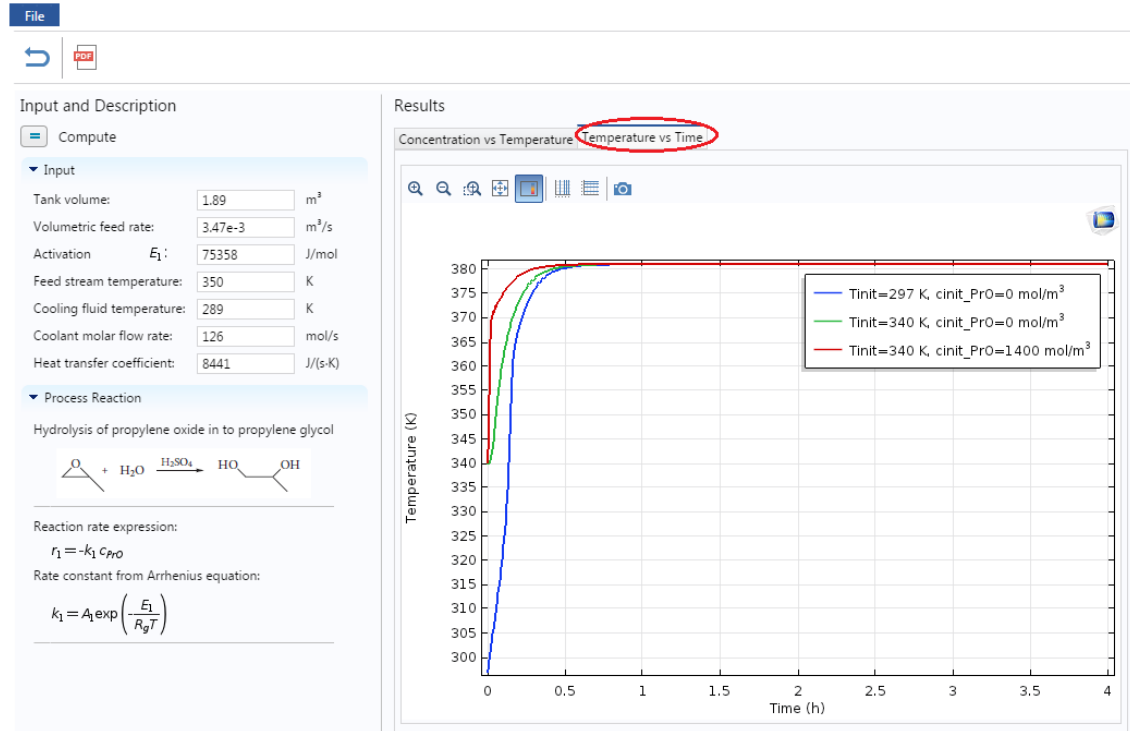
**Step 17:** Now let’s change another variable and see the effect on profiles. Change the feed stream temperature to 350 K from its initial value of 289 K and then click Compute



The following graph will be obtained for Concentration vs Temperature



The following graph will be obtained for Temperature vs Time



**Step 18:** Again, you can download the COMSOL file as was shown in **Step 12**. To open PDF documentation to view the detail of the COMSOL modeling steps, click on PDF button as shown below

File

PDF

Input and Description

Compute

Input

Tank volume: 1.89 m<sup>3</sup>

Volumetric feed rate: 3.47e-3 m<sup>3</sup>/s

Activation  $E_1$ : 75358 J/mol

Feed stream temperature: 297 K

Cooling fluid temperature: 289 K

Coolant molar flow rate: 126 mol/s

Heat transfer coefficient: 8441 J/(s·K)

Process Reaction

Hydrolysis of propylene oxide in to propylene glycol

C1CO1.O>>C1CO1.O

Reaction rate expression:

$$r_1 = -k_1 c_{PrO}$$

Rate constant from Arrhenius equation:

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

Results

Concentration vs Temperature Temperature vs Time

— Tinit=297 K, cinit\_PrO=0 mol/m<sup>3</sup>

— Tinit=340 K, cinit\_PrO=0 mol/m<sup>3</sup>

— Tinit=340 K, cinit\_PrO=1400 mol/m<sup>3</sup>

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

CSTR\_startup.pdf 1 / 16

Created in COMSOL Multiphysics 5.3

Startup of a Continuous Stirred Tank Reactor