Objectives:

1) Describe to a graduate student the difference between the prediction of the outlet conversion obtained from a model assuming plug flow and a laminar flow reactor model that contains both radial and axial diffusion and conduction.
2) This tutorial will have you compare the results of a POLYMATH plug flow reactor model with three models produced by COMSOL and solved using a finite element numerical method. The three models will be:
   a) Plug flow reactor in laminar flow
   b) Laminar flow reactor with axial and radial diffusion and conduction

Adiabatic Reactor

This second model with radial effects adds a heat balance to the material balance in the previous model. We assume the reactor is adiabatic, which means that its walls are insulated and do not exchange heat with the surroundings. To generate this model you should start with your previous comsol model or use the model linked to webct. In this new model that you will generate you will add an additional application mode for energy balances to the mass balances already included in the previous model.

Mole Balances

The governing equations for this problem can be derived from a shell balance on a ring shaped element in the cylindrical geometry. The resulting equation is

$$\frac{\partial C_A}{\partial t} = -\frac{\partial N_{Az}}{\partial z} - \frac{\partial (r N_{Ar})}{r\,\partial r} + r_A \tag{1}$$

For cylindrical coordinates r, z the following flux equations for convective and diffusive fluxes in the z and r directions are applicable:

$$N_{Az} = j_{Az} + y_A \sum N_i = -D_{AB}\frac{\partial C_A}{\partial z} + C_A u_z \tag{2}$$

$$N_{Ar} = j_{Ar} + y_A \sum N_i = -D_{AB}\frac{\partial C_A}{\partial r} + C_A u_r \tag{3}$$

Equation 3 can be simplified by eliminating the velocity term in the radial direction. Next substitute equations 2 and 3 into equation 1 to obtain

$$\frac{\partial C_A}{\partial t} = -\frac{\partial}{\partial z}\left(-D_{AB}\frac{\partial C_A}{\partial z} + C_A u_z\right) - \frac{\partial}{r\,\partial r}\left(-D_{AB} r \frac{\partial C_A}{\partial r}\right) + r_A \tag{4}$$

At steady state and assuming constant velocity in the z direction yields the following equation

$$u_z \frac{\partial C_A}{\partial z} = D_{AB}\frac{\partial^2 C_A}{\partial z^2} + D_{AB}\frac{\partial}{r\,\partial r}\left(r\frac{\partial C_A}{\partial r}\right) + r_A \tag{5}$$

Notice that if the diffusive flux in equation 5 is neglected then the familiar plug flow reactor equation results

$$u_z \frac{\partial C_A}{\partial z} = r_A \tag{6}$$

The steady-state energy balance on the fluid within the reactor can be transformed to the following equation (See Section 8.9 in Fogler 4th edition)

$$0 = -\frac{\partial}{\partial z}\left(-k\frac{\partial T}{\partial z} + C_p u_z T\right) - \frac{\partial}{r\,\partial r}\left(-kr\frac{\partial T}{\partial r}\right) + r_A \Delta H_{Rx} \tag{7}$$

The reaction stoichiometry is given by

$$A + B \Leftrightarrow 2C \tag{8}$$

The reaction rate is given by

$$r_A = -A\exp\left(-\frac{E}{RT}\right)\rho_{cat}\left(C_A C_B - \frac{C_c^2}{K_{eq}}\right) \tag{9}$$

In COMSOL the equation is written as:

$$rA = -A*\exp(-E/RT)*rhoCat*(cA*cB - cC\text{^}2/Keq) \tag{10}$$

For the isothermal reactor the T is set equal to T0.
The equilibrium constant is given by

$$K_{eq} = 1000\exp\left(\frac{\Delta H_{Rx}}{R}\left(\frac{1}{303K} - \frac{1}{T}\right)\right) \tag{11}$$

Using your previous polymath model, add an energy balance of a PFR to this model.

$$\frac{dT}{dV} = \frac{Ua(T_a - T) + \Delta H_R\big|_T r_A}{\left(\sum_{i=1}^{n} F_{i0}C_{pi} + F_{A0}X\Delta C_p\right)} \tag{12}$$

Assume that the heat capacity of the reaction mixture is Cp = 4180 J/kg·K (e.g. $\Delta C_p = 0$), the thermal conductivity of the reaction mixture is k = 0.559 J/m·s·K, and for the reactor with cooling the overall heat-transfer coefficient, Ua = 1300 J/m^2·s·K. Your previous model has a reaction with an activation energy E is 95,238 J/mol, the pre-exponential is A=1.1×10^8 m^6/(mol kg s), and the heat of reaction is $\Delta H_{Rx} = -83680\ J/mol$. The fluid is fed at an inlet temperature is 320K the inlet flowrate is 5×10^{-4} m^3/s. The reactant concentrations for A and B are equimolar at 500 mol/m^3. The density of the catalyst is 1500 kg/m^3 and the liquid phase density is 1000 kg/m^3. The reactor is 1 m in length with a radius of Ra=0.1 m. For the polymath model you will need the heat capacity with units of molar heat capacity which can be found as

$$C_{P(MOLAR)} = \frac{C_{P(MASS)}\rho\upsilon_0}{F_T} \tag{13}$$

Submit all work in email with the subject title, "Comsol Adiabatic Reactor." All "printouts" should be pasted into a word document and submitted by email. Answer any questions using text in the word document. Place figure captions on all figures to explain what you have plotted.

1) Submit your new POLYMATH model of this process (Paste the output into MS word document).
   a) This first model will be of an adiabatic reactor
   b) The second model will include an overall heat transfer term (U_k = 1300 J/m^2·s·K).
2) Plot the temperature and conversion of A as a function of volume of reactor and length of reactor. (remember constants in POLYMATH are given using the ! function).

Since we are in laminar flow the parabolic velocity profile for a pipe flow is given as

$$u_z = 2 * u_0 \left(1 - \left(\frac{r}{R_a} \right)^2 \right) \tag{14}$$

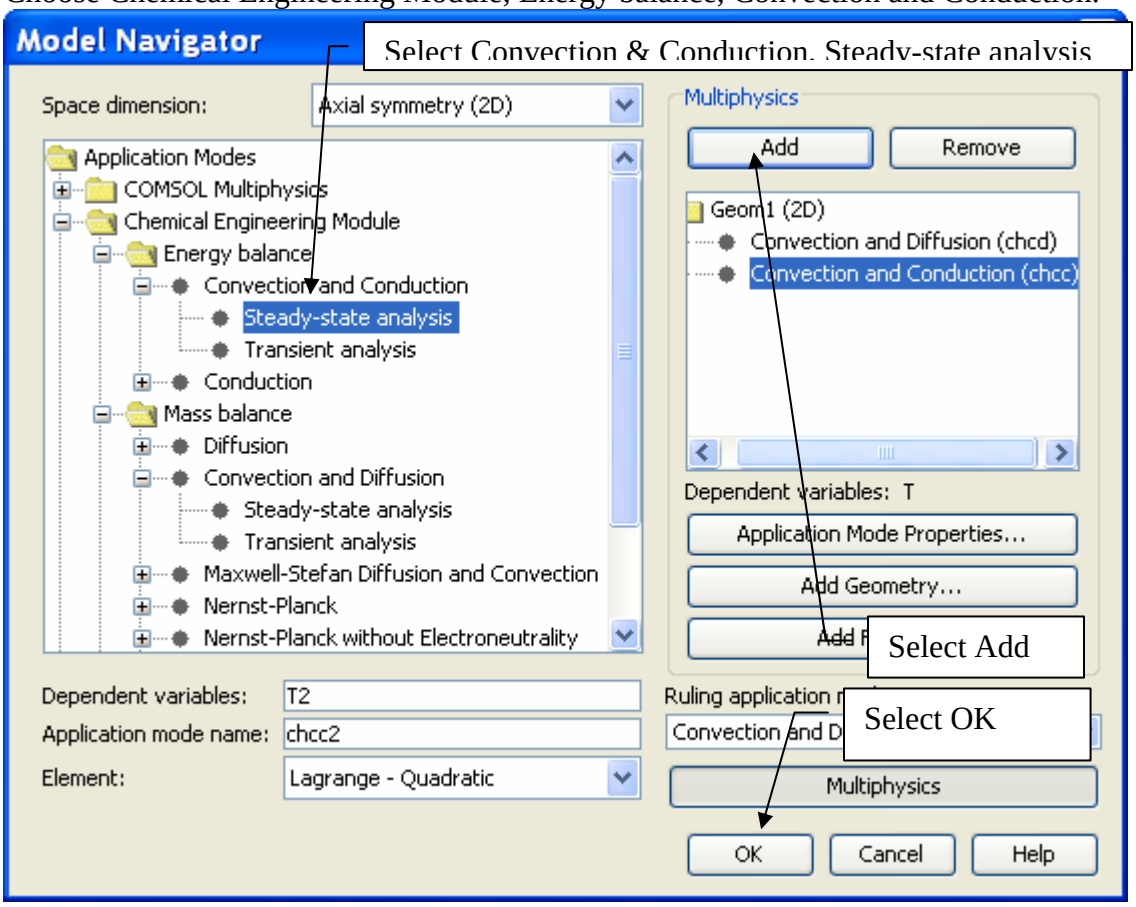
With the average velocity or superficial velocity given by

$$u_0 = \frac{5 \times 10^{-4}\ m^3/s}{\pi R_a^2} \tag{15}$$

1. Open Comsol Multiphysics and load your previous model. If this is not available load the file: 1-Isothermal_Reactor.fl from webCT.

2. Select Multiphysics, Model Navigator

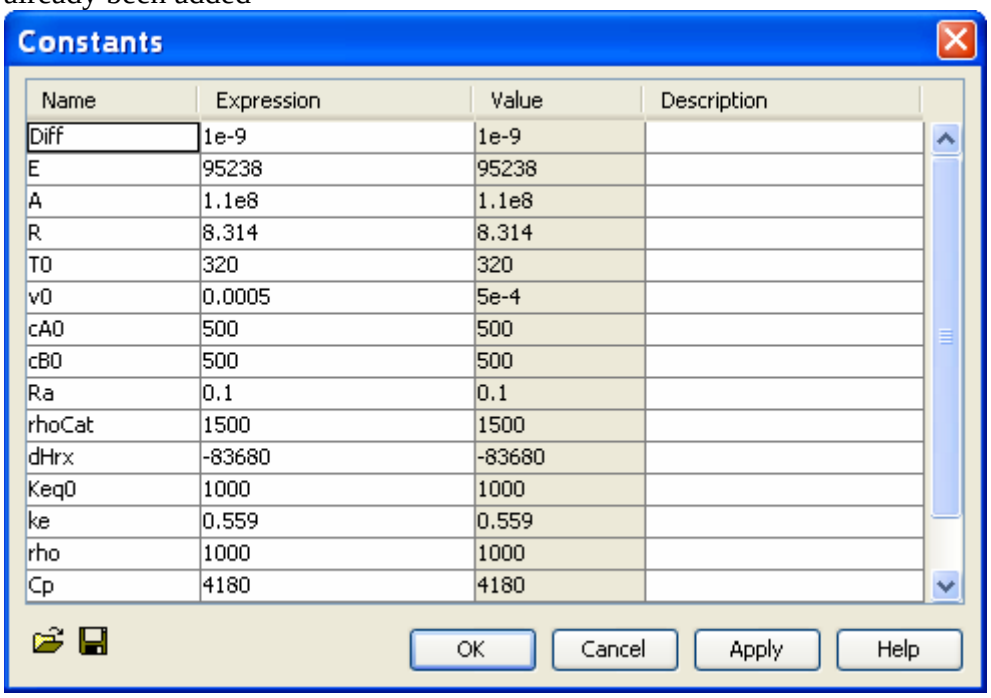
3. Choose Chemical Engineering Module, Energy balance, Convection and Conduction.



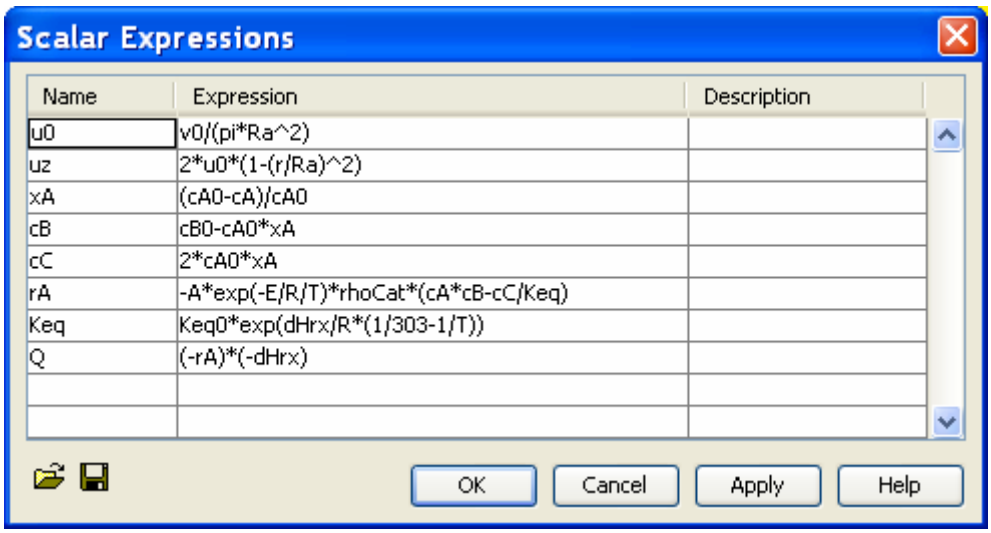
4. Select OK

5. Remember that the geometry of the tube a rectangle. The center of the pipe is at a radial position of 0 and the wall of the pipe is at a dimension of 0.1m. The length of pipe will be set at 1m.

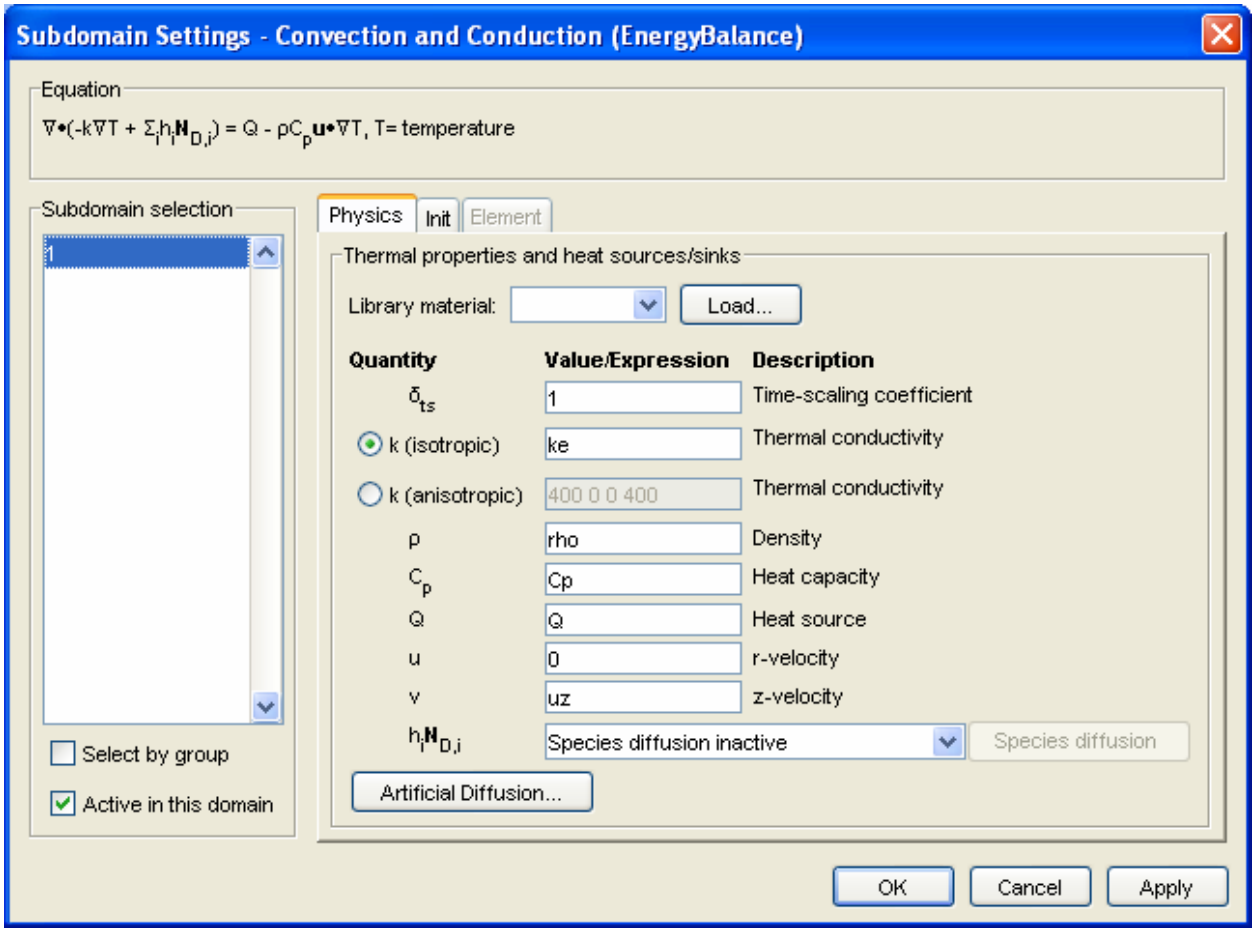
6. Enter the following Constants in **Options Constants** menu– Note some of these have already been added



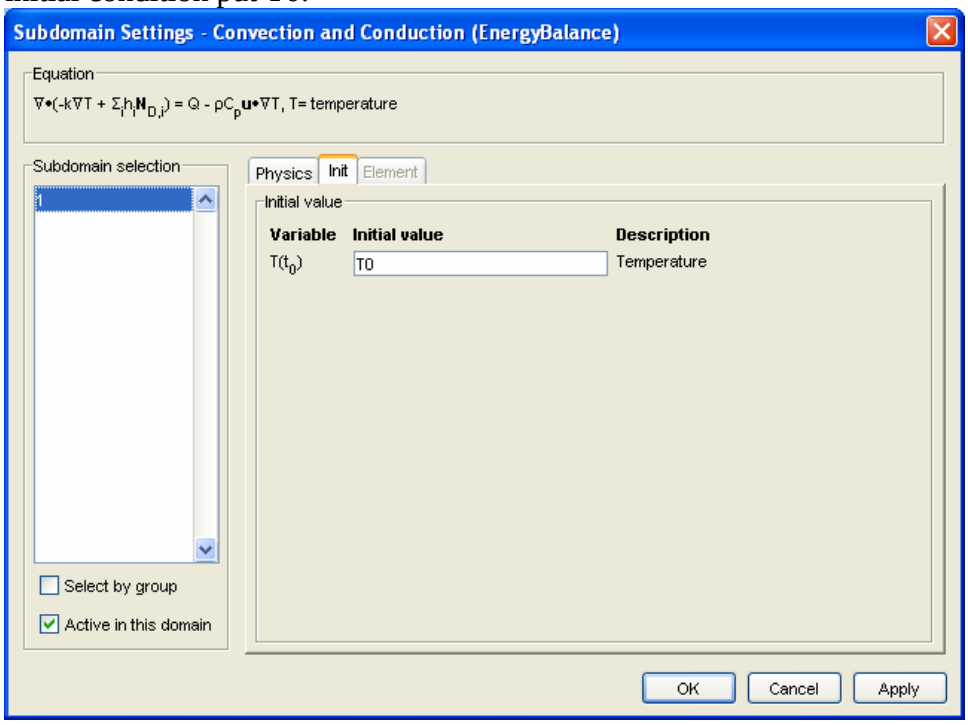
7. Enter in the **Options Expressions, Scalar Expressions** menu. **YOU MUST CHANGE YOUR TEMPERATURE VARIABLE IN THE REACTION RATE EXPRESSION.**



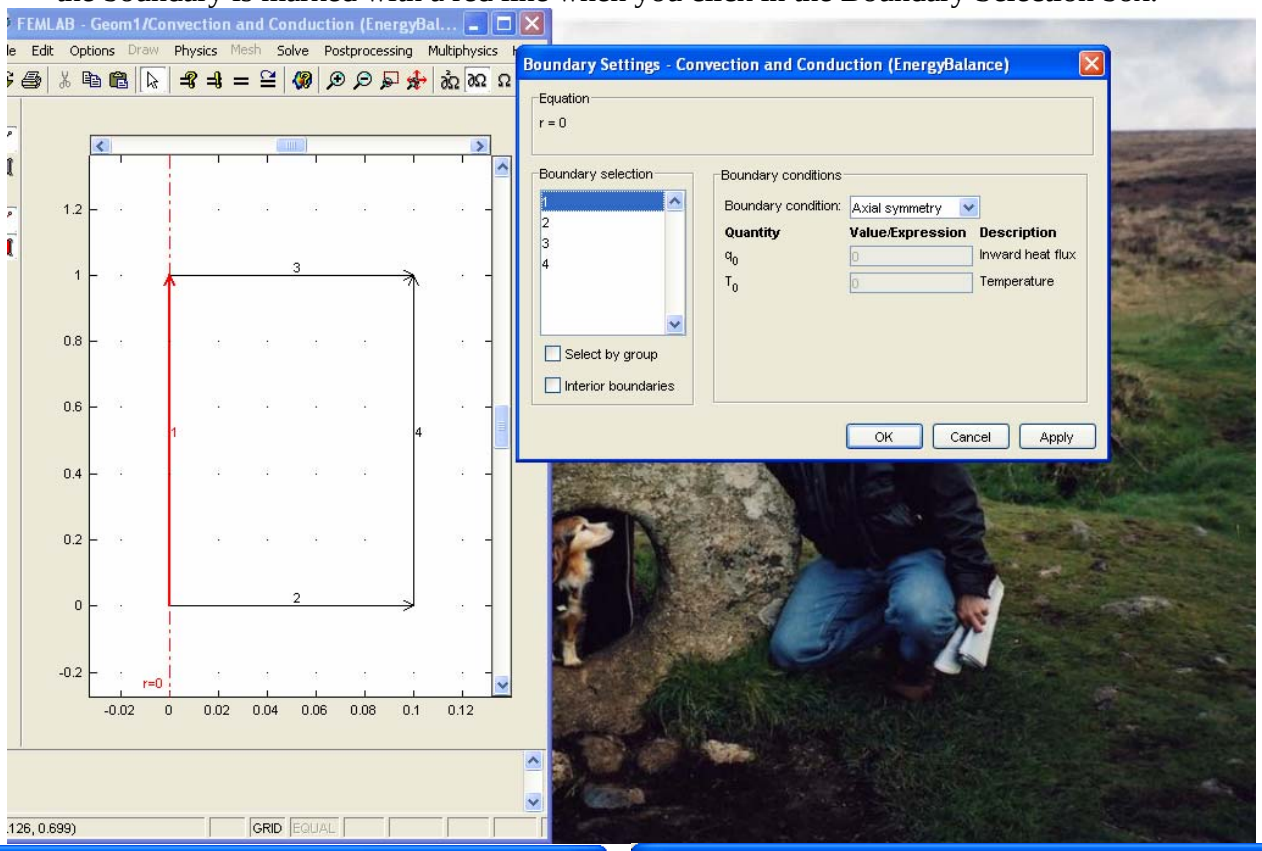
8. Select the **Physics** menu and select **Subdomain Settings** to open the corresponding dialog box. Select **subdomain 1** in the Subdomain selection list. This dialog box also displays the equation that forms the basis for the Conduction and Convection application mode, and the edit fields show the input data used in the energy balance. Note if you don't have a Time scaling coefficient that is ok.

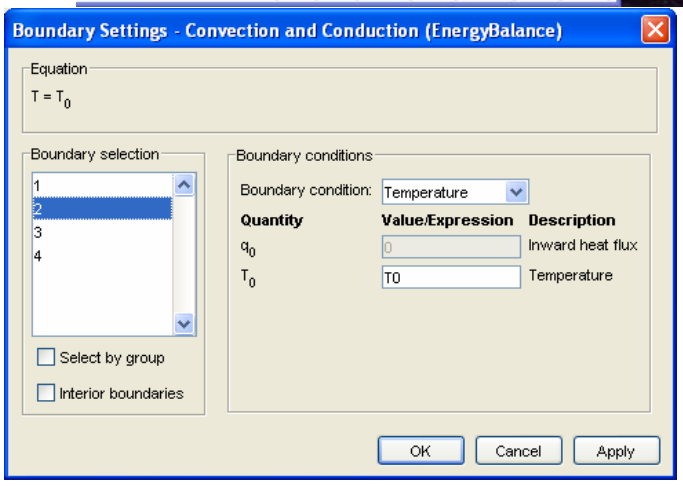


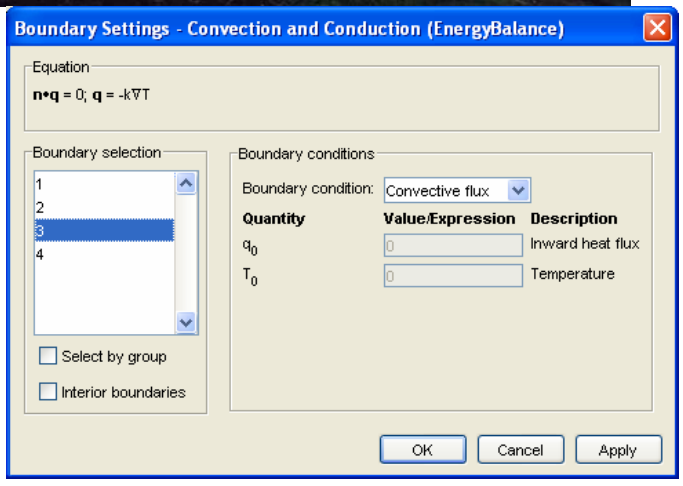
9. Here you are entering the variables that were given by equation 7. In the init tab for initial condition put T0.

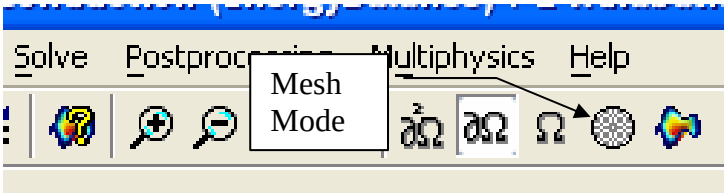


10. Enter boundary conditions, axial symmetry for 1 and insulation for 4, Temperature, T0 for the inlet boundary 2 and convective flux for the reactor outlet 3. Notice when you click on the number the figure of the reactor highlights in red the boundary condition. Notice how the boundary is marked with a red line when you click in the Boundary Selection box.



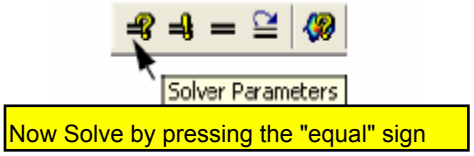






11. To visualize the mesh click the Mesh Mode button. Note that the scales on the r- and z-axes are not equal, which results in a distorted view. If desired, you can select equal scale settings by going to the **Options** menu and checking the **Axis** equal box in the **Axis/Grid Settings** menu item. In order to return to the original unequal scale settings, once again go to the **Axes/Grid Settings** menu and clear the **Axis** equal check box. Enter -0.1 in the r min edit field, 0.2 in the r max edit field and -0.1 and 1.1 in the z min and z max edit fields, respectively.

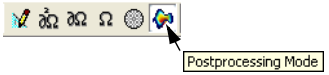
12. The model we solve in this exercise is nonlinear. To verify the solver settings, click the Solver Parameters button and make certain that the Stationary nonlinear solver is selected.

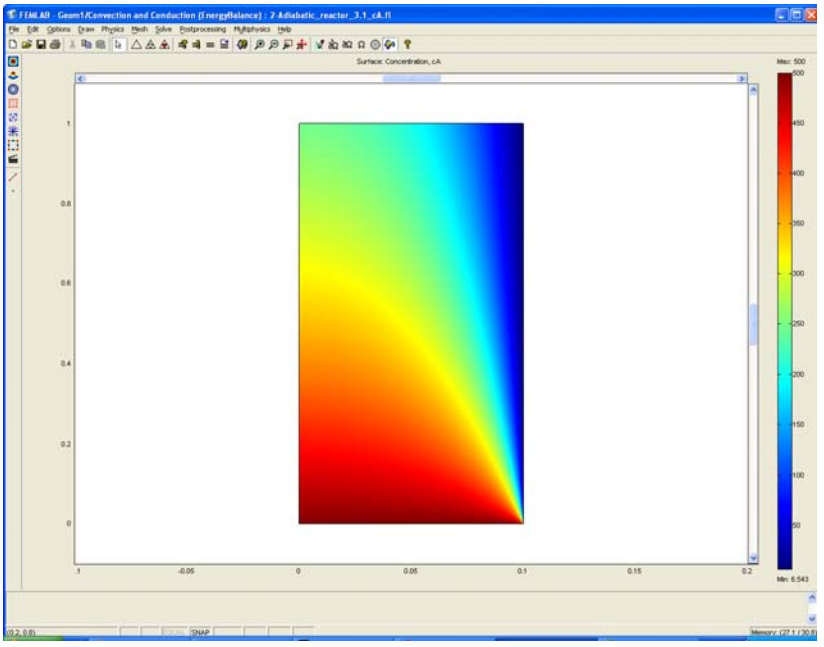


13. The manual explaining a portion of today's tutorial is located on the following pages and also on webct.rowan.edu page under the heading **3 Additional Materials, 3.1 FEMLAB ECRE Manual and is on CD with Book.** This will open a pdf file titled FEMLAB3 ECRE version. You will be entering this model in the REAL version of COMSOL and must turn in all assignments using the COMSOL model. You are of course welcome to compare your answers with the prepackaged models on your CD FEMLAB3 ECRE-VERSION that came with the book.
14. You will now refer to the instructions in the ECRE manual which are given on the next page. This is written in the form of *look at what is in the ECRE model*. (This section was taken from page 39 step 1 of the manual which is 43 of 88 in the ECRE pdf file.)

GO to the next page

1 Click the **Postprocessing Mode button**. The default plot shows the concentration of species A in the reactor.

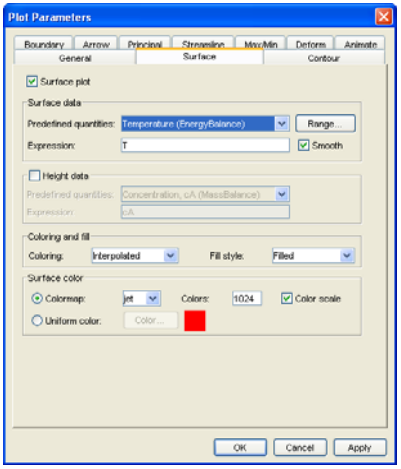




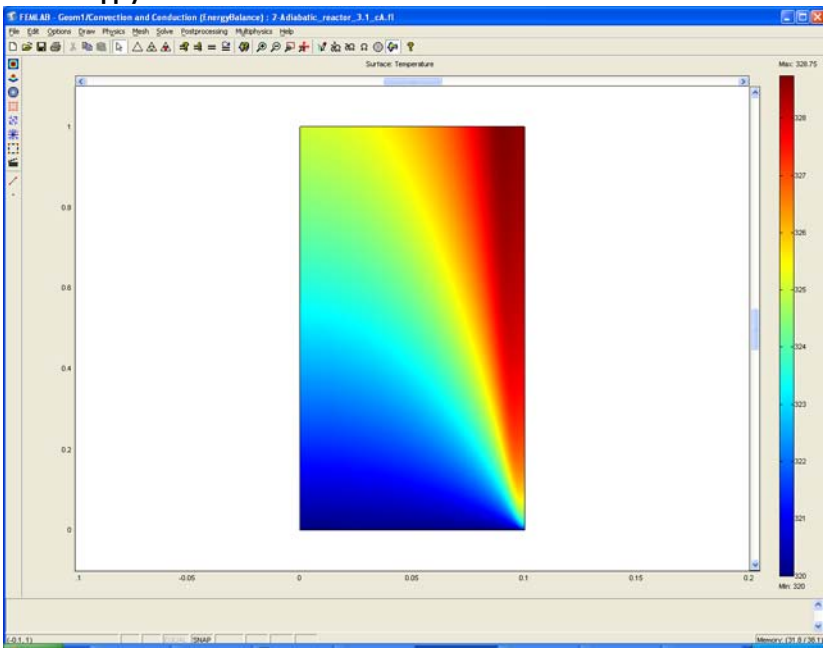
2 Click the **Plot Parameters** button.

3 Click the **Surface** tab.

4 On the **Surface** page, go to the **Predefined quantities** drop-down list and select **Temperature**.

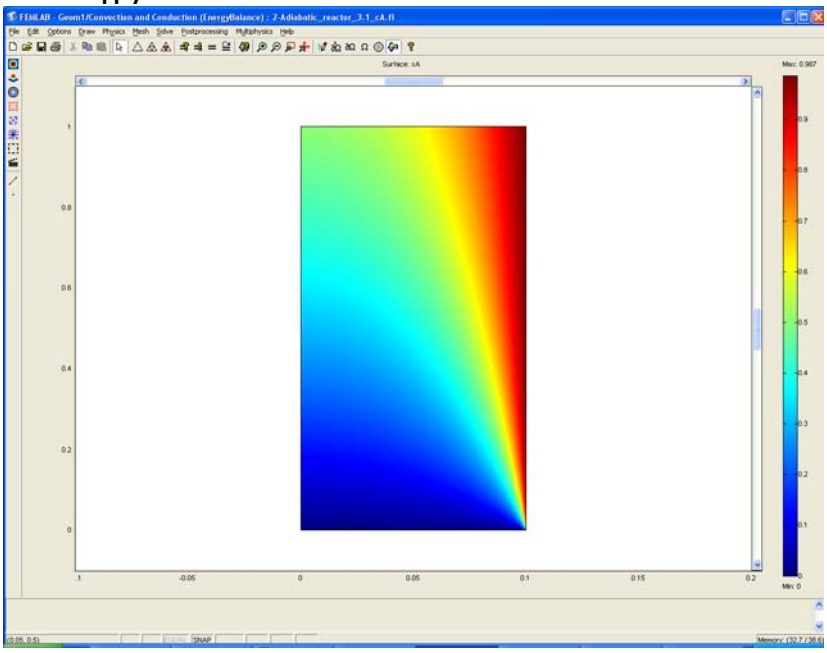


5 Click **Apply**.



6 To plot the conversion of A, enter `xA` in the **Expression** edit field in the **Surface** page.

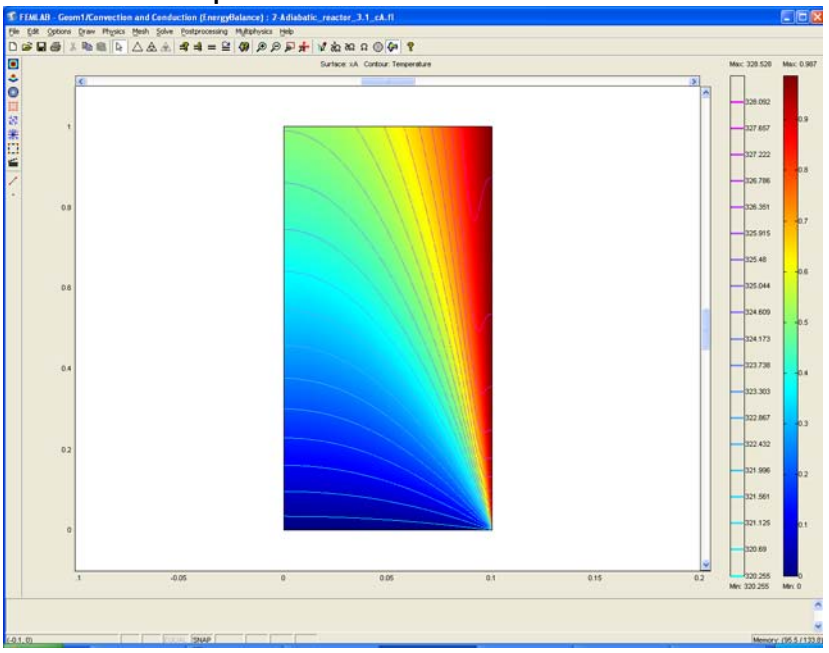
7 Click **Apply**.



8 To visualize the relation between temperature and conversion, first click the **Contour** tab.

9 Select `Temperature (EnergyBalance)` in the **Predefined quantities** drop-down list.

10 Click the **Contour plot** check box and click OK.



11 To visualize the local conversion in selected cross sections along the length of the reactor, go to the **Postprocessing** menu and select **Cross-Section Plot Parameters**.

12 Click the **Line/Extrusion** tab.

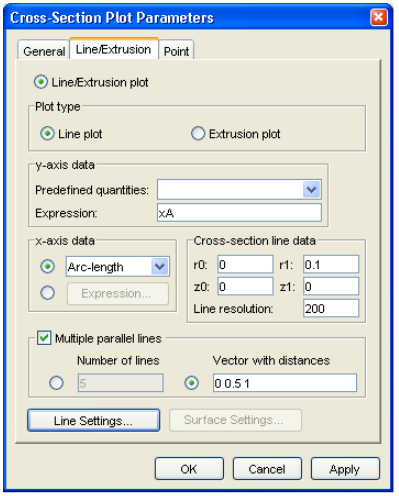
13 Enter xA in the **Expression** edit field.

14 Enter 0 in the **r0** edit field and 0.1 in the **r1** edit field.

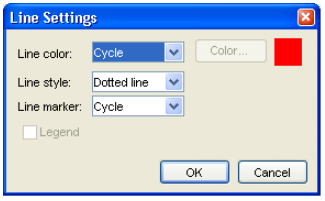
15 Enter 0 in both the **z0** and **z1** edit fields.

16 Check the **Multi parallel lines** box and click the **Vector with distances** option.

I7 Enter `0 0.5 1` in the **Vector with distances** edit field to generate three cross-section plots at the inlet, in the middle of the reactor, and at the outlet, respectively.



I8 Click the **Line Settings** button. In the dialog box that opens, select the **Cycle** option in the **Line color** drop-down list; select **Dotted line** in the **Line style** drop-down list; and select **Cycle** in the **Line marker** drop-down list.



19 To generate the following plot, click **OK** twice: first in the **Line Settings** dialog box, then again in the **Cross-Section Plot Parameters** dialog box.

See page 15 of 19 for more details on making this graph.

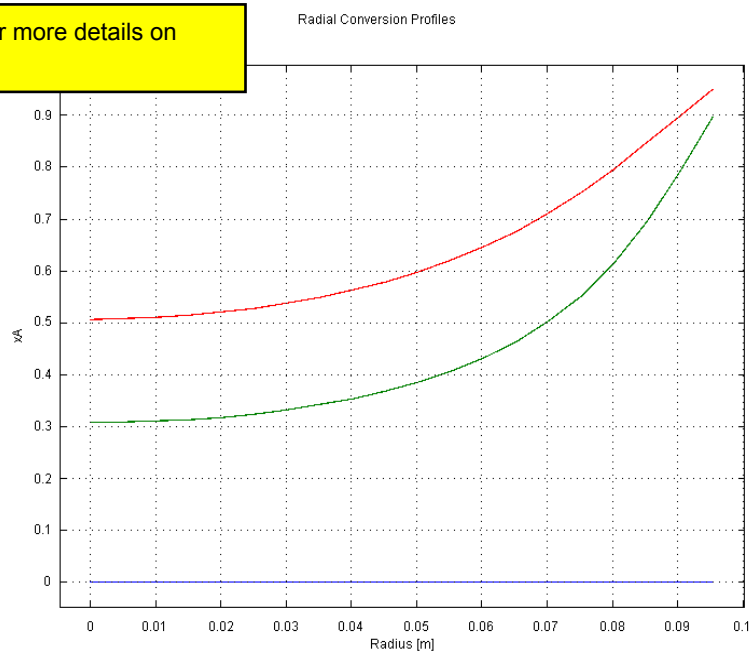


Figure 2-3: Radial conversion profiles at the inlet, outlet and halfway through an adiabatic reactor.

You can now calculate the mixing cup outlet concentration (see the previous example for its definition). Start by calculating the integral of the outlet flux over the outlet boundary.

20 Go to the **Postprocessing** menu and select **Boundary Integration**.

21 Select boundary 3 in the **Boundary selection** list.

22 Enter `2*pi*r*cA*uz` in the **Expression** edit field.

23 Click **Apply**.

The value of the integral appears in the status bar at the bottom of the user interface and reads `0.088836`. You can now calculate the integral of u_z.

24 Enter `2*pi*r*uz` in the **Expression** edit field and click **Apply**.

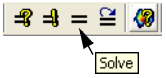
The value of this integral is `5e-4`, which gives an average concentration of `0.088836/5e-4`, which is approximately `178` mole m^{-3}.

You have now completed a review of the model and are ready to run it with varying input parameters.

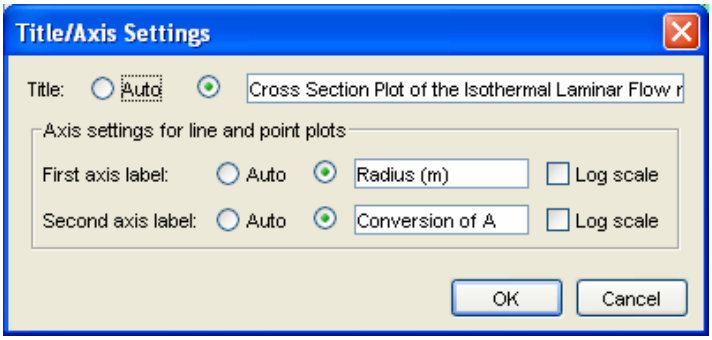
Questions and Exercises

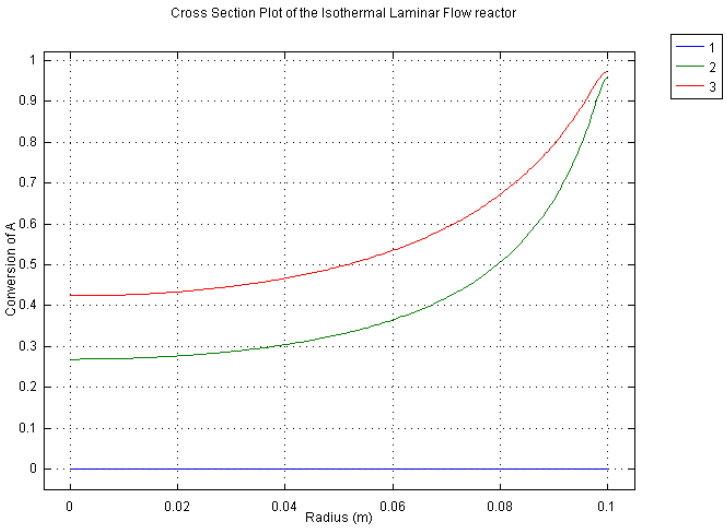
To answer the following questions and perform the exercises, you can either use the results in the model just presented, or you can solve it again with new input data.

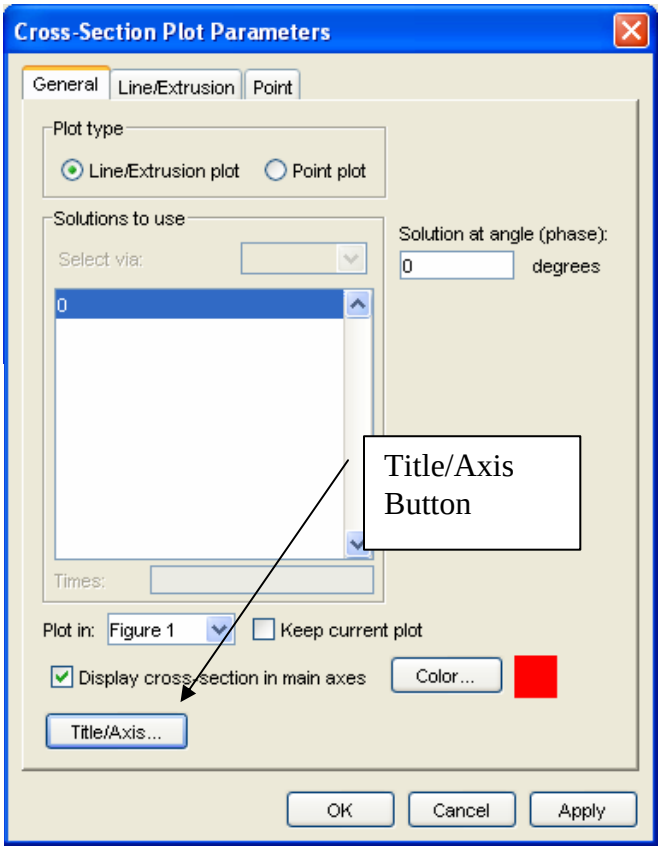
1. How do you explain the difference in outlet conversion between the isothermal and non-isothermal adiabatic reactor? (For a clue, examine the temperature plot.)
2. This section deals with the model of an adiabatic reactor. What is special about the solution's surface plot of the temperature? Explain the resulting radial temperature distribution.
3. Increase the thermal conductivity, `ke`, by a factor of 10 and explain how this affects the temperature profiles. At what radial position do you find the highest conversion? You can change the thermal conductivity by going to the **Options** menu and then the **Constants** item. Click the **Solve** button to solve the problem with the new thermal conductivity.

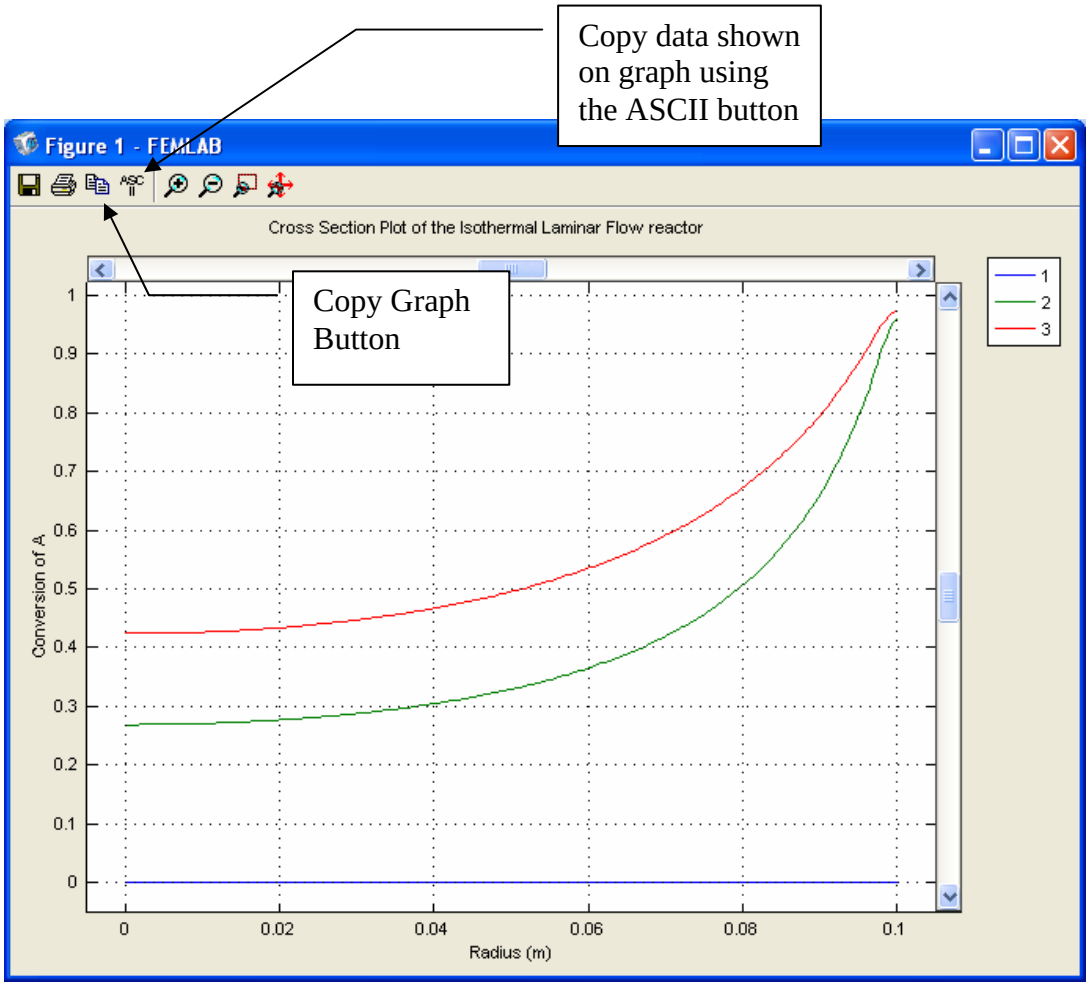


15. In Step 19 of page 44 in the ECRE manual (and on page 13 of 19 in this pdf file) it asked you to make a Cross-Section plot. I prefer to use as the x-axis data either the z or the r coordinate. Also in the line Settings box I always request a legend.
16. Also a title to the graph as well as axis labels can be specified. Select the General tap and the Title/Axis button.
17. This plot can now be pasted into a word document by selecting the MS windows copy icon.

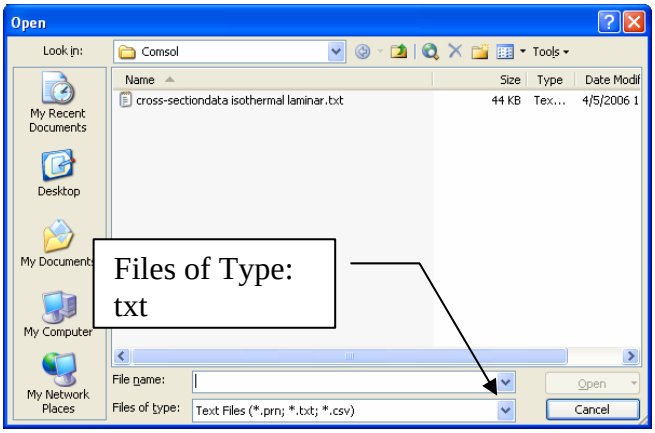


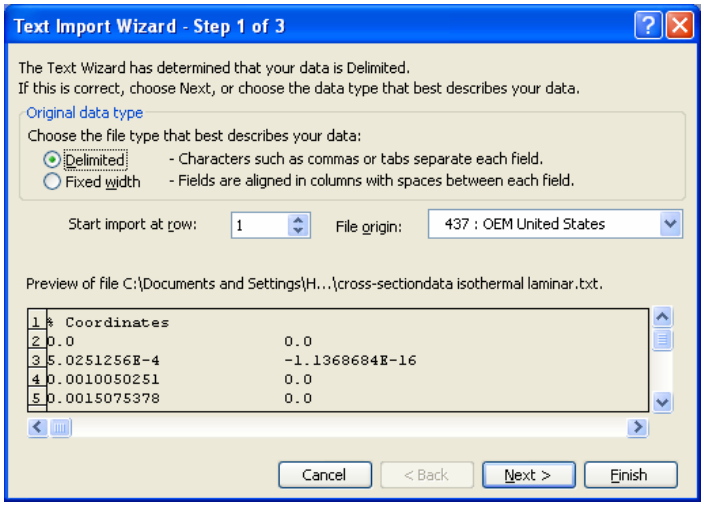


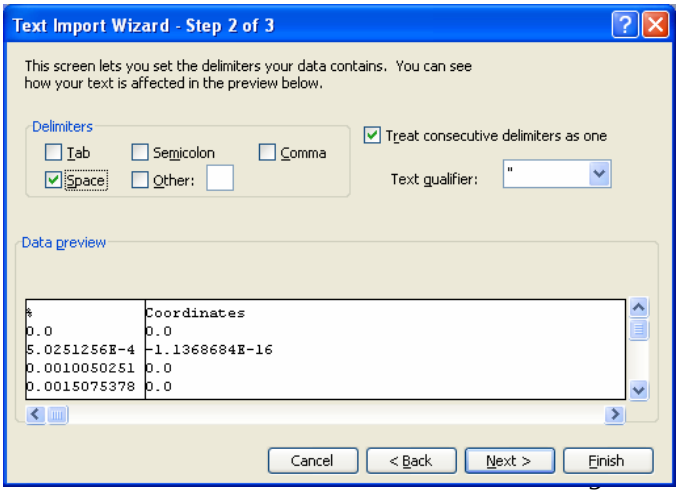




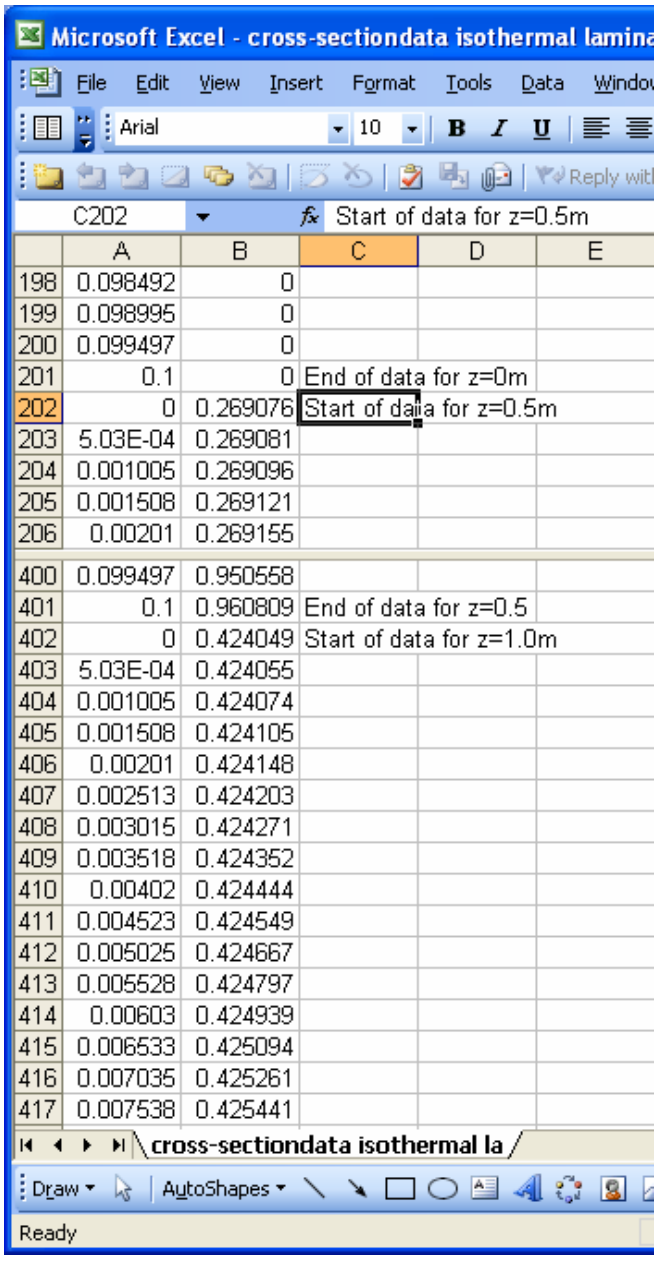
18. To obtain a table of data shown on the cross section plot then you must click on the ASCII button and then save this file.
19. The file will be a text file that can be opened by excel for further analysis. Open the txt file by having excel look for text files.
20. Then start the conversion of the data using a delimited file.\



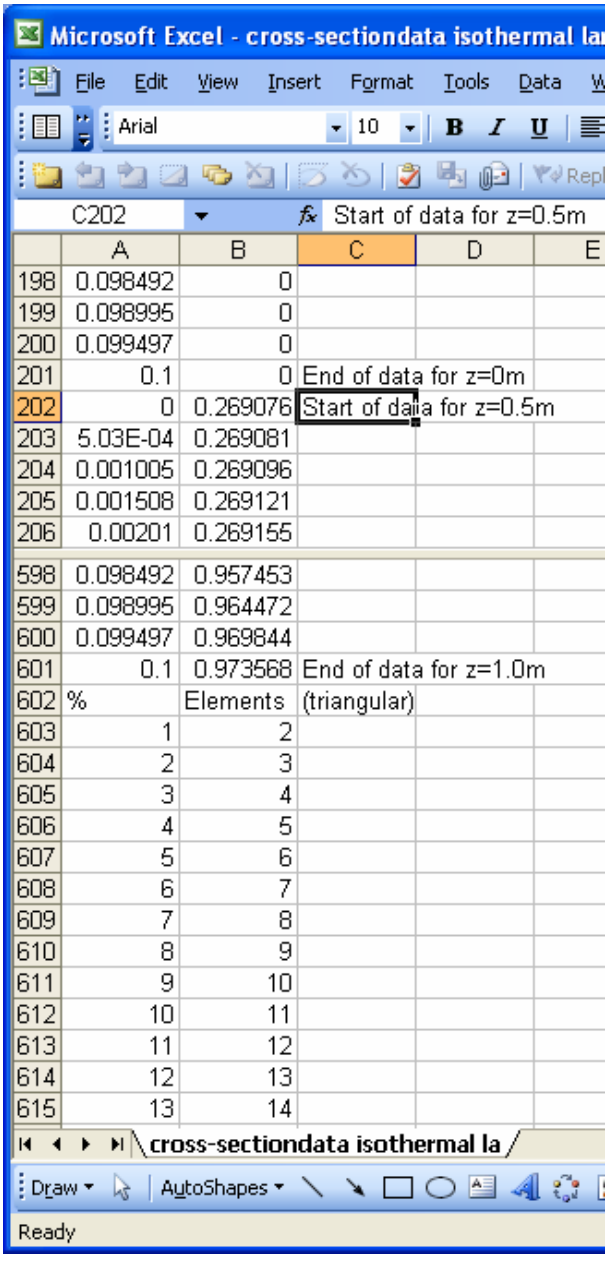




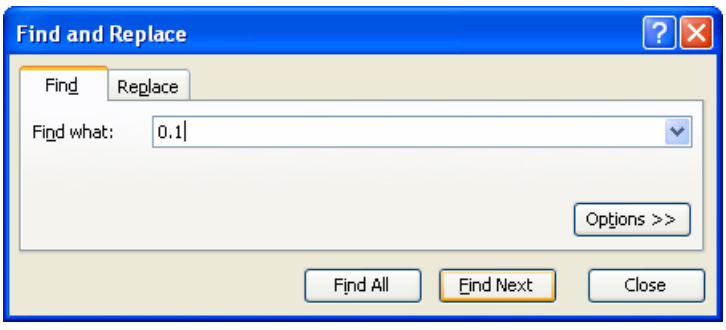
21. The data is placed in two columns (x,y). The first cross-section at z=0m is listed, followed by the second cross-section z=0.5m, followed by the third cross-section at z=1.0m. To find these I always use the Edit, Search feature and find the ending r data point.



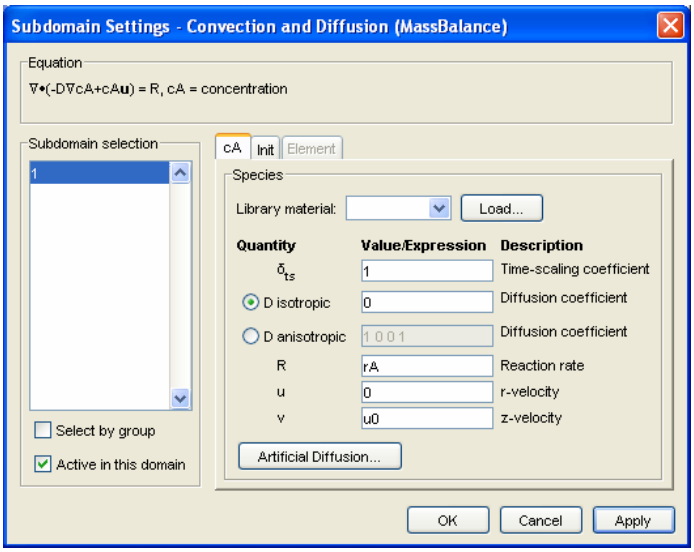
	A	B	C	D	E
198	0.098492	0			
199	0.098995	0			
200	0.099497	0			
201	0.1	0	End of data for z=0m		
202	0	0.269076	Start of data for z=0.5m		
203	5.03E-04	0.269081			
204	0.001005	0.269096			
205	0.001508	0.269121			
206	0.00201	0.269155			
400	0.099497	0.950558			
401	0.1	0.960809	End of data for z=0.5		
402	0	0.424049	Start of data for z=1.0m		
403	5.03E-04	0.424055			
404	0.001005	0.424074			
405	0.001508	0.424105			
406	0.00201	0.424148			
407	0.002513	0.424203			
408	0.003015	0.424271			
409	0.003518	0.424352			
410	0.00402	0.424444			
411	0.004523	0.424549			
412	0.005025	0.424667			
413	0.005528	0.424797			
414	0.00603	0.424939			
415	0.006533	0.425094			
416	0.007035	0.425261			
417	0.007538	0.425441			



	A	B	C	D	E
198	0.098492	0			
199	0.098995	0			
200	0.099497	0			
201	0.1	0	End of data for z=0m		
202	0	0.269076	Start of data for z=0.5m		
203	5.03E-04	0.269081			
204	0.001005	0.269096			
205	0.001508	0.269121			
206	0.00201	0.269155			
598	0.098492	0.957453			
599	0.098995	0.964472			
600	0.099497	0.969844			
601	0.1	0.973568	End of data for z=1.0m		
602	%	Elements	(triangular)		
603	1	2			
604	2	3			
605	3	4			
606	4	5			
607	5	6			
608	6	7			
609	7	8			
610	8	9			
611	9	10			
612	10	11			
613	11	12			
614	12	13			
615	13	14			



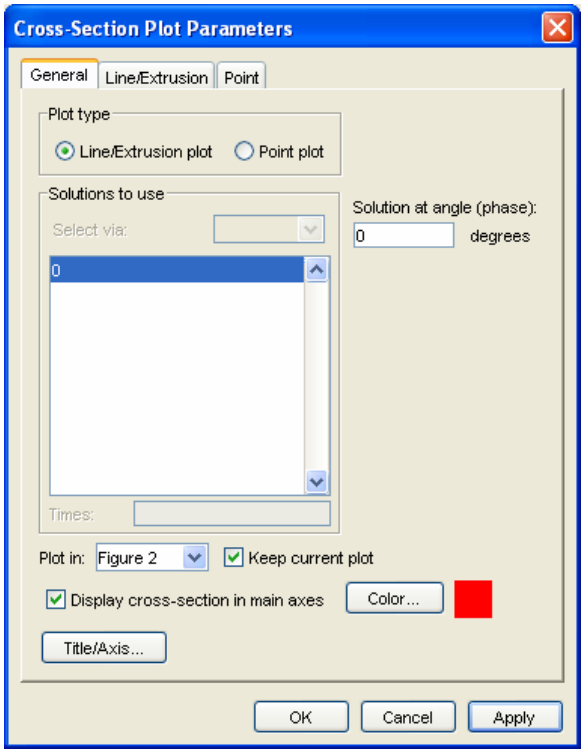
To be Submitted:
Submit all work in email with the subject title, "Comsol Adiabatic Reactor." All "printouts" should be pasted into a word document and submitted by email. Answer any questions using text in the word document. Place figure captions on all figures to explain what you have plotted.

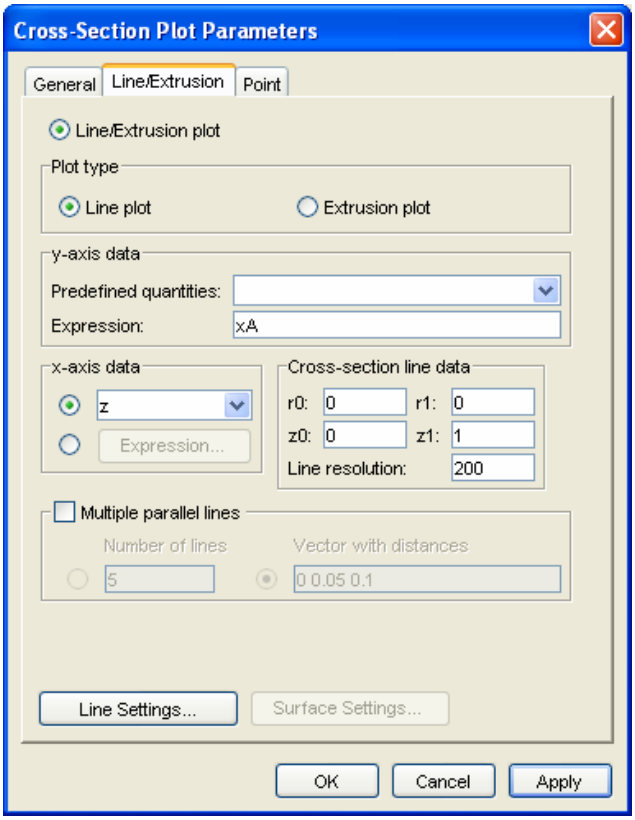


1) POLYMATH model and requested plots
2) Answer Questions 1-3 on page 14 of 19 in this tutorial (page 45 of the ECRE manual).
3) Reset your model to the base case conditions given in the above tutorial (Diff=1×10^{-9}m^2/s and ke = 0.559 J/m·s·K.)
   a) Run the following cases: (Remember to change a parameter in either the mass balance or energy balance you must select it using the Multiphysics

Case	Diffusivity (m^2/s)	Thermal Conductivity (J/(m s K)	Velocity Profile
Base Case	1×10^{-9}	0.559	$u_z = 2*u_0\left(1-\left(\frac{r}{R_a}\right)^2\right)$
Case 1	0	0.559	$u_z = u_0$
Case 2	0	0	$u_z = u_0$

   b) Compare the base case with Case 1 and Case 2. Do this using surface plots and cross-section plots of conversion and temperature.
   c) Compare Case 1 and Case 2 with your POLYMATH model results. Make plots of T and X_A vs L that show predictions of cases 1 & 2 and your POLYMATH results from a plug flow reactor.
   d) Compare the average outlet conversion and temperature from the COMSOL laminar flow adiabatic reactor model (base case) with the outlet conversions and temperatures obtained from the POLYMATH PFR. Write a statement on the comparison of the conversion of these two data sets.





In the Table for anisotropic the Diffusivities are:

Dr (radial)	
	Dz (axial)