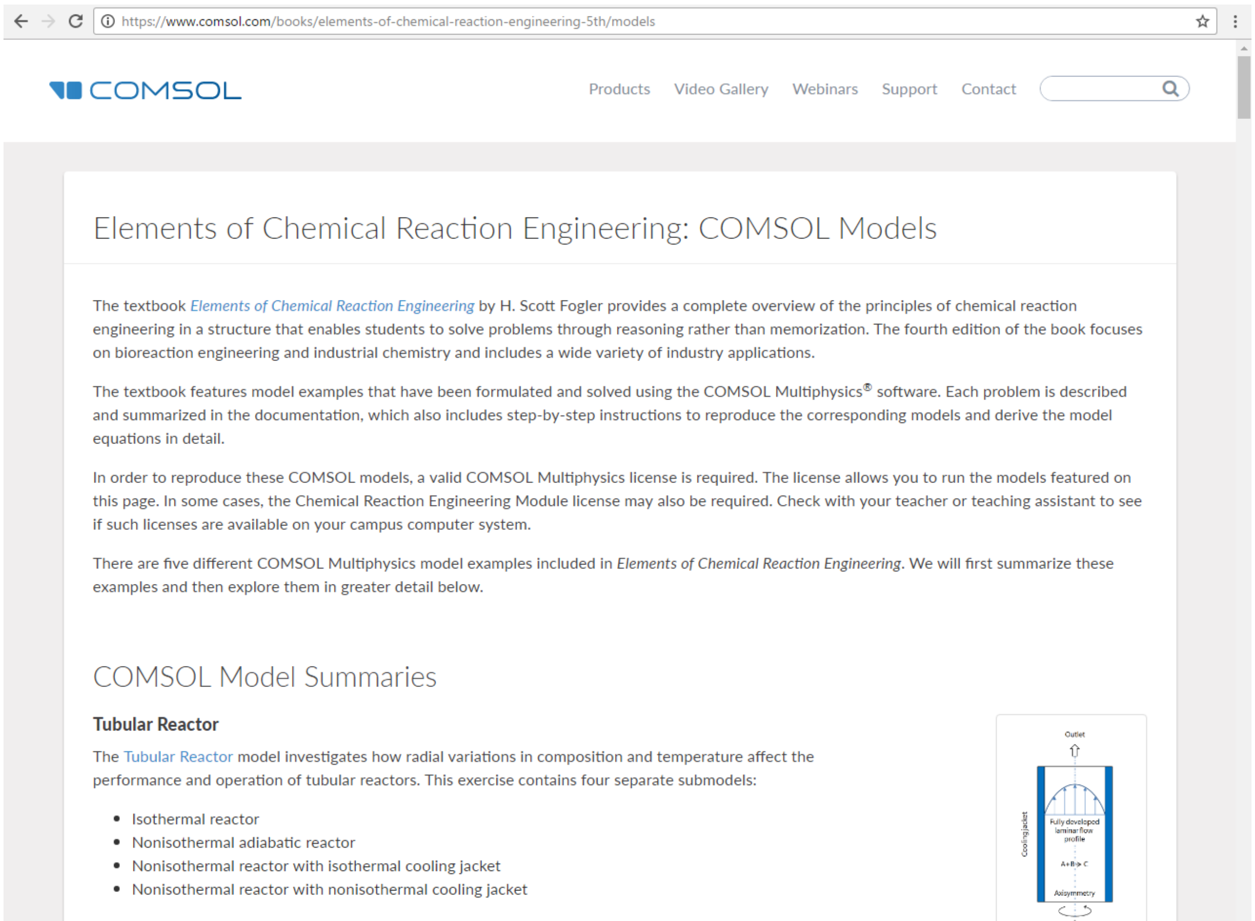
Tutorial for running COMSOL files from COMSOL website

Step 1: Open your browser (Chrome/explorer etc.) and enter the below link

https://www.comsol.com/books/elements-of-chemical-reaction-engineering-5th/models

You will see that following page opens


https://www.comsol.com/books/elements-of-chemical-reaction-engineering-5th/models

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Elements of Chemical Reaction Engineering: COMSOL Models

The textbook *Elements of Chemical Reaction Engineering* by H. Scott Fogler provides a complete overview of the principles of chemical reaction engineering in a structure that enables students to solve problems through reasoning rather than memorization. The fourth edition of the book focuses on bioreaction engineering and industrial chemistry and includes a wide variety of industry applications.

The textbook features model examples that have been formulated and solved using the COMSOL Multiphysics® software. Each problem is described and summarized in the documentation, which also includes step-by-step instructions to reproduce the corresponding models and derive the model equations in detail.

In order to reproduce these COMSOL models, a valid COMSOL Multiphysics license is required. The license allows you to run the models featured on this page. In some cases, the Chemical Reaction Engineering Module license may also be required. Check with your teacher or teaching assistant to see if such licenses are available on your campus computer system.

There are five different COMSOL Multiphysics model examples included in *Elements of Chemical Reaction Engineering*. We will first summarize these examples and then explore them in greater detail below.

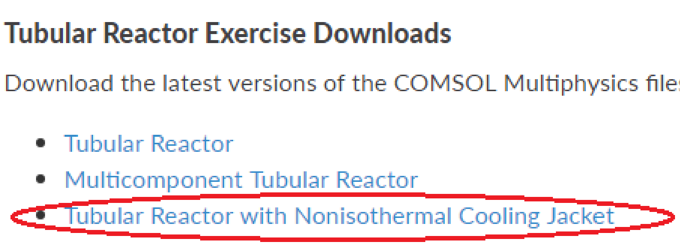
COMSOL Model Summaries

Tubular Reactor

The Tubular Reactor model investigates how radial variations in composition and temperature affect the performance and operation of tubular reactors. This exercise contains four separate submodels:

- Isothermal reactor
- Nonisothermal adiabatic reactor
- Nonisothermal reactor with isothermal cooling jacket
- Nonisothermal reactor with nonisothermal cooling jacket

Step 2: You will find that there are many COMSOL exercises available to download. Scroll down the page and find "**Tubular Reactor Exercise Downloads**". Click on "Tubular Reactor with Nonisothermal cooling Jacket" under this section


Tubular Reactor Exercise Downloads

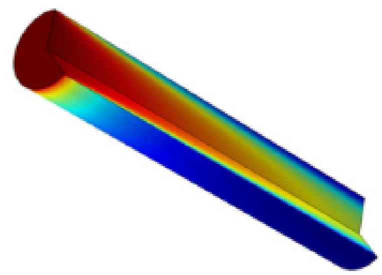
Download the latest versions of the COMSOL Multiphysics files for the application and the embedded model:

- Tubular Reactor
- Multicomponent Tubular Reactor
- Tubular Reactor with Nonisothermal Cooling Jacket

Step 3: You will see that the following page opens. Click on Download the application files. Currently you can't download any COMSOL file (.mph file). To access any COMSOL files, you need to have a COMSOL account which can be created for ***FREE***. Click on "COMSOL Access" present at the bottom of the page

Tubular Reactor with Nonisothermal Cooling Jacket

Application ID: 67



Chemical engineering students can model a nonideal tubular reactor, including radial and axial variations in temperature and composition, and investigate the impact of different operating conditions with this easy-to-use app. The process described by the Tubular Reactor with Nonisothermal Cooling Jacket app is the exothermic reaction of propylene oxide with water to form propylene glycol, assuming first-order reaction kinetics.

The reactor also contains a cooling jacket, and the application consists of an energy and material balance. The student can change the activation energy of the reaction, the thermal conductivity, and the heat of reaction to investigate a variety of scenarios.

The resulting solution gives the axial and radial reaction conversion as well as the temperature profile.

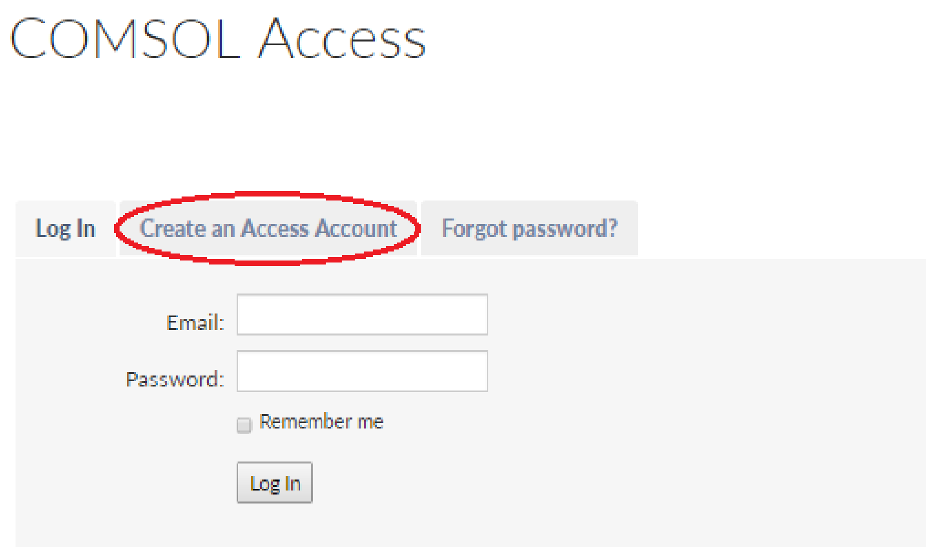
Suggested Products | **Download the application files**

COMSOL 5.2a | COMSOL 5.2 | COMSOL 5.1

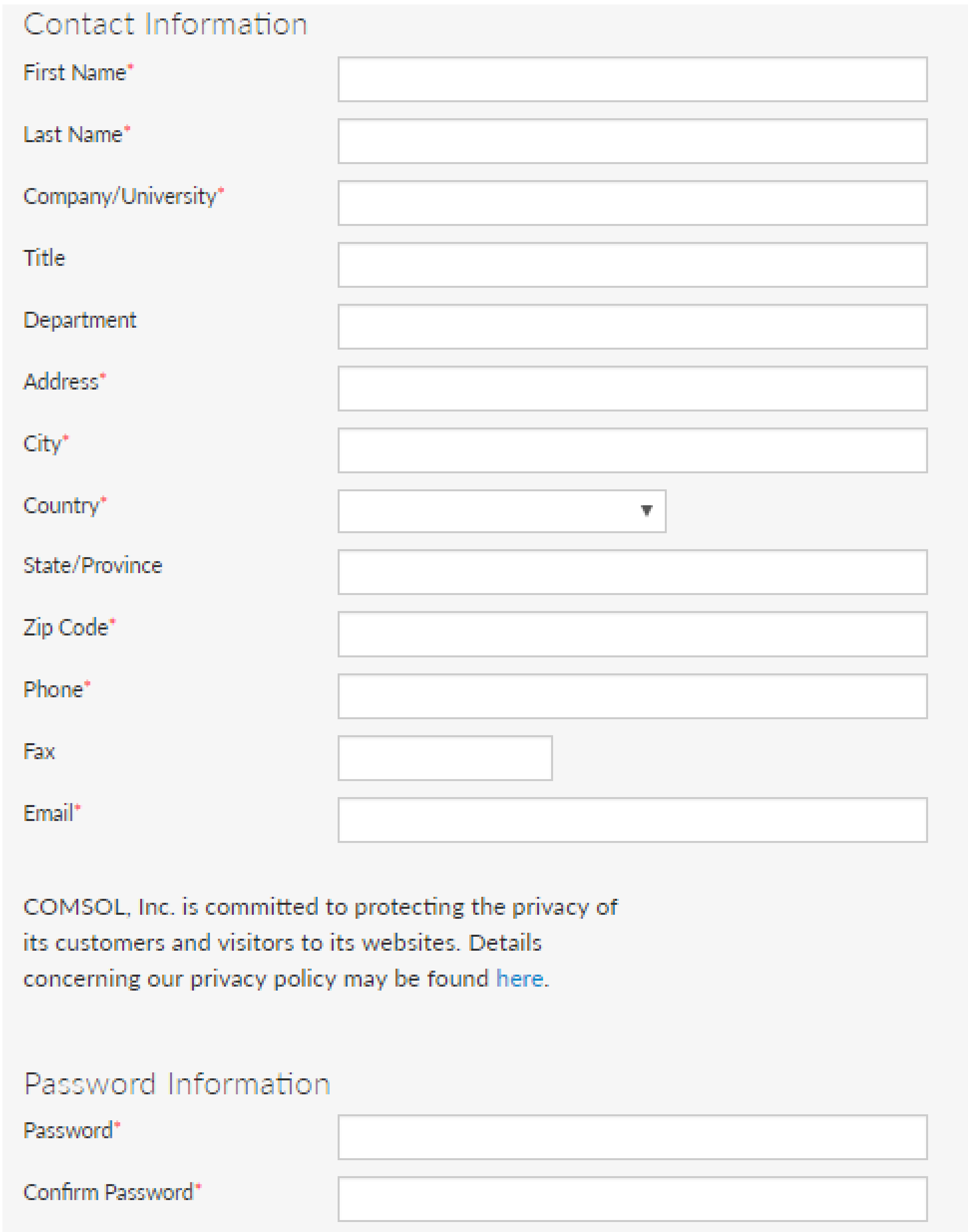
models.mph.tubular_reactor.pdf - 0.53MB
tubular_reactor.mph (includes app design) *
tubular_reactor.mph *
tubular_reactor_parameters.txt - 0MB
tubular_reactor_variables.txt - 0MB

*To download the files, please sign into your COMSOL Access account.

Step 4: The following page will appear. If you already have a COMSOL account then move to Step 6. If you don't have an account, then click on "Create an Access Account" to create one



Step 5: The following page will appear where you need to provide few details and create a password. Fill in the details and submit. You will receive an email from COMSOL with an activation link. Click on the link to activate your COMSOL account


Contact Information

First Name*

Last Name*

Company/University*

Title

Department

Address*

City*

Country*

State/Province

Zip Code*

Phone*

Fax

Email*

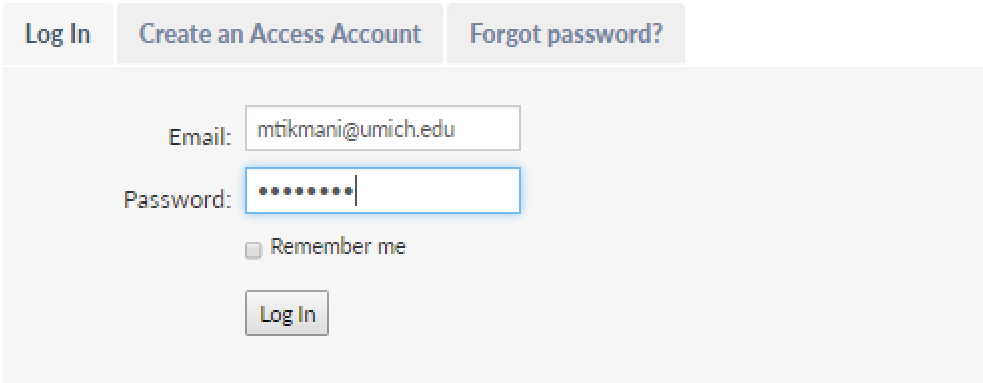
COMSOL, Inc. is committed to protecting the privacy of its customers and visitors to its websites. Details concerning our privacy policy may be found here.

Password Information

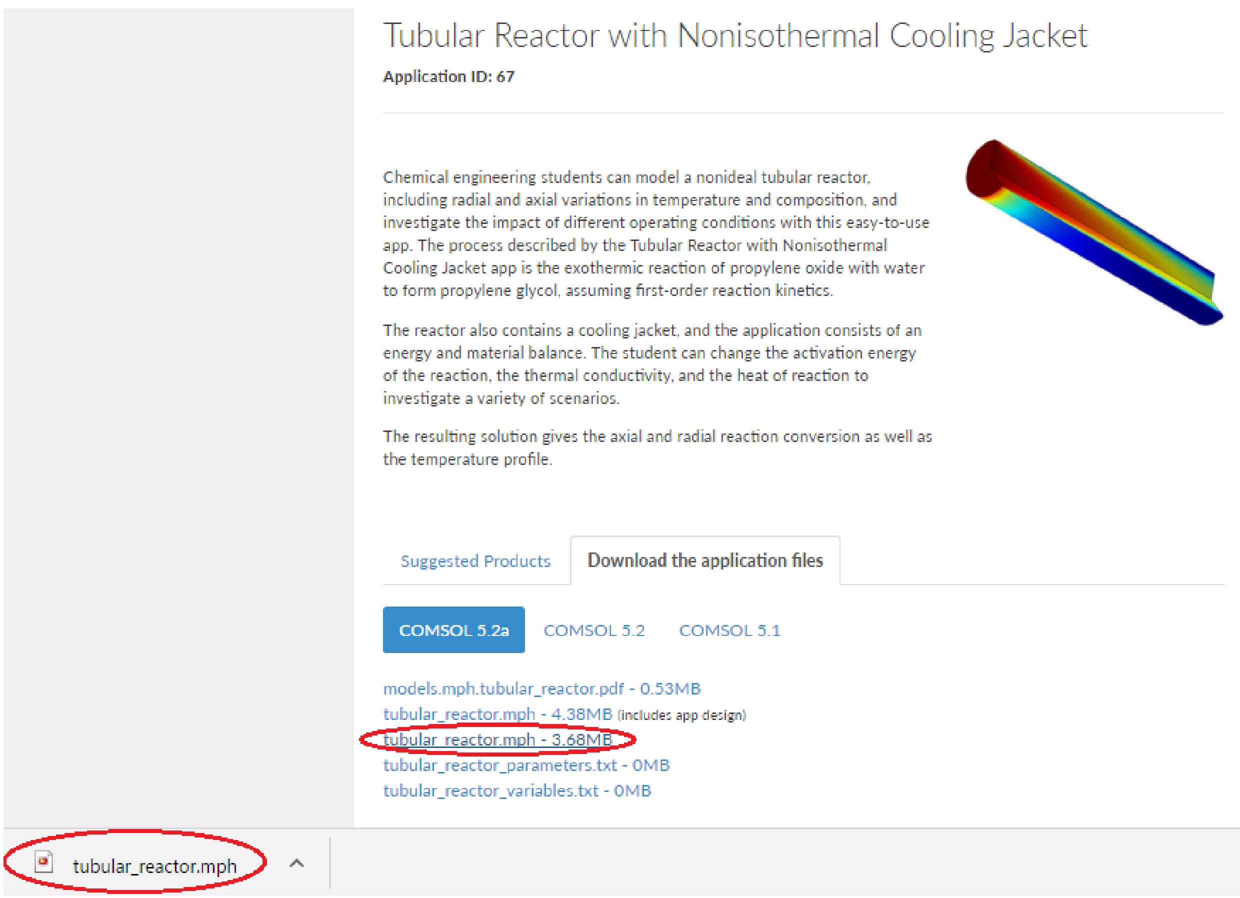
Password*

Confirm Password*

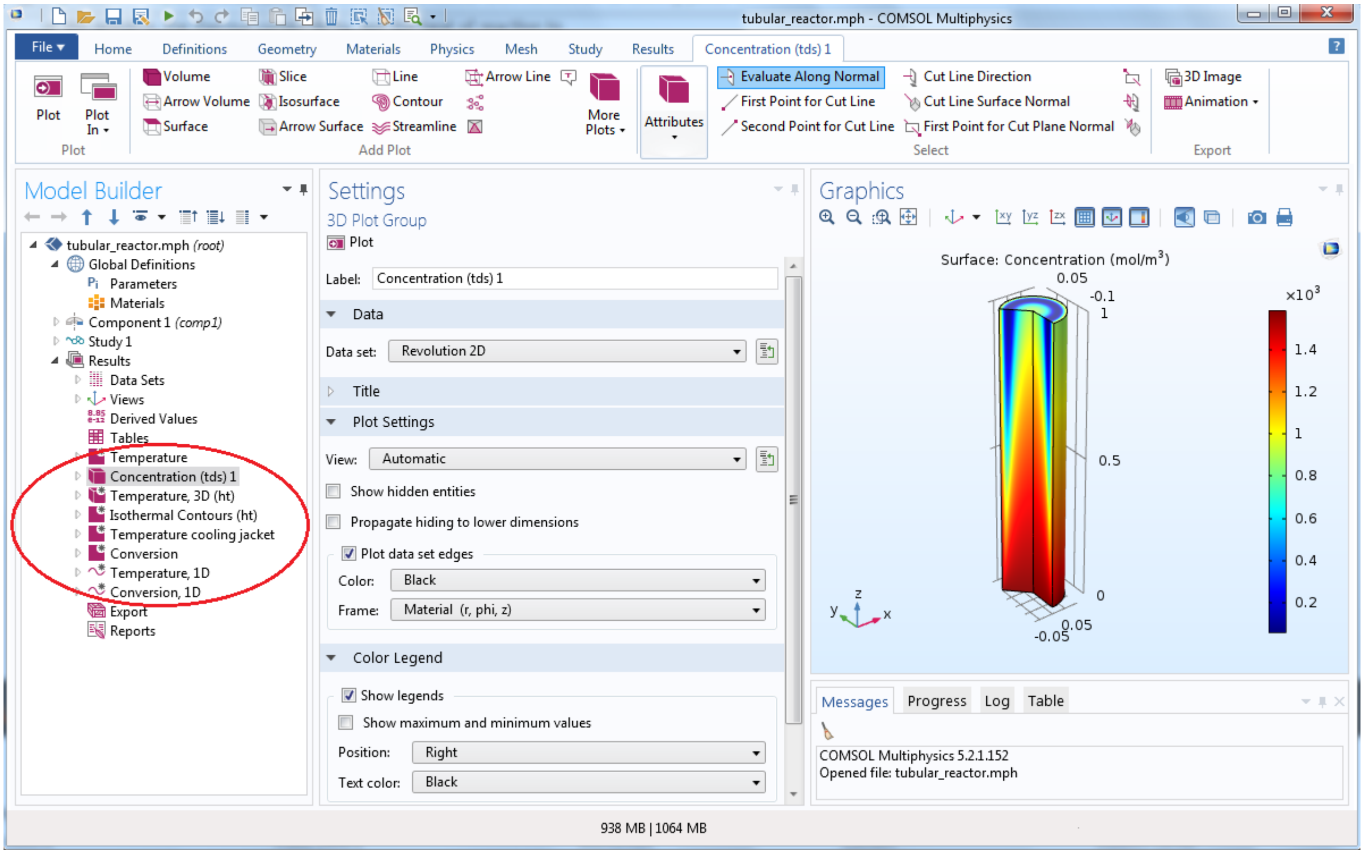
Step 6: After you have created your account, Log In with your registered Email Id and password.



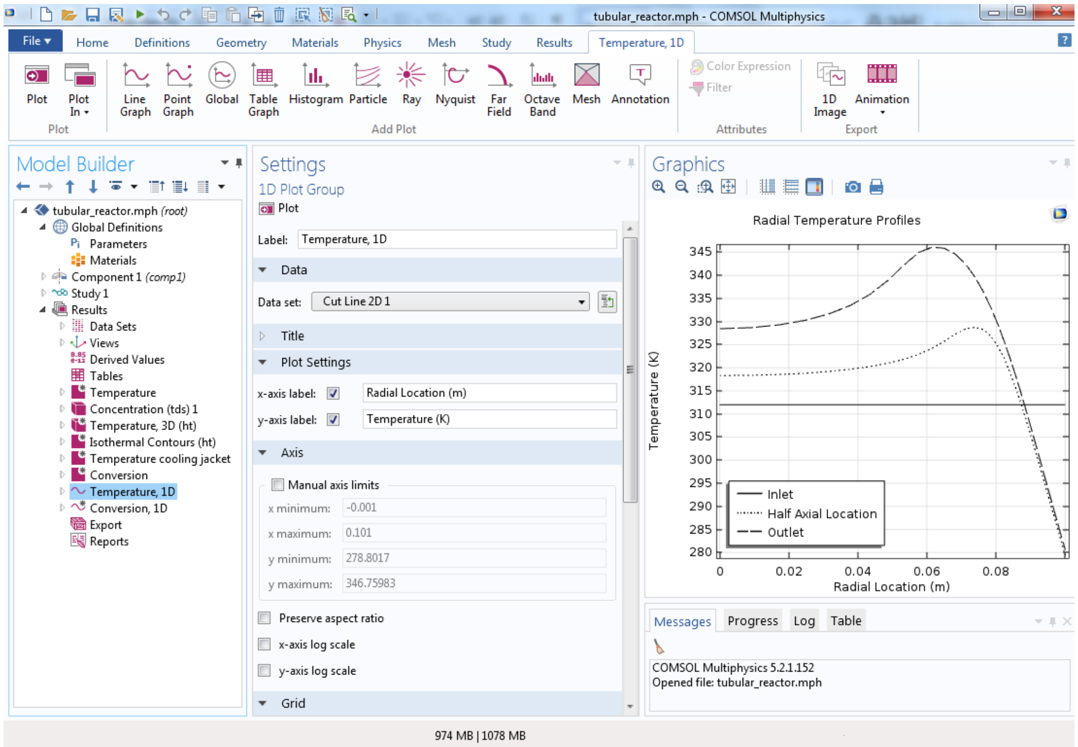
Step 7: This will again open up the same page as was obtained in Step 3. However, now you can download any COMSOL file. Click on "tubular_reactor.mph-3.68 MB" to download the file. The file will get downloaded at the bottom of the browser



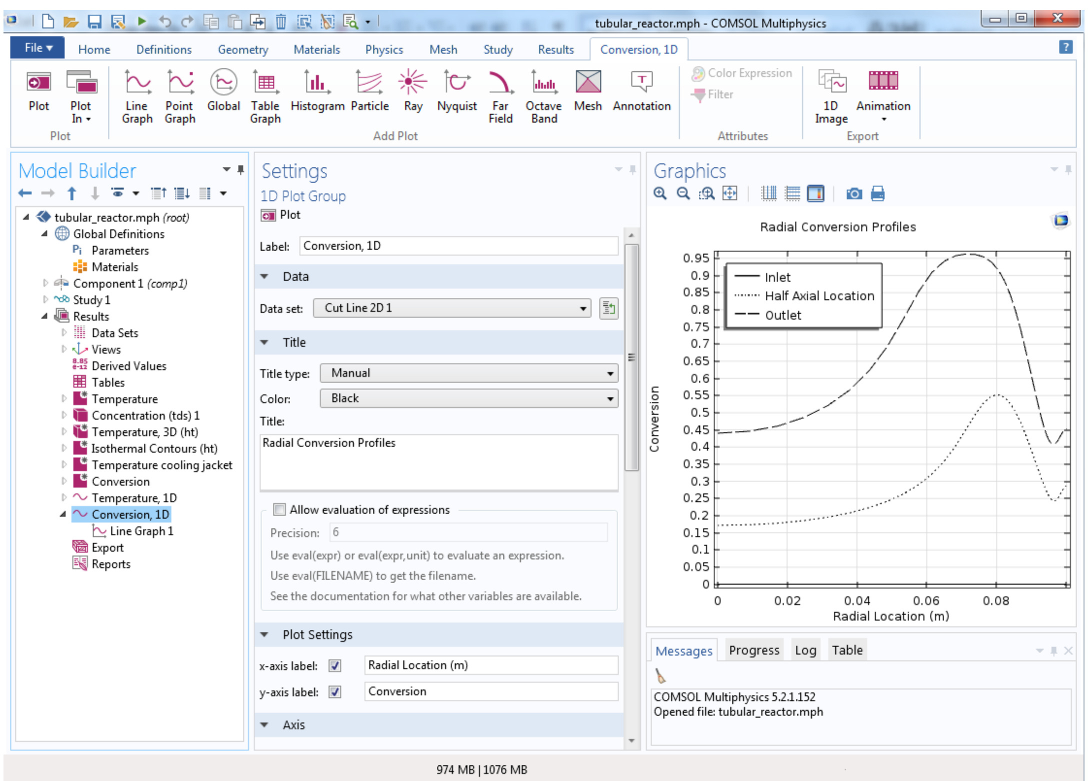
Step 8: Click on the downloaded file. You will see that your model opens up in COMSOL. Click on the various buttons present under Model Builder to view 1D, 2D or 3D profiles for Temperature, Concentration and Conversion.



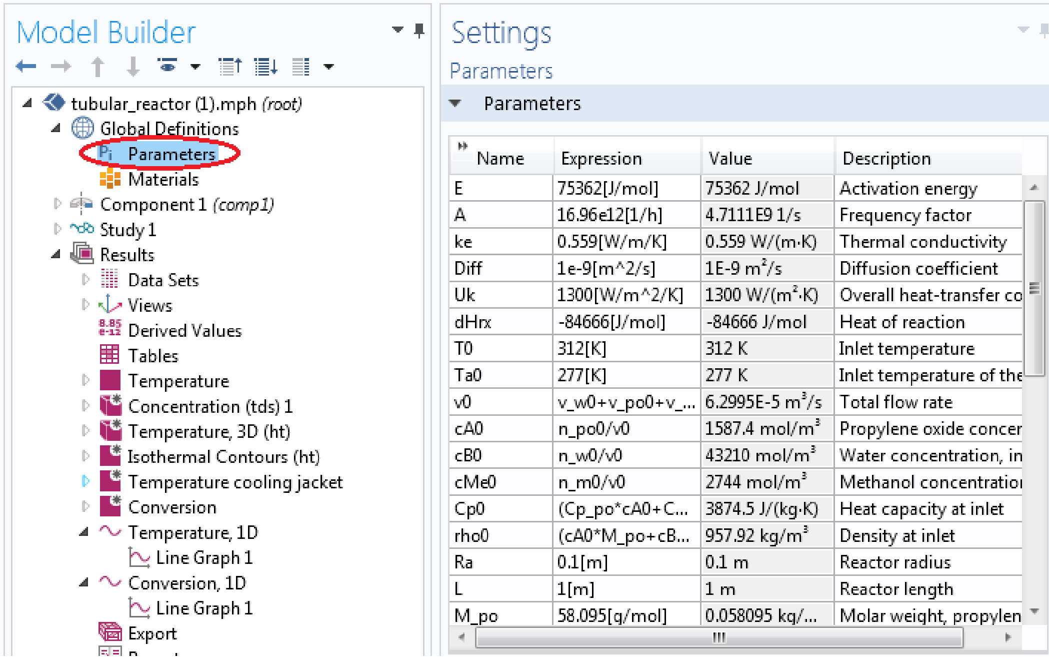
Step 9. Click on Temperature, 1D under Model Builder to view Temperature 1D Plot



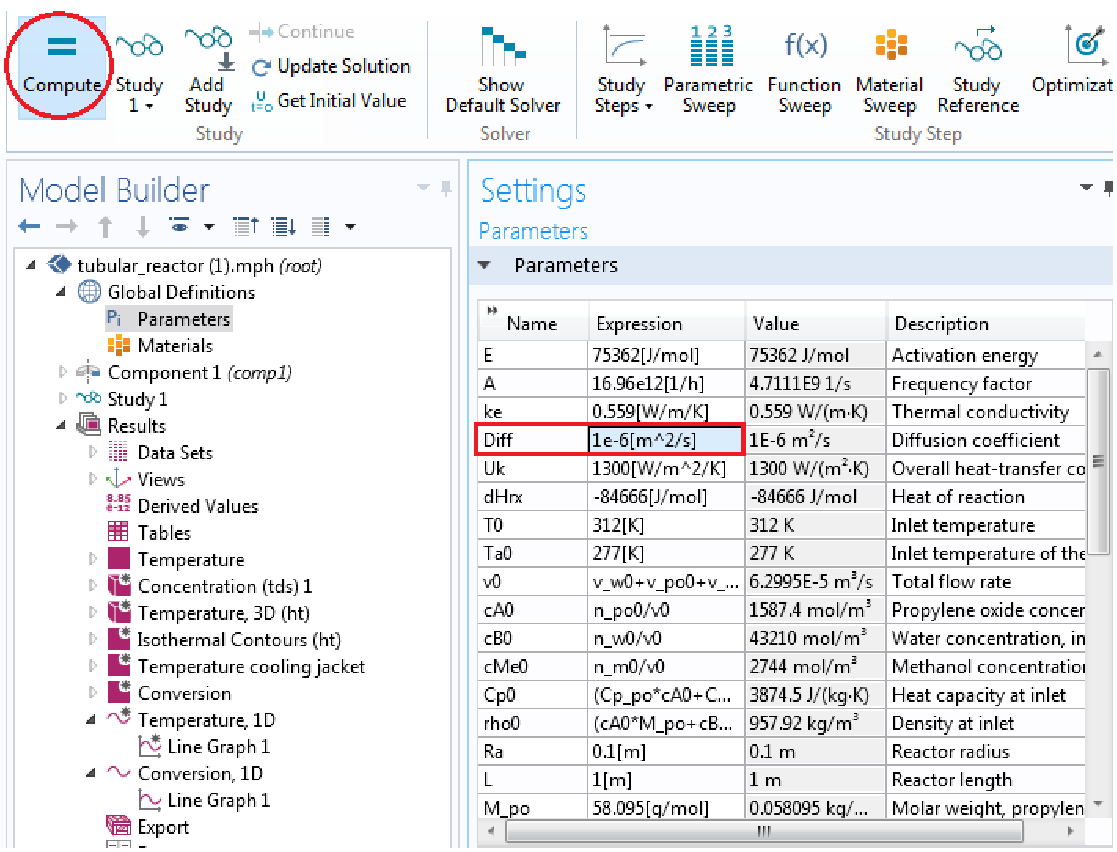
Step 10. Click on Conversion, 1D under Model Builder to view Conversion 1D Plot



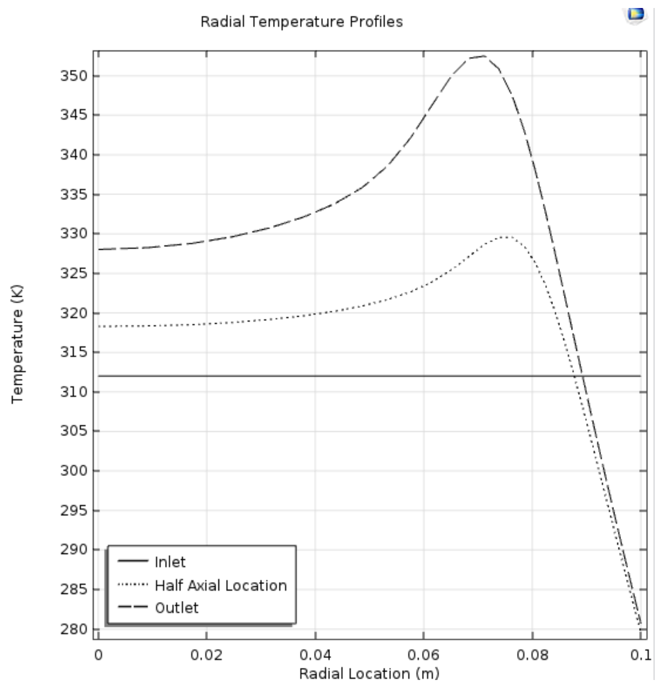
Step 11: Click on Parameters under "Model Builder" to view and change any parameter values



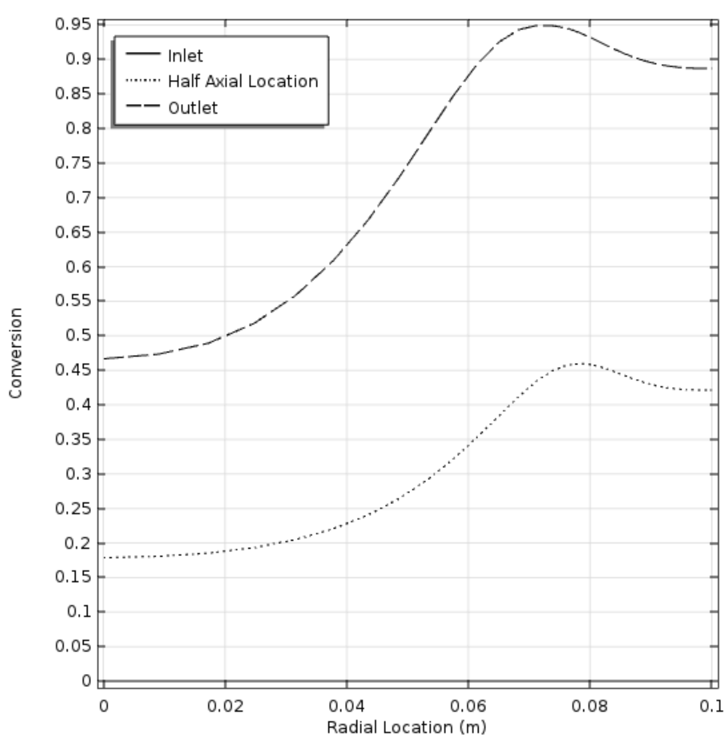
Step 12: Let's change a parameter and see the effect on the profile. Change the Diff value to 1e-6 from 1e-9. After you are done, Click on Compute present under Home toolbar or Study toolbar



Step 13: Click on Temperature,1 D to view Temperature profile when diffusivity is decreased. The following graph will be obtained

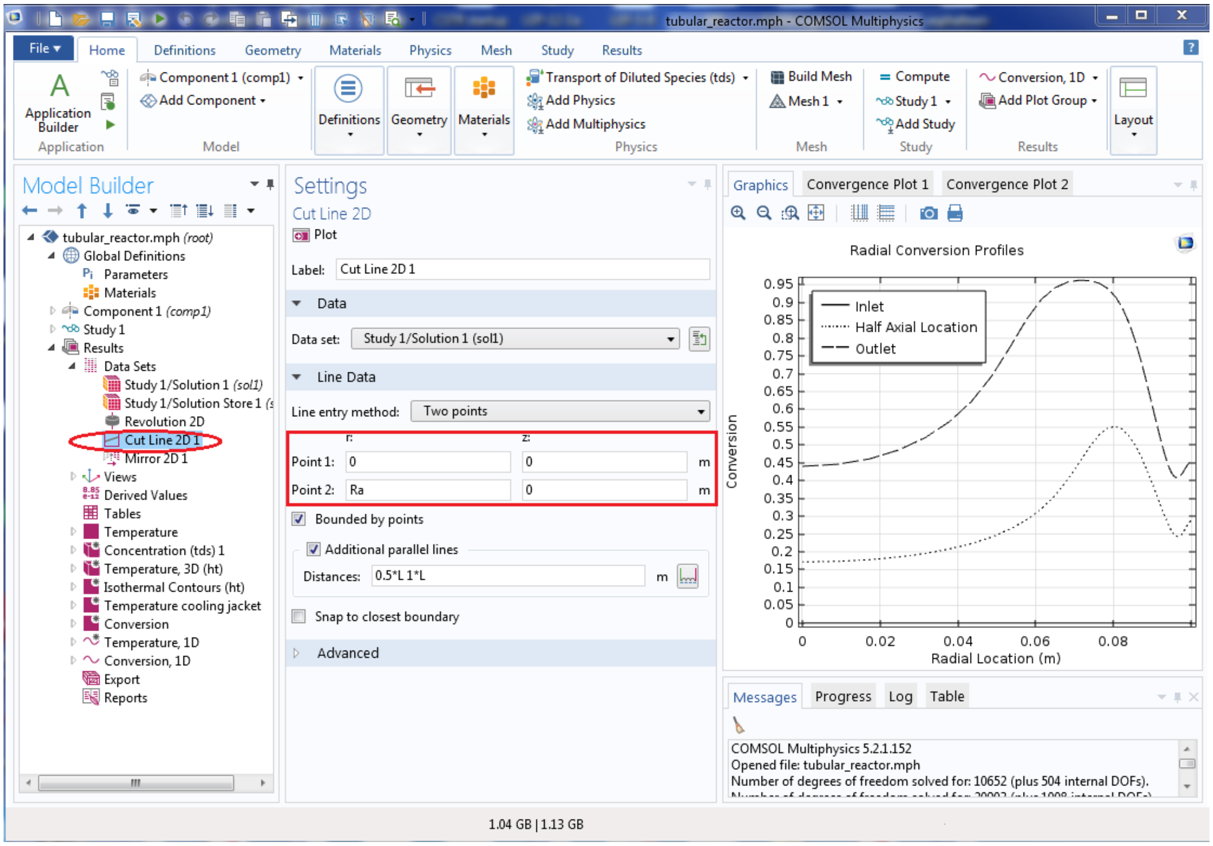


Now click on Conversion, 1D to view Conversion profile

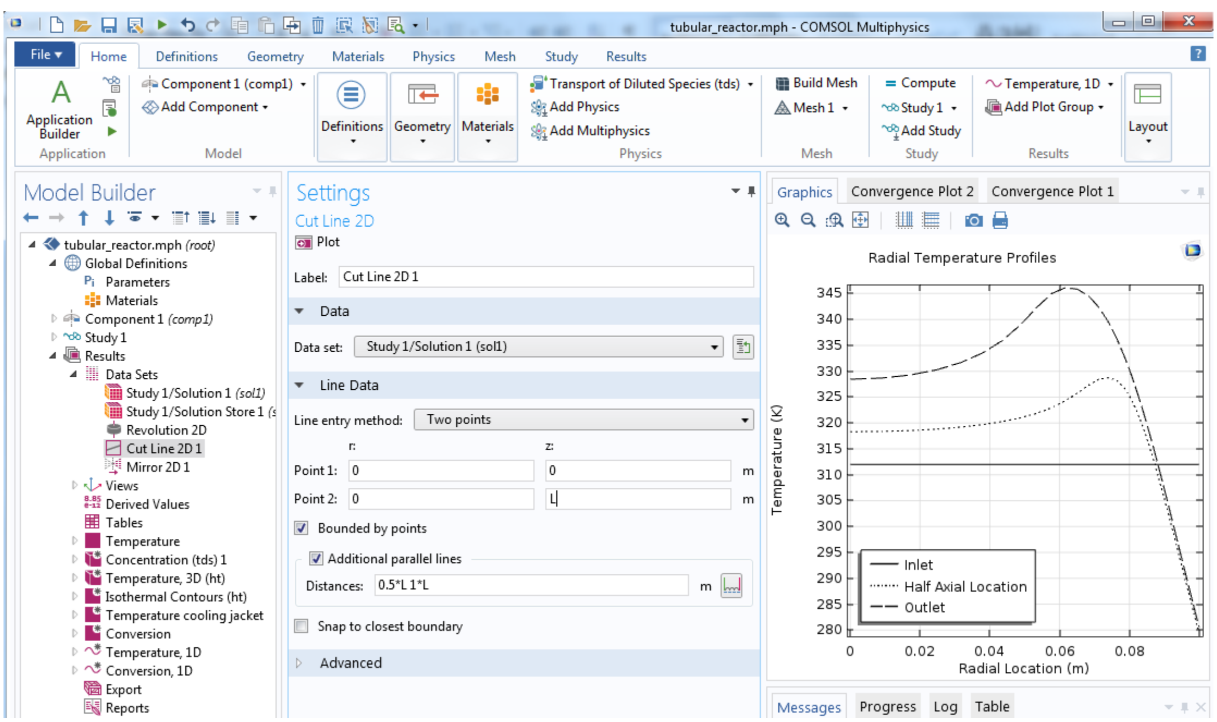


Step 14: Similarly, change other parameters and analyze the change in Temperature and Conversion profiles

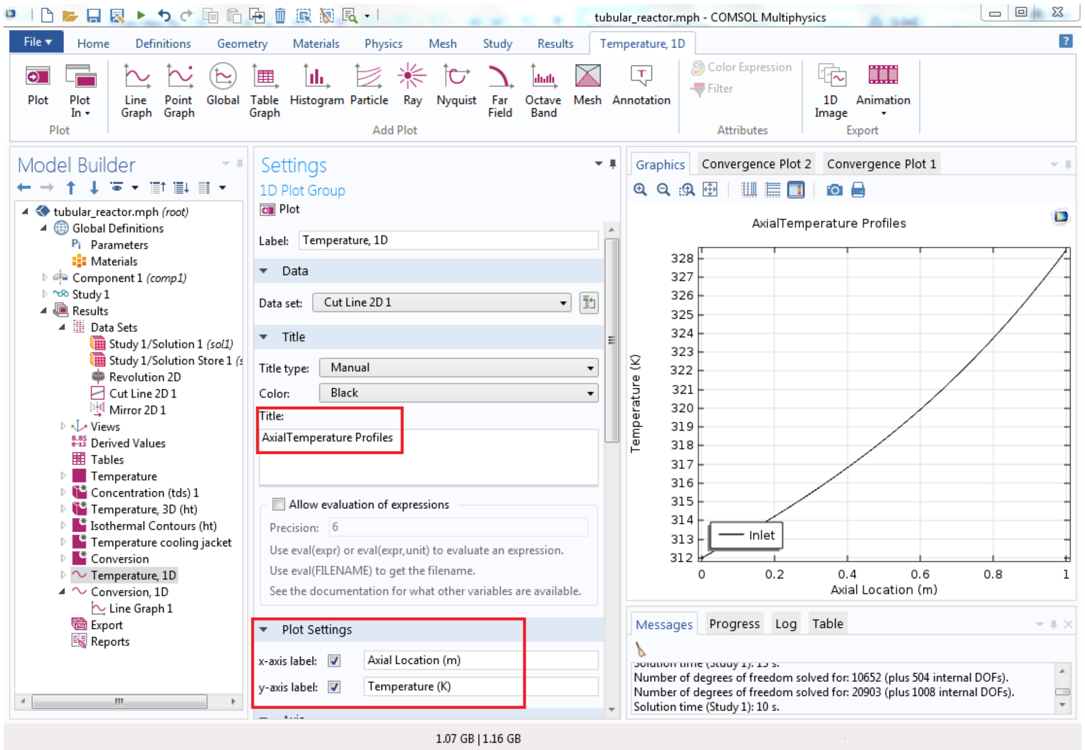
Step 15: To view the axial profiles, click on cut Line 2D 1 present under Data sets



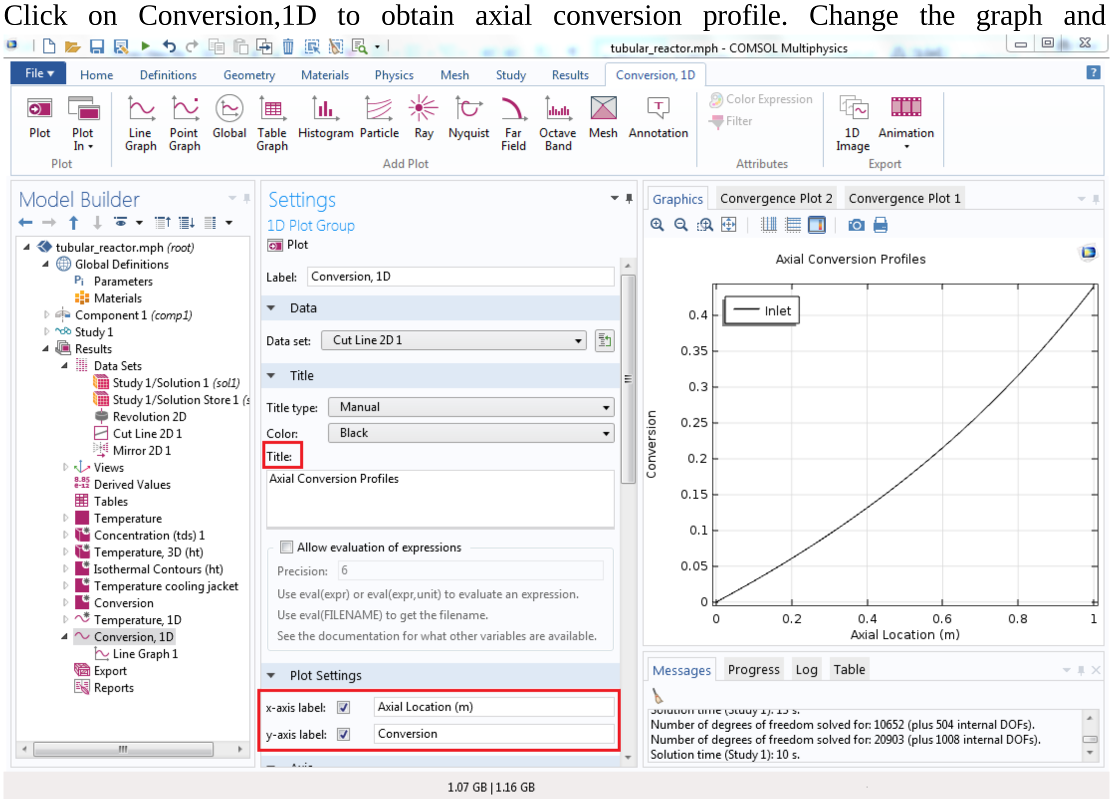
Change point 1 and 2 as shown below. Vary z from 0 to L keeping r fixed at 0



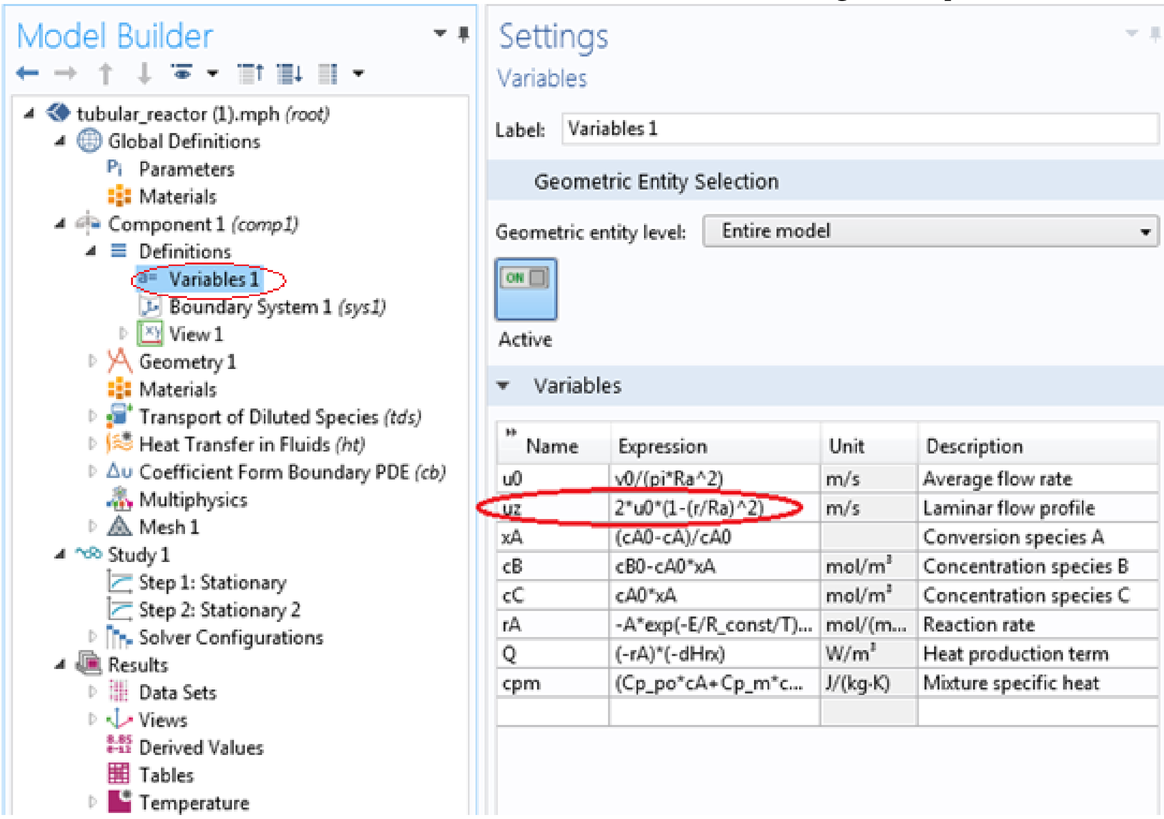
Step 16: Click on Temperature,1D to obtain axial temperature profile. Change the graph and axis titles as shown below



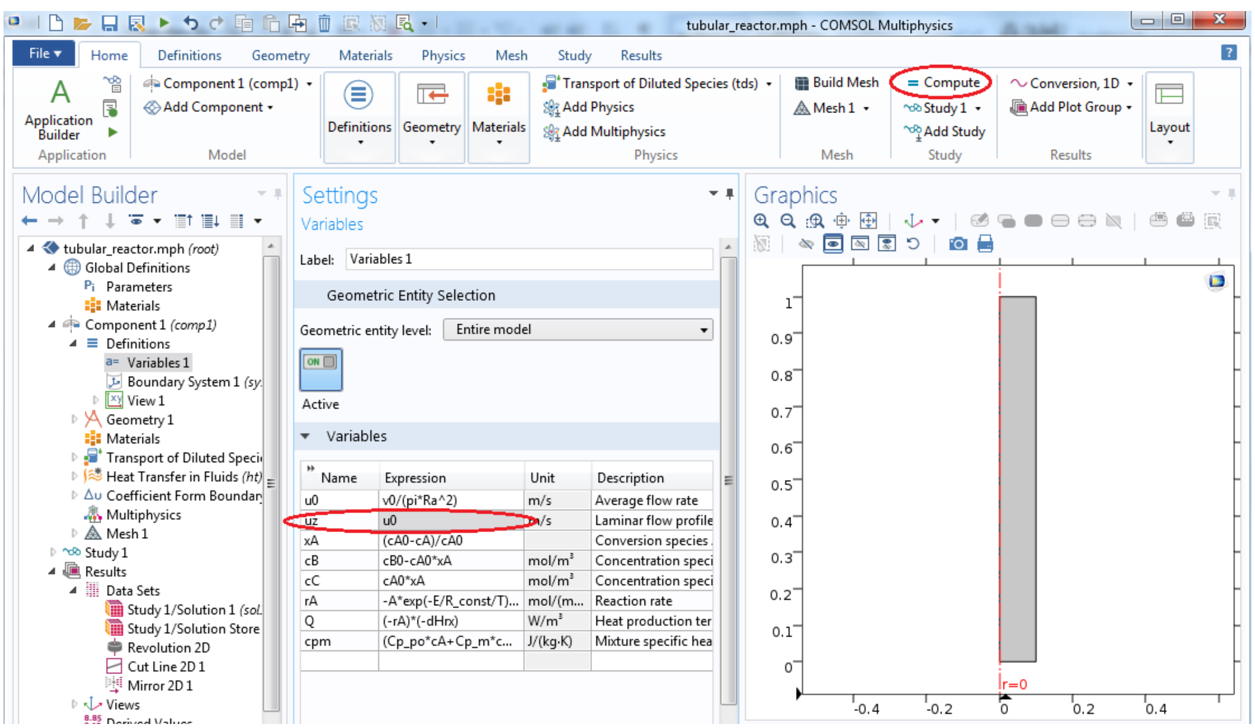
Click on Conversion,1D to obtain axial conversion profile. Change the graph and axis titles



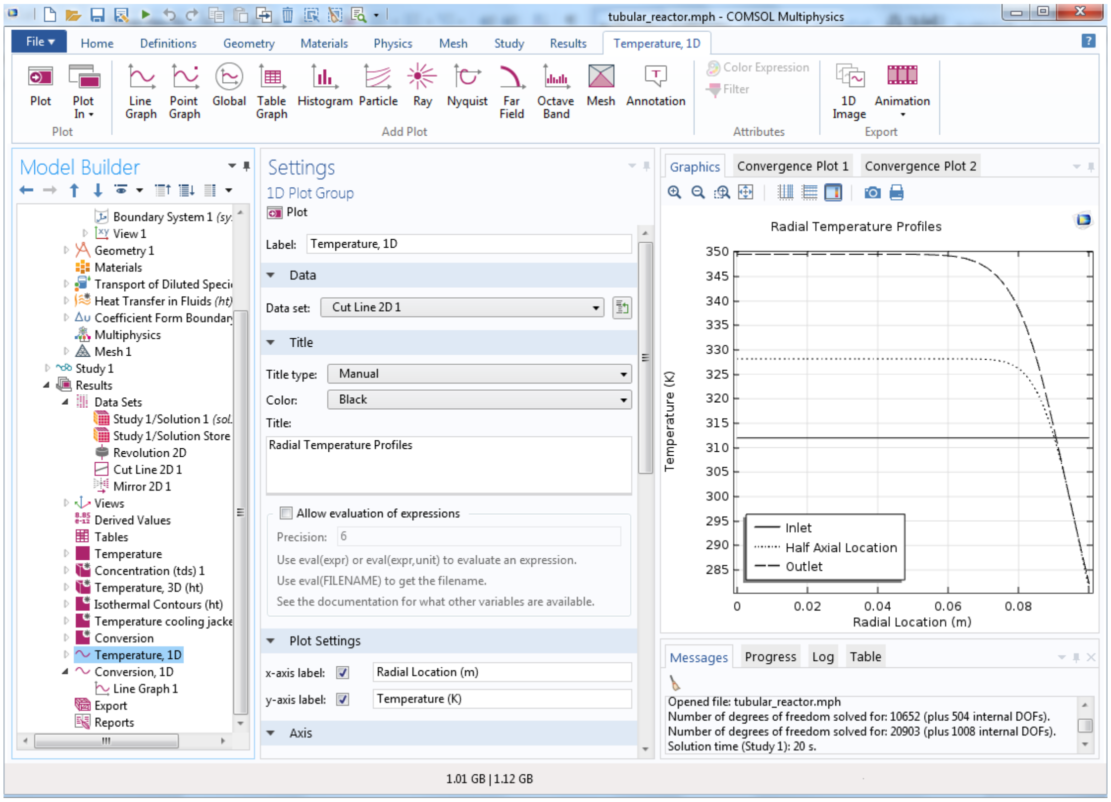
Step 17: To change the flow conditions from laminar flow to plug flow, expand Definitions and click on Variables 1. You will see a list of defined variables. We want to change the expression for velocity (uz)



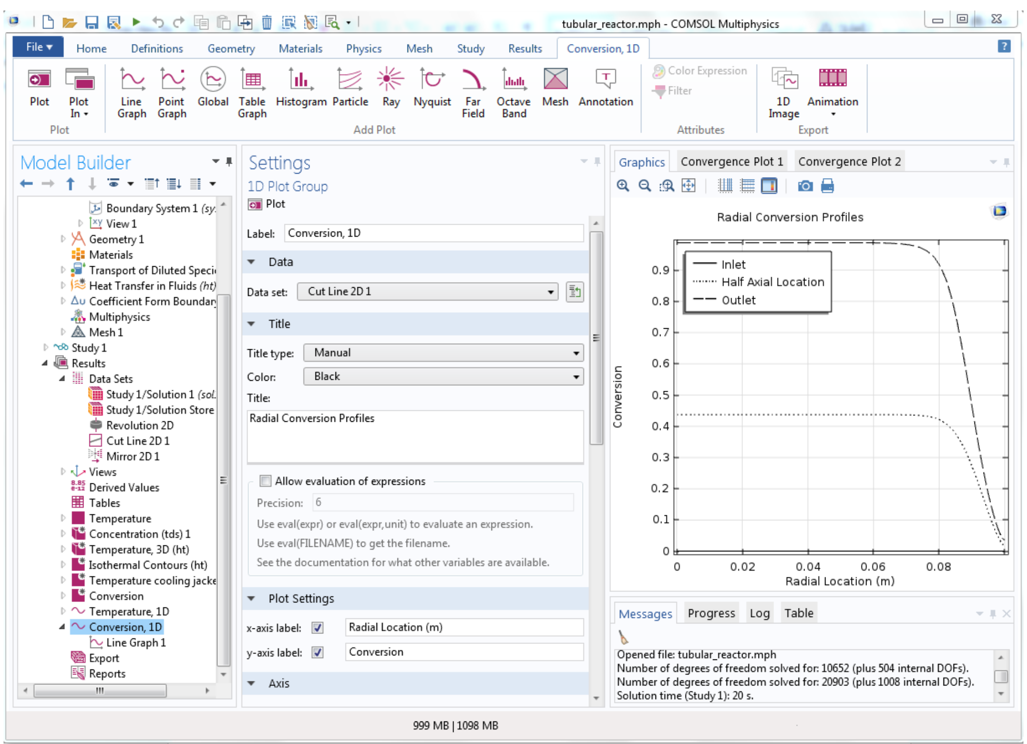
Change the expression of uz by entering "u0" in the text field. Click on Compute Button



Step 18: Now, again click on Temperature,1 D graph to obtain temperature profile for plug flow

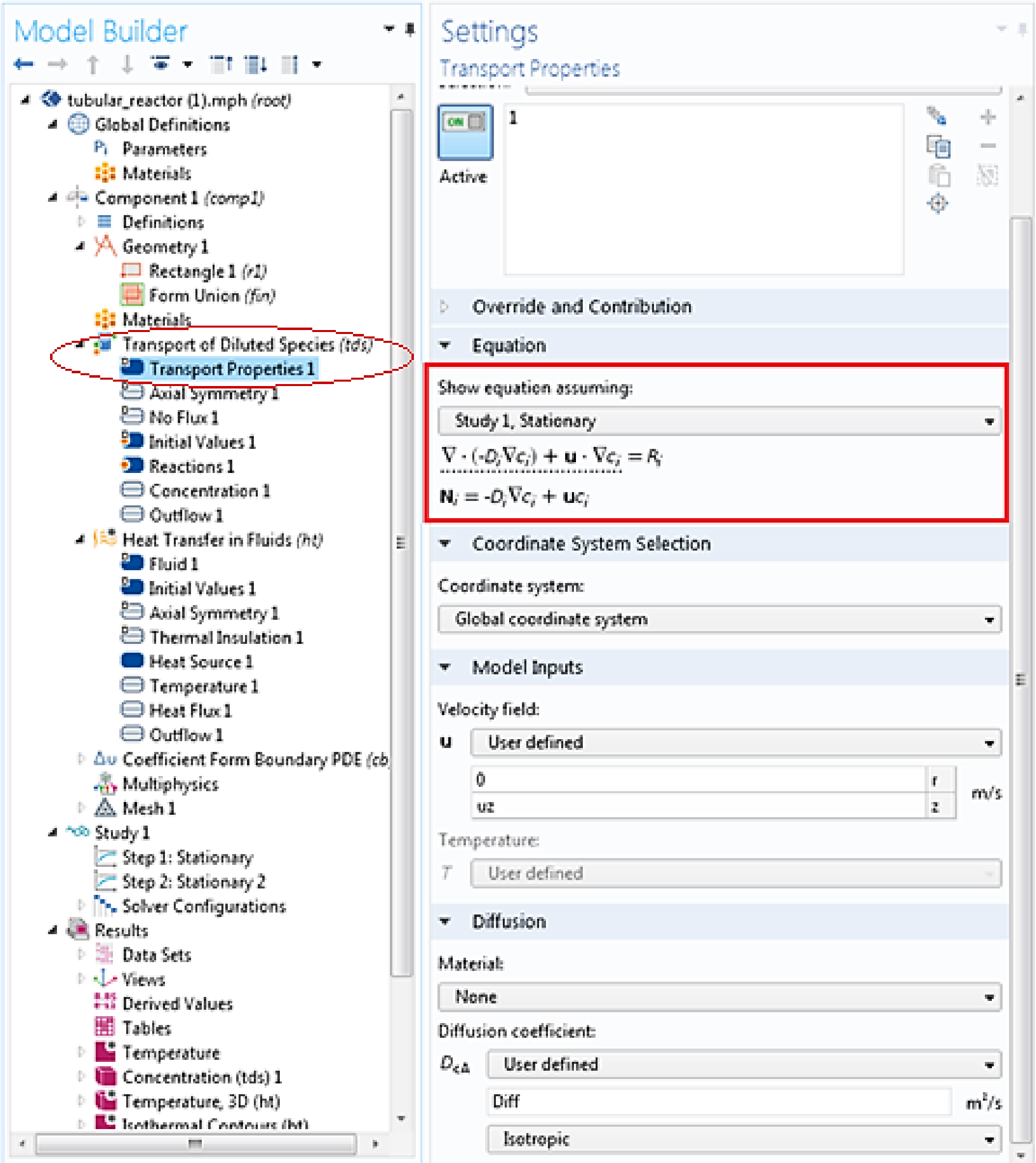


Click on Conversion,1 D graph to obtain conversion profile for plug flow

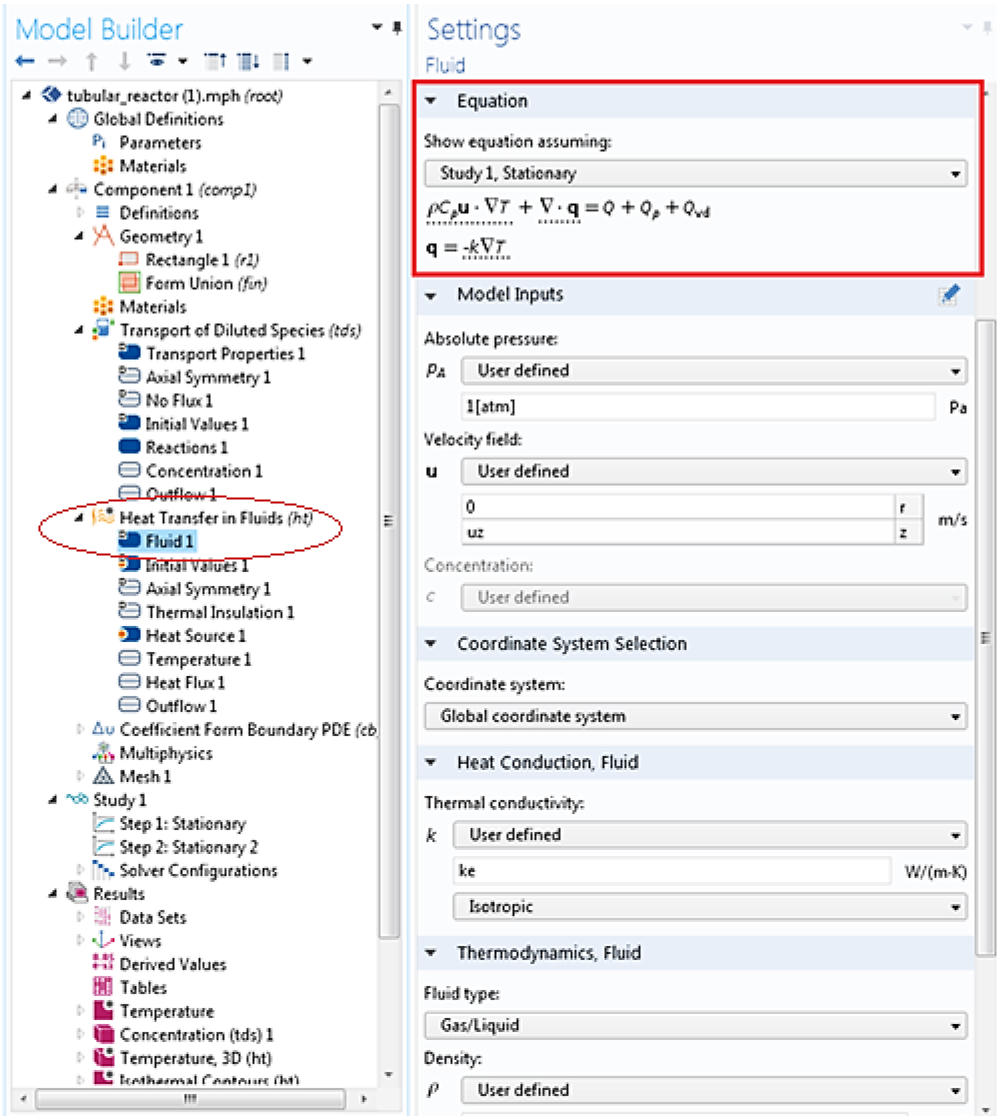


Step 19: Now obtain axial profile for plug flow reactor in a similar way as was done for laminar flow

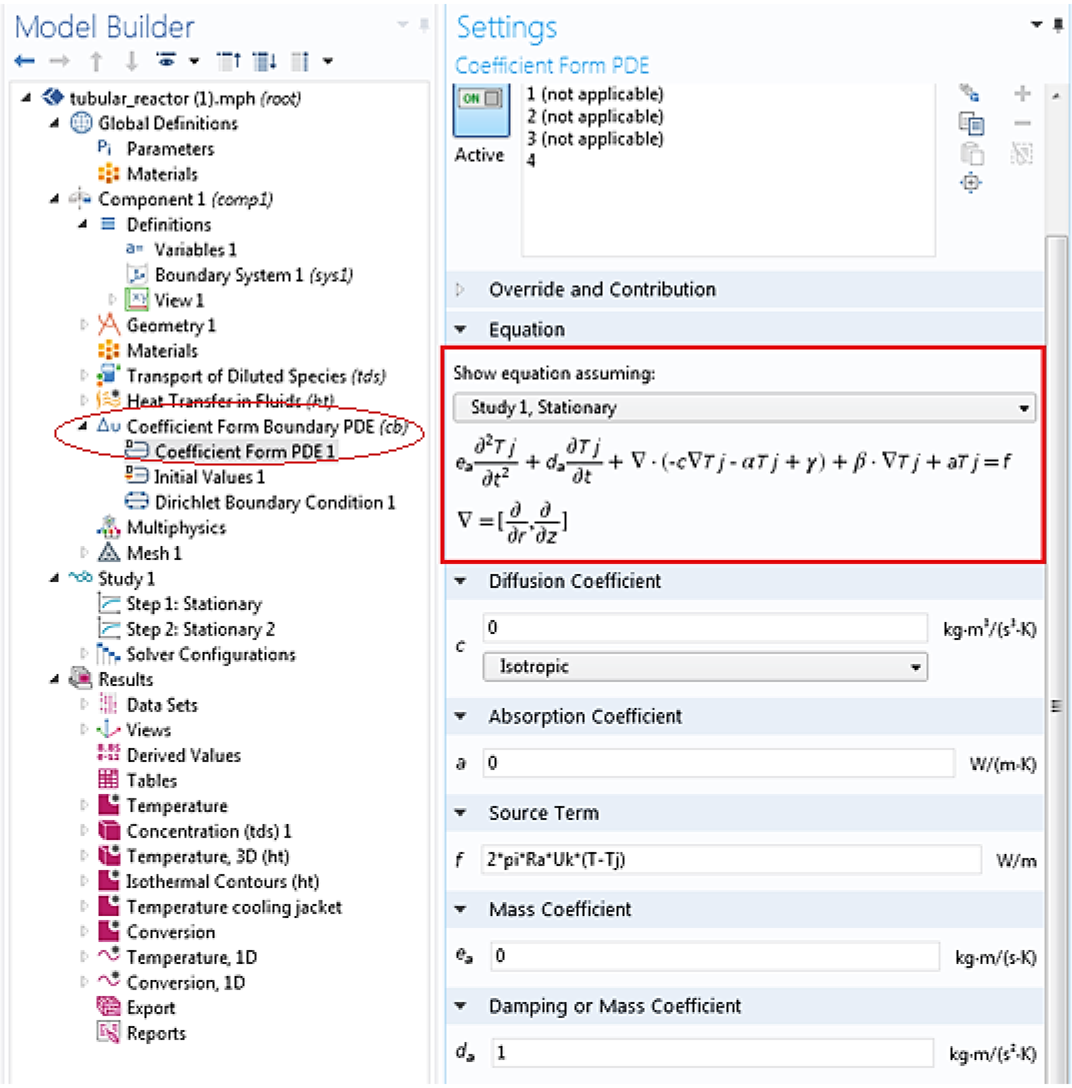
Step 20: To view the mass transfer equations being used by COMSOL, expand Transport of Diluted Species (tds) and click on Transport Properties 1



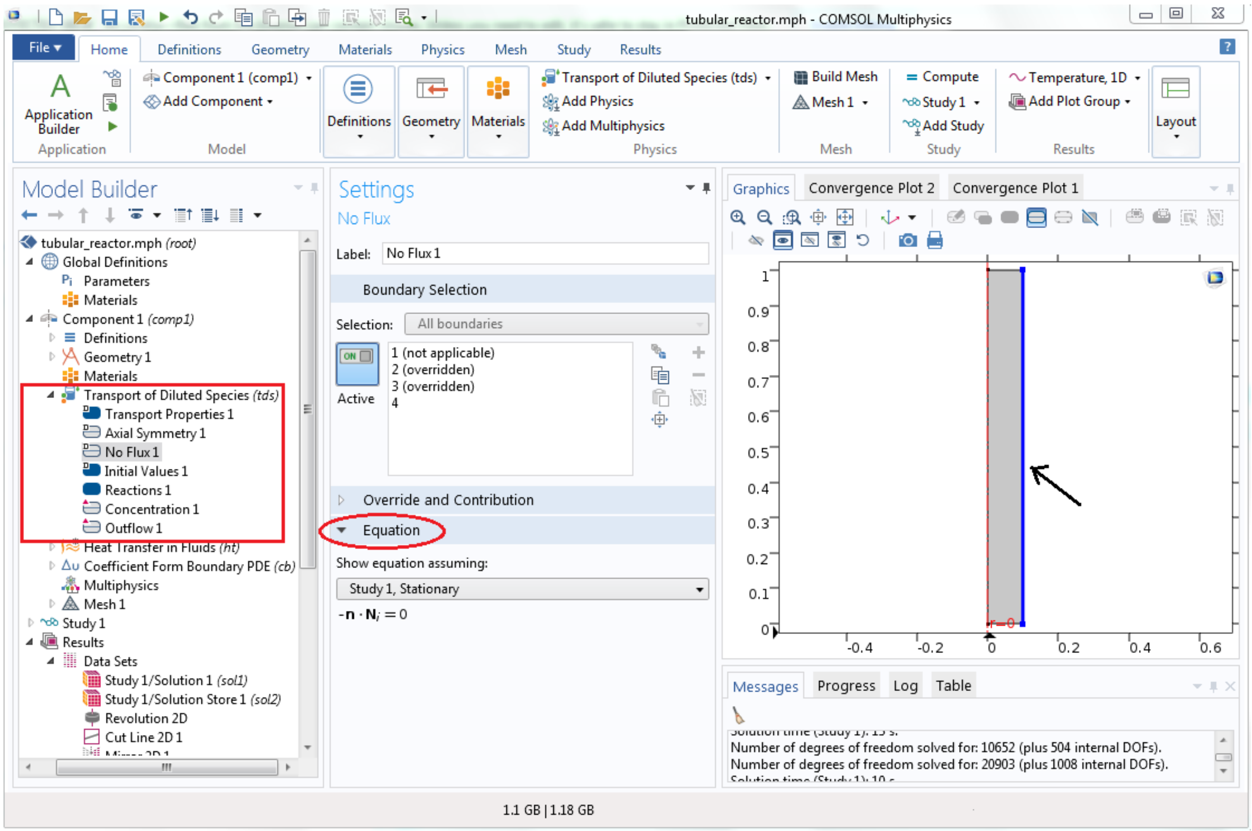
Step 21: To view the heat transfer equations being used by COMSOL, expand Heat Transfer in Fluids (ht) and click on Fluid 1



Step 22: To view the equations for Coolant flow being used by COMSOL, expand Coefficient Form Boundary PDE (cb) and click on Coefficient Form PDE1



Step 23: To view the mass transfer boundary conditions, expand the "Transport of Diluted species" and view the various tabs which include boundary conditions and initial values. If you click on "No Flux 1" you can find the equation that is applied (under equation) and the boundary on which this equation is applied (dark blue color on the geometry)



Step 24: Similarly, you can check the boundary conditions for heat transfer and coolant flow