

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.
- 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 diffusion
 - c) Laminar flow reactor with axial and radial diffusion

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

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

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

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

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

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

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

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

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

Notice that if the diffusive flux in equation 5 is neglected ($D_{AB} = 0$) then the familiar plug flow reactor equation results

$$u_z \frac{\partial C_A}{\partial z} = r_A \quad (6)$$

The reaction stoichiometry is given by



The reaction rate is given by

$$r_A = -A \exp\left(-\frac{E}{RT}\right) \rho_{cat} \left(C_A C_B - \frac{C_c^2}{K_{eq}} \right) \quad (8)$$

In COMSOL the equation is written as:

$$rA = -A * \exp(-E/RT) * rhoCat * (cA * cB - cC^2 / Keq) \quad (9)$$

For the isothermal reactor the T is set equal to T_0 .

The equilibrium constant is given by

$$K_{eq} = 1000 \exp\left(\frac{\Delta H_{Rx}}{R} \left(\frac{1}{303K} - \frac{1}{T}\right)\right) \quad (10)$$

Construct a polymath model for this problem given that the activation energy E is 95,238 J/mol, the preexponential is $A=1.1 \times 10^8 \text{ m}^6/(\text{mol kg s})$, and the heat of reaction is

$\Delta H_{Rx} = -83680 \text{ J/mol}$. The fluid is fed at an inlet temperature is 320K the inlet flowrate is $5 \times 10^{-4} \text{ m}^3/\text{s}$. The reactant concentrations for A and B are equimolar at 500 mol/m^3 . The density of the catalyst is 1500 kg/m^3 . The reactor is 1 m in length with a radius of $R_a=0.1 \text{ m}$.

To save time you can copy and paste the model given below. Make sure there are no mistakes in this model.

```
d(FA)/d(V) = rA # molA/m^3
rA = -k * 1500 * (cA * cB - cC ^ 2 / Keq) # molA/m^3/s
d(FC)/d(V) = -2 * rA
FC(0) = 0
d(FB)/d(V) = rA
FB(0) = .25
FA(0) = 0.25
cA = FA / flow
cB = FB / flow
cC = FC / flow
delH = -83680
Keq = 1000 * exp(delH / 8.314 * (1 / 303 - 1 / T))
L = V / (pi * 0.1 ^ 2)
pi = 3.14159265359
k = 1.1e8 * exp(-95238 / 8.314 / T)
T0 = 320
flow = 5e-4 # m^3/s
FT = FA + FB + FC
T = T0
FT0 = 0.5
X = (0.25 - FA) / 0.25
V(0) = 0
V(f) = 0.03141
```

- 1) Calculate the Reynolds number of this flow if the average density is 1000 kg/m^3 and viscosity is 0.0016 kg/(m s) .
- 2) Submit a POLYMATH model of this process. Plot the molar flowrates and the 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

$$u_z = 2 * u_0 \left(1 - \left(\frac{r}{R_a}\right)^2\right) \quad (11)$$

With the average velocity or superficial velocity given by

$$u_0 = \frac{5 \times 10^{-4} \text{ m}^3/\text{s}}{\pi R_a^2} \quad (12)$$

The manual explaining today's tutorial is located on the webct.rowan.edu page under the heading **3.1 FEMLAB ECRE Manual. This manual is also on the CD that came with you textbook.** I have attached the appropriate pages from the manual that you need to skim in several pages following this one. 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.

1. Quickly review the model description on the following pages and make a sketch of the geometry and the boundary conditions for this geometry.

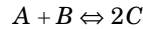
FEMLAB[®] 3

FEMLAB ECRE

VERSION 3.1

Model Description, Equations, and Input Data

This chapter uses the FEMLAB ECRE Version to study an elementary, exothermic, 2nd-order reversible reaction



in a tubular reactor (liquid phase, laminar flow regime). To keep its temperature down, the reactor uses a cooling jacket with a variable coolant temperature. The following model setup proceeds in stages, gradually leading to the final configuration. The first version of the model deals with an isothermal tubular reactor with composition variations in both the radial and axial directions. The second stage extends the model to include the energy balance for the reactor. By this addition, the isothermal reactor is turned into an adiabatic reactor. The third stage introduces an isothermal cooling jacket, and finally the fourth stage models a non-isothermal cooling jacket.

The following section provides a general description for all of the above-mentioned models.

Model Description

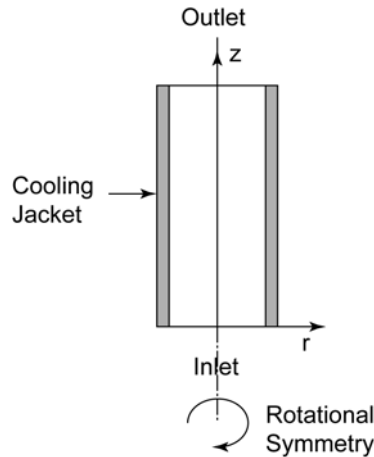


Figure 2-1: Model geometry for the 2-dimensional rotationally symmetric models.

Figure 2-1 illustrates the model geometry. We assume that the variations in angular direction around the central axis are negligible, and therefore the model can be axi-symmetric.

The system is described by a set of differential equations on a 2D surface that represents a cross section of the tubular reactor in the z - r plane. That 2D surface's borders represent the inlet, the outlet, the reactor wall, and the center line. Assuming that the diffusivity for the three species is of the same magnitude, you can model the reactor using three differential equations; one mass balance for one of the species (as noted in the next section, mass balances are not necessary for the other two species), one heat balance for the reactor core, and one heat balance for the heating jacket. Due to rotational symmetry, the software need only solve these equations for half of the domain shown in Figure 2-1.

Model Equations

You describe the mass balances and heat balances in the reactors with partial differential equations (PDEs), while one ordinary differential equation (ODE) is required for the heat balance in the cooling jacket. The equations are defined as follows.

MASS BALANCE, SPECIES A:

$$D_p \frac{1}{r} \frac{\partial C_A}{\partial r} + D_p \frac{\partial^2 C_A}{\partial r^2} + D_p \frac{\partial^2 C_A}{\partial z^2} - 2U \left(1 - \left(\frac{r}{R} \right)^2 \right) \frac{\partial C_A}{\partial z} + r_A = 0$$

where D_p denotes the diffusion coefficient, C_A is the concentration of species A, U is the flow velocity, R gives the radius of the reactor, and r_A is the reaction rate. In this model we assume that the species A, B, and C have the same diffusivity, which implies that we must solve only one material balance; we know the other species' concentrations through stoichiometry.

BOUNDARY CONDITIONS FOR THE MASS BALANCE:

- Inlet ($z = 0$)

$$C_A(r, 0) = C_{A0}$$

- At the wall ($r = R$)

$$\frac{\partial C_A}{\partial r}(R, z) = 0$$

- Center (symmetry) line

$$\frac{\partial C_A}{\partial r}(0, z) = 0$$

The boundary condition selected for the outlet does not set any restrictions except that convection dominates transport out of the reactor. Thus this condition keeps the outlet boundary open and does not set any restrictions on the concentration.

- Outlet ($z = L$)

$$\frac{\partial C_A}{\partial z}(r, L) = 0$$

where L denotes the length of the reactor.

ENERGY BALANCE INSIDE THE REACTOR:

$$k \frac{1}{r} \frac{\partial T}{\partial r} + k \frac{\partial^2 T}{\partial r^2} + k \frac{\partial^2 T}{\partial z^2} - 2U \left(1 - \left(\frac{r}{R} \right)^2 \right) \rho C_p \frac{\partial T}{\partial z} - r_A (-\Delta H_{Rx}) = 0$$

where k denotes the thermal conductivity, T is temperature, ρ is density, C_p equals the heat capacity, and ΔH_{Rx} is the reaction enthalpy.

BOUNDARY CONDITIONS FOR THE ENERGY BALANCE:

- Inlet ($z = 0$)

$$T(r, 0) = T_0$$

- At the wall ($r = R$)

$$-\frac{\partial T}{\partial r}(R, z) = \frac{U_k}{k}(T - T_a)$$

where T_a denotes the temperature in the cooling jacket.

- Center (symmetry) line

$$-\frac{\partial T}{\partial r}(0, z) = 0$$

As for the mass balance, choose the boundary condition at the outlet for the energy balance such that it keeps the outlet boundary open. This condition sets only one restriction, that the heat transport out of the reactor be convective.

- Outlet ($z = L$)

$$-\frac{\partial T}{\partial z}(r, L) = 0$$

ENERGY BALANCE OF THE COOLANT IN THE COOLING JACKET:

Here we assume that only axial temperature variations are present in the cooling jacket. This assumption gives a single ODE for the heat balance:

$$\frac{\partial T_a}{\partial z} = \frac{2\pi R U_k (T - T_a)}{m_c C_{Pc}}$$

where m_c is the mass flow rate of the coolant, C_{Pc} represents its heat capacity, and U_k gives the heat-transfer coefficient between the reactor and the cooling jacket. You can neglect the contribution of heat conduction in the cooling jacket and thus assume that heat transport takes place only through convection.

BOUNDARY CONDITION FOR THE COOLING JACKET:

You can describe the cooling jacket with a 1D line. Therefore you need only an inlet boundary condition.

- Inlet ($z = 0$)

$$T_a(0) = T_{a0}$$

Model Parameters

We now list the model's input data. You define them either as constants or as logical expressions in FEMLAB's **Option** menu. In defining each parameter in FEMLAB, for the constant's **Name** use the left-hand side of the equality in the following list (in the first entry, for example, **Diff**), and use the value on the right-hand side of the equality (for instance, **1E-9**) for the **Expression** that defines it.

The constants in the model are:

- Diffusivity of all species, **Diff** = **1E-9** m²/s
- Activation energy, **E** = **95238** J/mol

- Rate constant, $A = 1.1 \text{E}8 \text{ m}^6/(\text{mol}\cdot\text{kg}\cdot\text{s})$
- Gas constant, $R = 8.314 \text{ J/mol}\cdot\text{K}$ (do not confuse this constant with the geometrical extension of the radius)
- Inlet temperature, $T_0 = 320 \text{ K}$
- Total flow rate, $v_0 = 5 \text{ E-}4 \text{ m}^3/\text{s}$
- Reactant concentrations in the feed, $CA_0 = CB_0 = 500 \text{ mol/m}^3$
- Reactor radius, $Ra = 0.1 \text{ m}$
- Catalyst density, ρ_{Cat} , $\rho_{\text{Cat}} = 1500 \text{ kg/m}^3$
- Heat of reaction, $\Delta H_{R,x}$, $dH_{R,x} = -83680 \text{ J/mol}$
- Equilibrium constant at 303 degrees K, $Keq_0 = 1000$
- Thermal conductivity of the reaction mixture, $ke = 0.559 \text{ J/m}\cdot\text{s}\cdot\text{K}$
- Average density of the reaction mixture, ρ , $\rho = 1000 \text{ kg/m}^3$
- Heat capacity of the reaction mixture, $Cp = 4180 \text{ J/kg}\cdot\text{K}$
- Overall heat-transfer coefficient, $Uk = 1300 \text{ J/m}^2\cdot\text{s}\cdot\text{K}$
- Inlet temperature of the coolant, $Ta_0 = 298 \text{ K}$
- Heat capacity of the coolant, $CpJ = 4180 \text{ J/kg}\cdot\text{K}$
- Coolant flow rate, $mJ = 0.01 \text{ kg/s}$

Next, the following section lists the definitions for the expressions this model uses. Again, to put each expression in FEMLAB form, use the left-hand side of the equality (for instance, u_0) for the variable's **Name**, and use the right-hand side of the equality (for instance, $v_0 / (\pi \cdot Ra^2)$) for its **Expression**.

- The superficial flow rate is defined according to the analytical expression

$$u_0 = \frac{v_0}{\pi(Ra)^2}$$

which we define in FEMLAB as $u_0 = v_0 / (\pi \cdot Ra^2)$.

- The superficial, laminar flow rate

$$u_z = 2u_0 \left(1 - \left(\frac{r}{Ra} \right)^2 \right)$$

in FEMLAB form becomes $uz = 2 \cdot u_0 \cdot (1 - (r/Ra)^2)$.

- The conversion of species A is given by

$$x_A = \frac{C_{A0} - C_A}{C_{A0}}$$

which in FEMLAB form is $x_A = (cA0 - cA) / cA0$.

- The concentration of B is according to

$$C_B = C_{B0} - C_{A0} x_A$$

which in FEMLAB form becomes $cB = cB0 - cA0 * xA$.

- The concentration of C is expressed as

$$C_c = 2C_{A0} x_A$$

which in FEMLAB form becomes $cC = 2 * cA0 * xA$.

- The rate of reaction takes two forms:
 - Before adding the heat balance, the reaction looks like

$$r_A = -A \exp\left(-\frac{E}{RT_0}\right) \rho_{cat} \left(c_A c_B - \frac{c_c^2}{K_{eq}} \right),$$

which in FEMLAB form is $rA = -A * \exp(-E/R/T0) * \rho cat * (cA * cB - cC^2/Keq)$.

- After you add the energy balance, the reaction expression becomes

$$r_A = -A \exp\left(-\frac{E}{RT}\right) \rho_{cat} \left(c_A c_B - \frac{c_c^2}{K_{eq}} \right),$$

which in FEMLAB form is $rA = -A * \exp(-E/R/T) * \rho cat * (cA * cB - cC^2/Keq)$.

- The temperature-dependent equilibrium constant is given by the following expressions:
 - For the isothermal case

$$K_{eq} = K_{eq0} \exp\left(\frac{\Delta H_{Rx}}{R} \left(\frac{1}{303} - \frac{1}{T_0} \right)\right)$$

which in FEMLAB form is $Keq = Keq0 * \exp(dHrx/R * (1/303 - 1/T0))$.

- After adding the energy balance you obtain

$$K_{eq} = K_{eq0} \exp\left(\frac{\Delta H_{Rx}}{R} \left(\frac{1}{303} - \frac{1}{T}\right)\right)$$

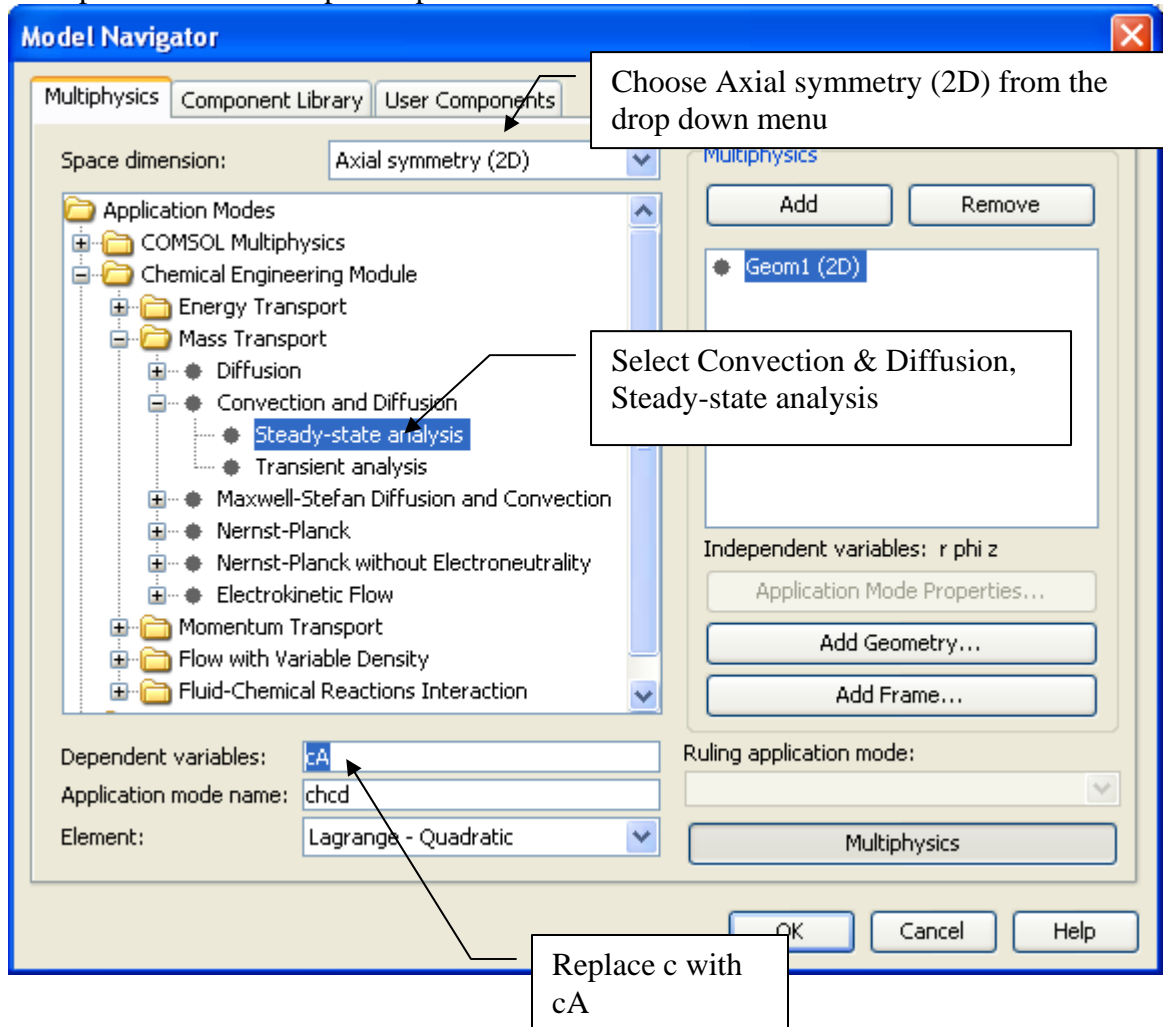
which in FEMLAB form is $Keq = Keq0 * \exp(dHrx/R * (1/303 - 1/T))$.

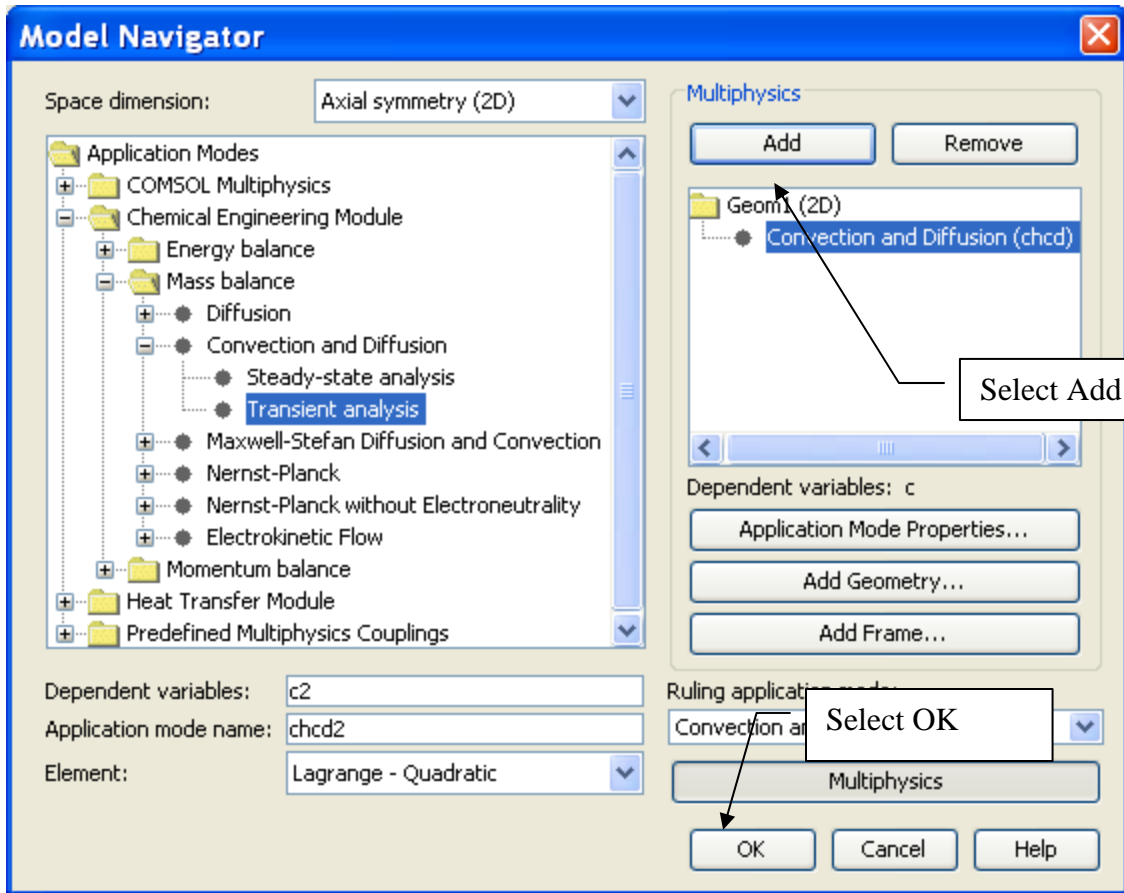
- The heat-production term becomes

$$Q = -r_a \Delta H_{Rx}$$

which in FEMLAB form is $Q = -rA*dHrx$.

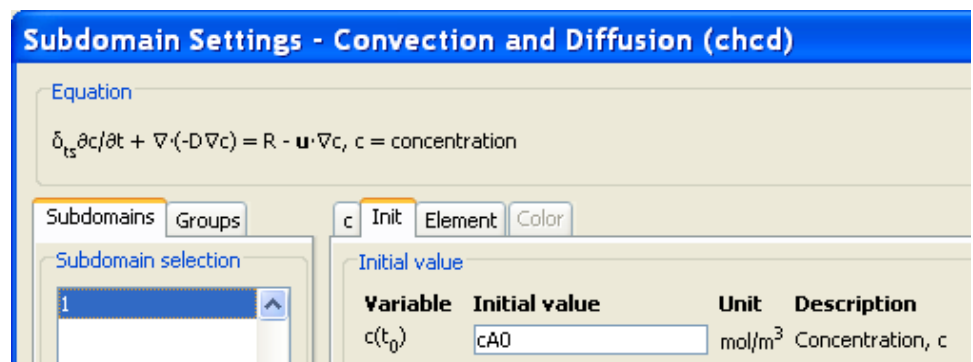
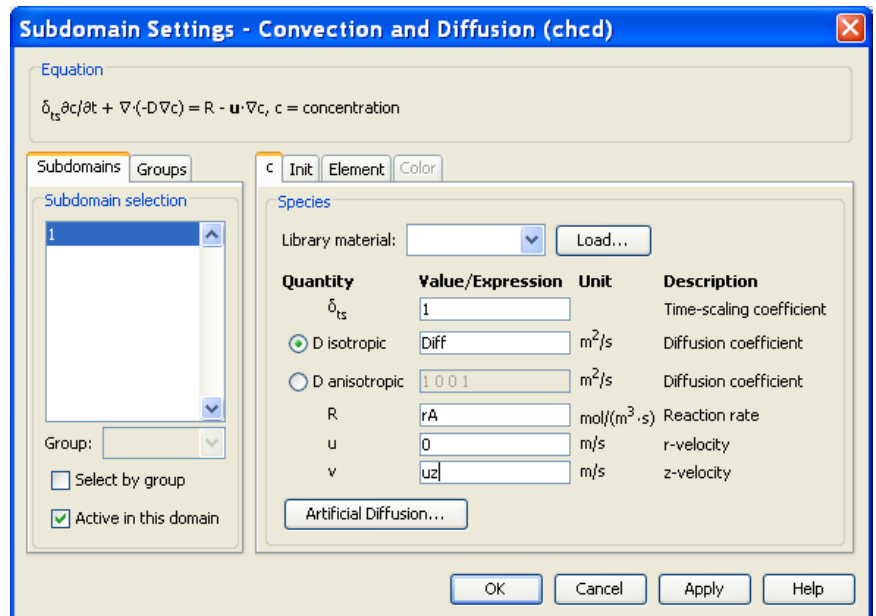
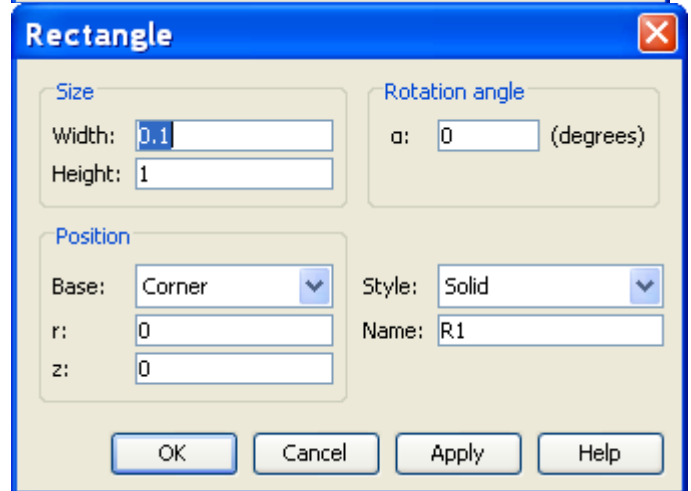
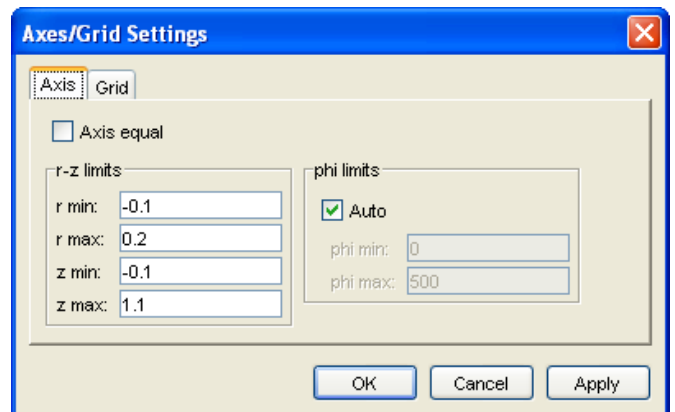
2. Open Comsol Multiphysics 3.4, Select the New Tab, Choose Axial symmetry (2D).
3. Choose Chemical Engineering Module, Mass balance, Convection and Diffusion, Steady-state analysis.
4. In the Dependent variables space replace the c with cA



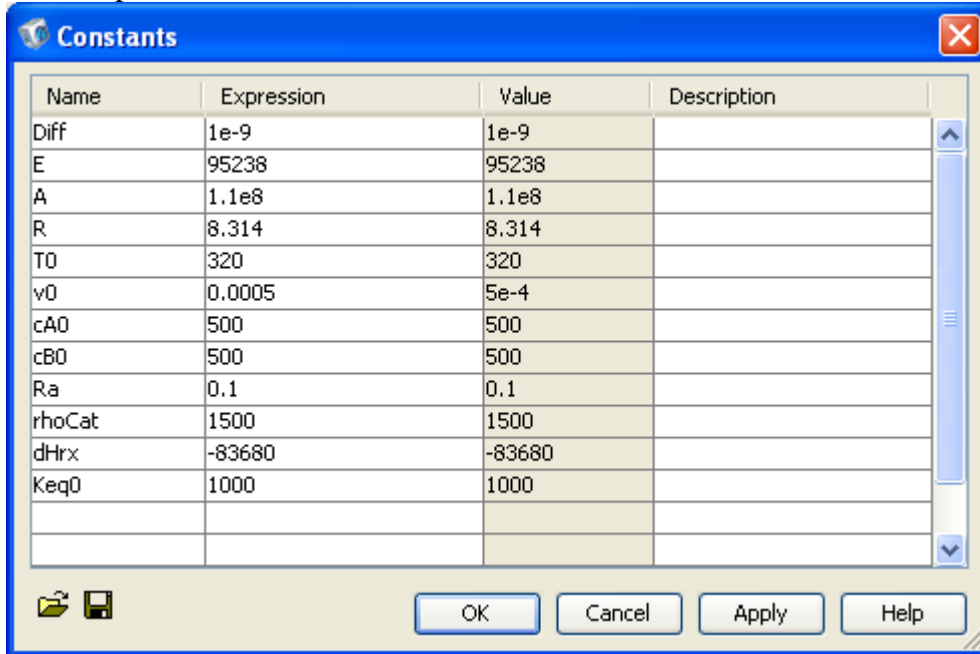


5. Select Add
6. Select OK
7. Now you must draw the geometry of a tube in COMSOL. This is a rectangle. Remember that the center of the pipe is at a radial position of 0 and the wall of the pipe is at a dimension of 0.1m. The length of pipe will be set at 1m.

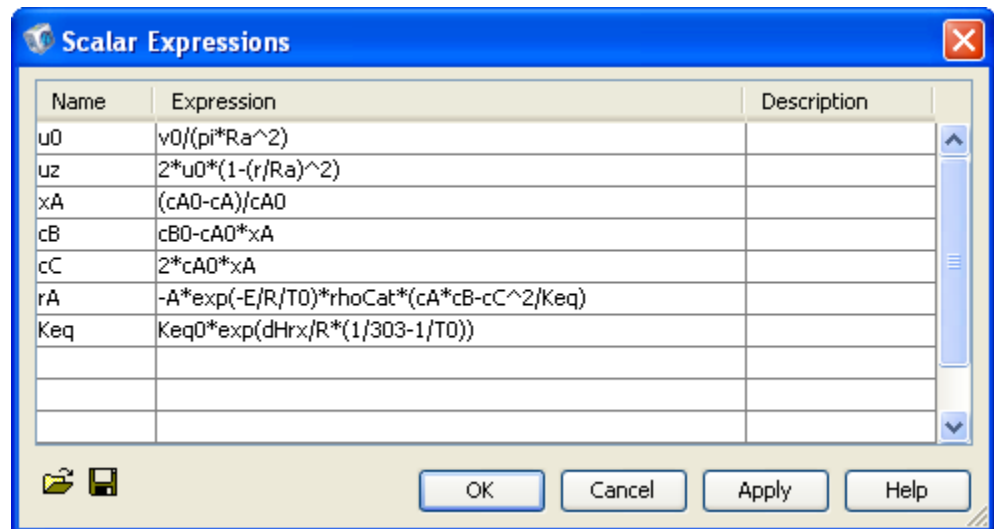
8. For this model the length of the reactor is much longer than radius. To see the trends in both directions a set of unequal axes can be obtained. To obtain an “unequal” axes setting, Choose Options, Axis/Grid settings and select the Axis tab and then clear the Axis equal check box. Enter -0.1 in the 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. To obtain a Grid spacing of 0.1 go to the Grid tab and click on the Auto box. Change the settings to 0.1 and 0.1. Then Click OK
9. Now draw the rectangle that represents half of a reactor. (eg. from r=0 to r=0.1m and z=0 to z=1.0m.
10. Go to the Physics menu and select Subdomain Settings, which opens up the corresponding dialog box. Select subdomain 1 in the Subdomain Settings list. This dialog box displays the equation that forms the basis for this application mode, while the edit fields show the input data used in the equation.
11. Now choose Physics, subdomain Settings and select subdomain 1. Enter Diff, rA, 0 and uz as shown in the figure below. The edit fields correspond to the diffusion coefficient, reaction-rate expression, and velocity distribution in the reactor—all of which you can freely define. To review and change the definition of the input data, follow this procedure
12. Select the Init tab (this sets the initial conditions for the reactor) Now enter cA0 in the initial value box.



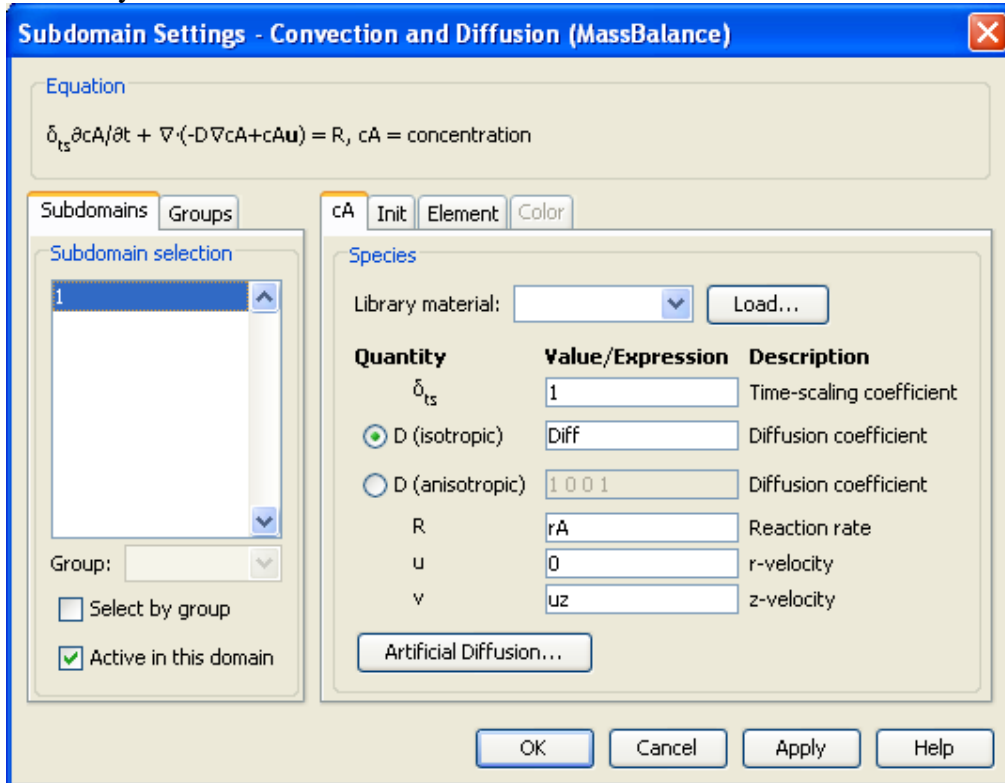
13. Select Options, Constants and then enter Constants –



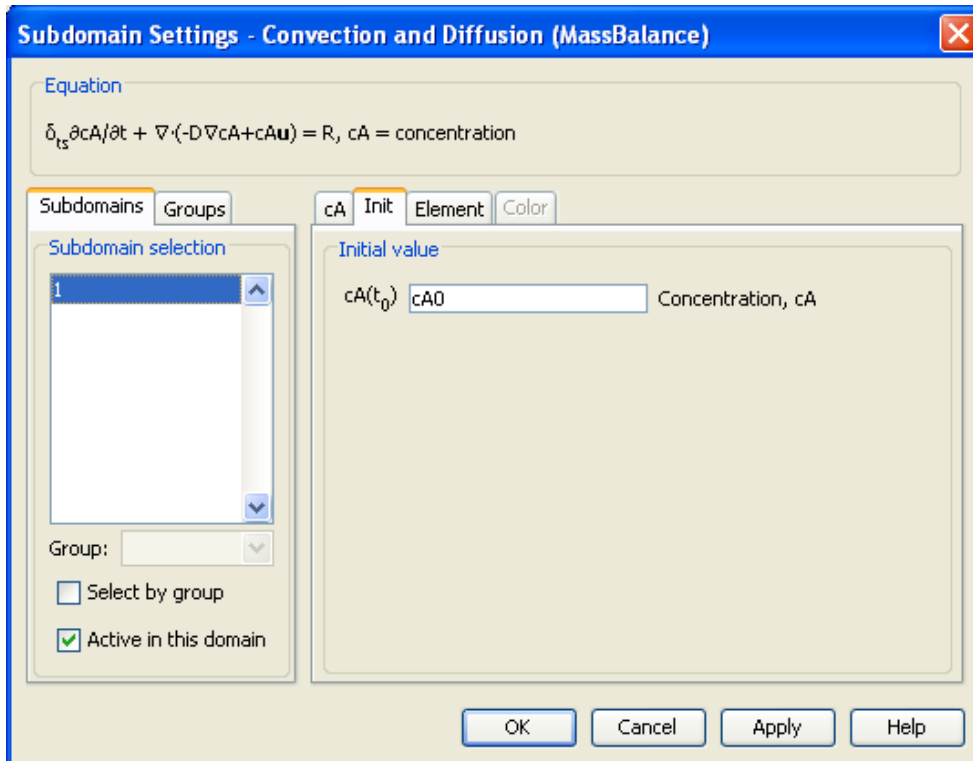
14. Select Options, Scalar Expressions and enter the following expressions. Some of these expressions will be used in later models.



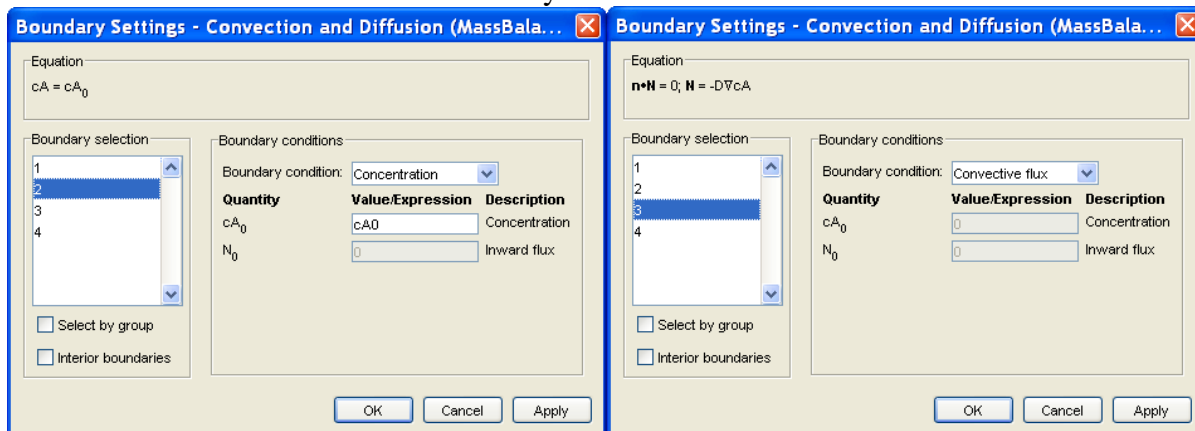
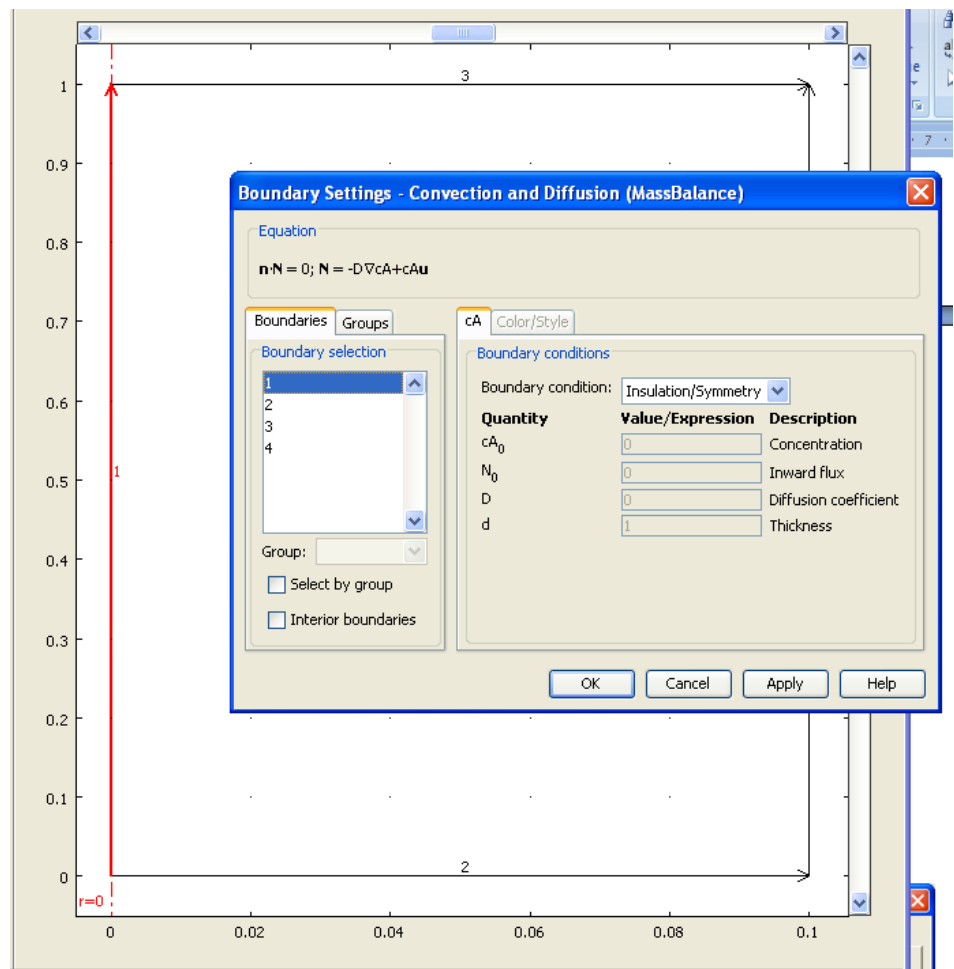
- Go to the **Physics** menu and select **Subdomain Settings**, which opens up the corresponding dialog box. Select subdomain 1 in the Subdomain Settings list. Enter the reaction rate r_A , the z -velocity and the diffusion coefficient $Diff$



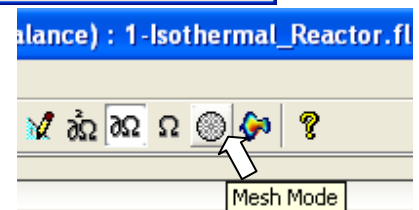
- Go to the **Init** tab and enter the initial concentration variable c_{A0} and then select **OK**



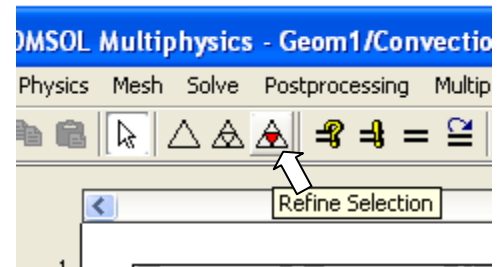
17. Go to the **Physics** menu and select **Boundary Settings**. Enter the boundary conditions, insulation for 1 and 4 which corresponds to no flow of mass through the wall and the centerline ($r=0$). You can click on the figure to verify which boundary is 1 and which is 4. The boundary that you click on turns red and the number in the boundary settings selection menu is highlighted in blue. Then give the concentration of A entering the reactor, cA_0 , at the inlet boundary 2 and specify a convective flux for the reactor outlet 3. This term means that fluid will flow out of the reactor at boundary 3.



18. Now create a mesh. Go to the Mesh mode by pressing the mesh mode button.
19. Select Mesh, Initialize Mesh. This will automatically create a mesh for you.



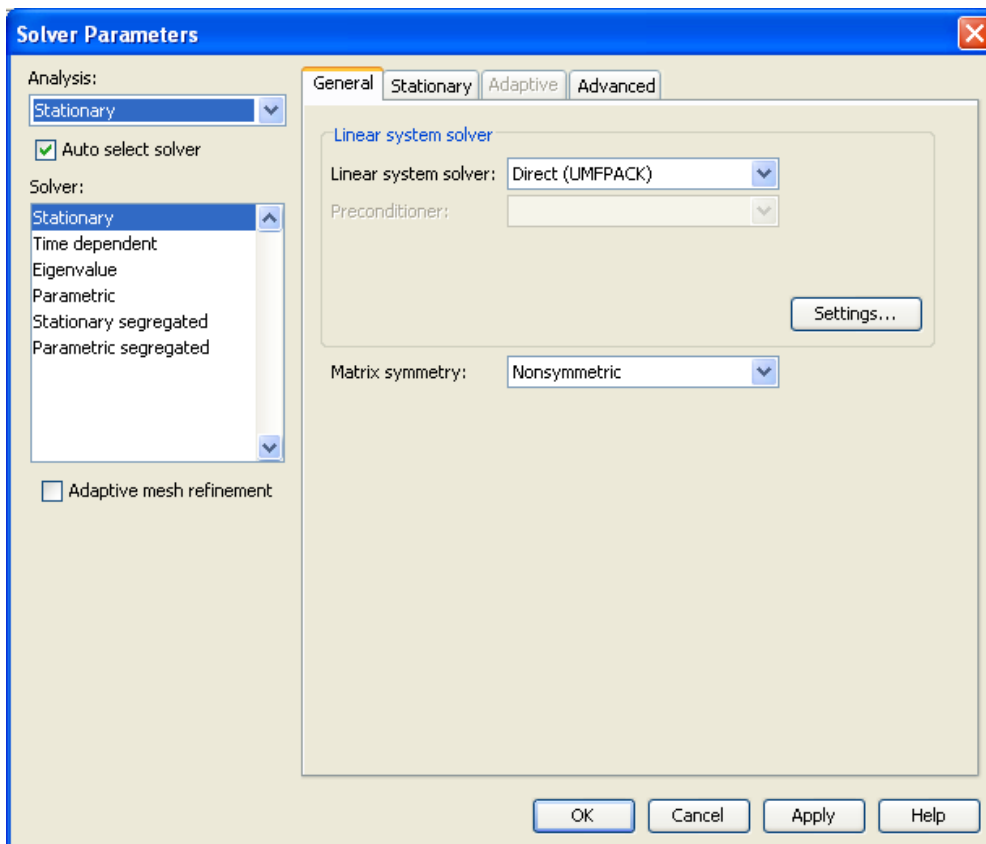
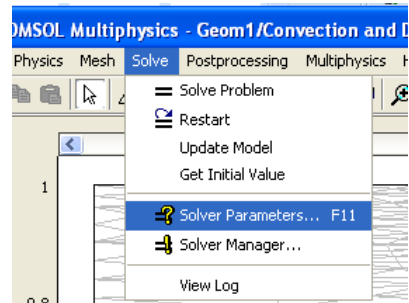
20. You should probably refine this mesh by choosing the Mesh, Refine Mesh option. Notice the short cut figure for later refining of the mesh. To obtain the images that are shown later you will need to refine certain areas of the mesh. This can be done by choosing the Mesh, Refine Selection button or option.



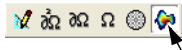
21. Note in this case that the scales on the r- and z-axes are not equal, which gives a distorted view. If desired, you can select equal scale settings in the Axis/Grid Settings menu item under the Options menu. In order to return to the original unequal scale settings, once again go to the Axes/Grid 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.

22. The model in this exercise is nonlinear; thus press the Solver Parameters and verify that the Stationary nonlinear solver is selected.

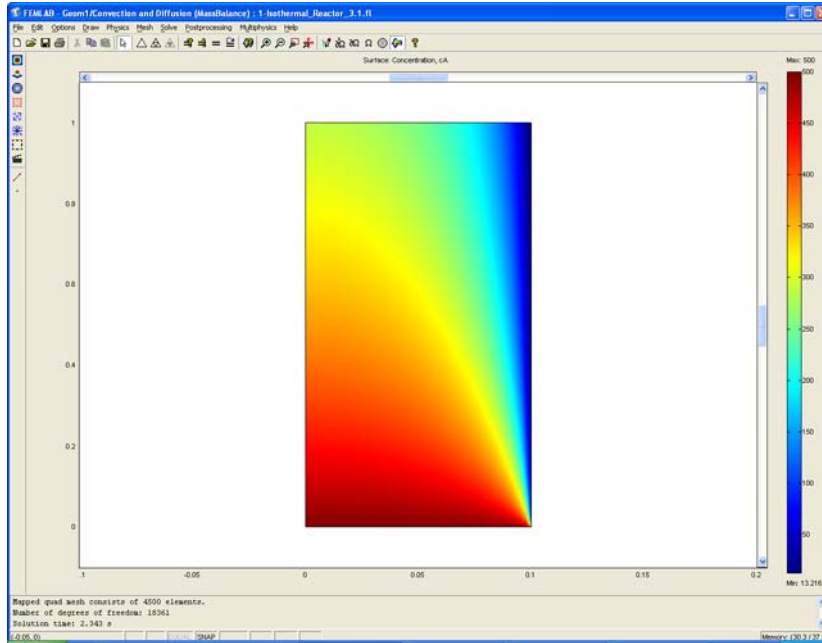
23. Solve the problem using the Solve Problem button or drop down menu.



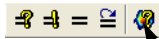
- 1 Click the **Postprocessing Mode** button. The default plot shows the concentration of species A in the reactor.



Postprocessing Mode



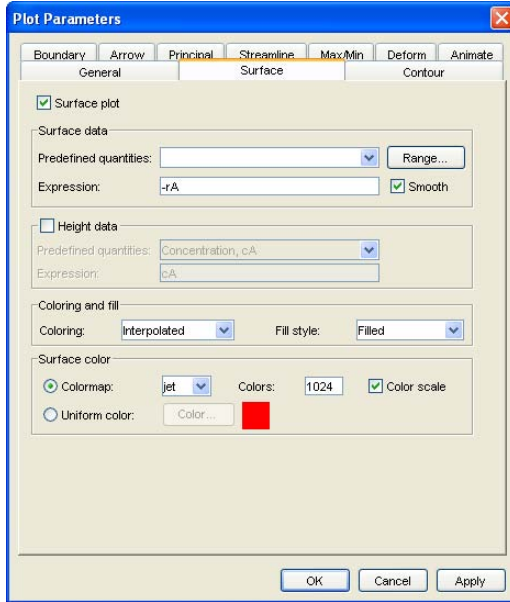
- 2 Click the **Plot Parameters** button.



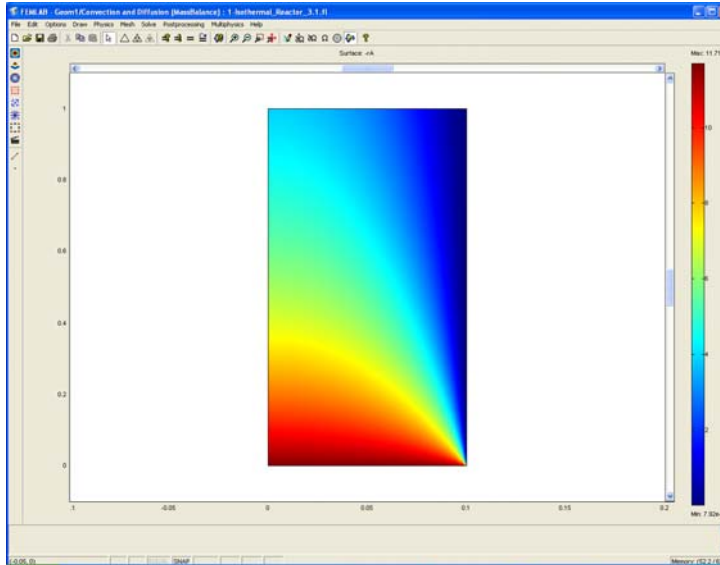
Plot Parameters

- 3 Click on the **Surface** tab.

4 On the **Surface** page, enter $-r_A$ in the **Expression** edit field.

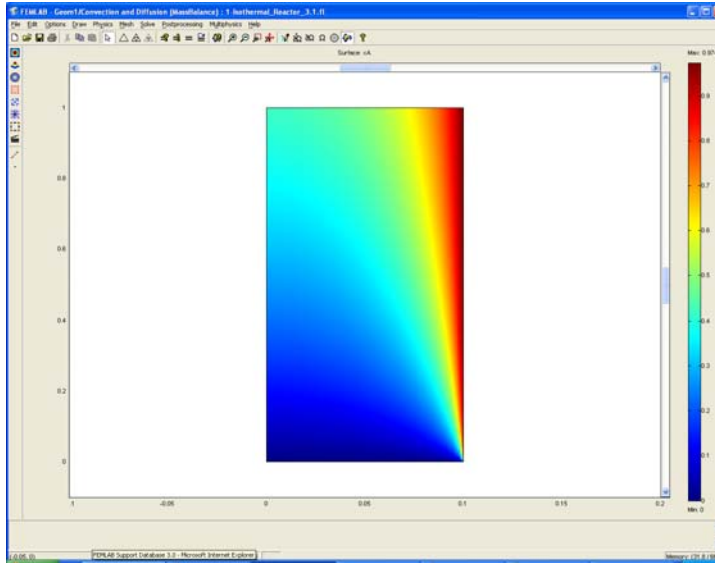


5 Click **Apply**.



6 To plot the conversion of species A, enter x_A in the **Expression** edit field in the **Plot Parameters** dialog box.

7 Click **Apply**.



8 In order to define the location of the maximum and minimum conversion, click the **Max/Min** tab.

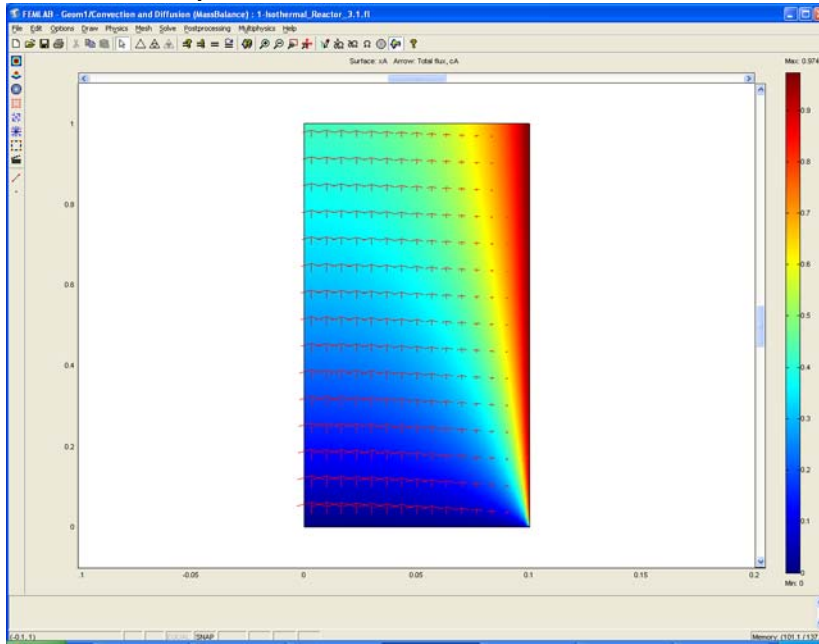
9 Enter x_A in the **Expression** edit field in the **Subdomain max/min data** dialog box.

10 Click the **Max/min marker** check box and click **Apply**.

11 To visualize the relation between residence time and conversion, first click the **Max/min marker** check box to deselect it and click the **Arrow** tab in the **Postprocessing** menu.

12 Select **Total flux, c_A** in the **Predefined quantities** drop-down list.

B Click the **Arrow plot** check box and click **OK**.



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

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

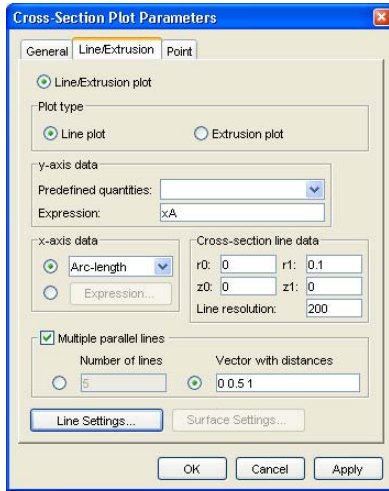
16 Enter x_A in the **Expression** edit field.

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

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

19 Check the **Multi parallel lines** box, then click the **Vector with distances** option.

20 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.



21 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.



See note on making graphs on page 27 of 31 of this pdf file step 15 and then return

22 Finally, to generate the following plot, click **OK** twice: first in the **Line Settings** dialog box, and then in the **Cross-Section Plot Parameters** dialog box.

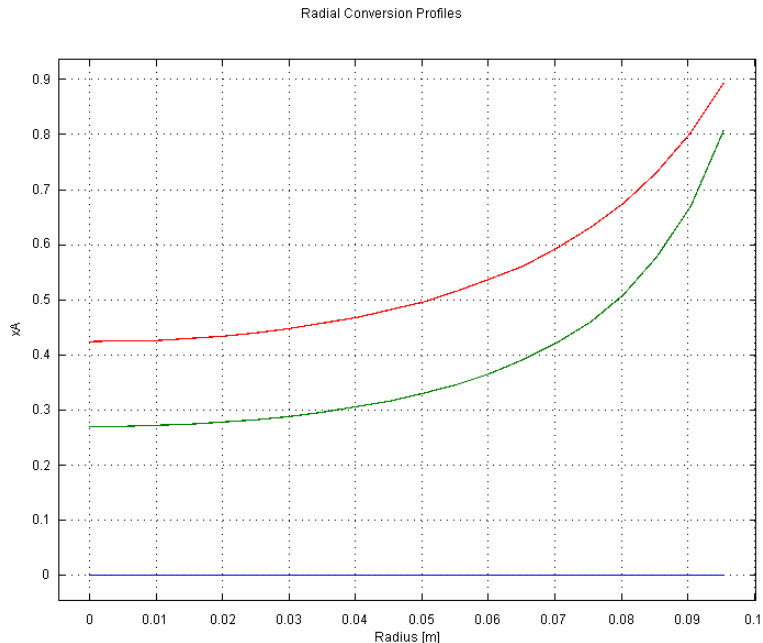
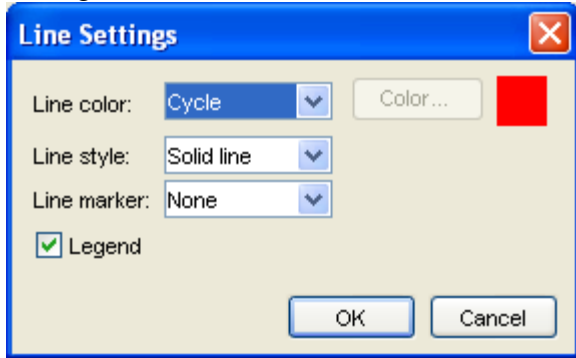


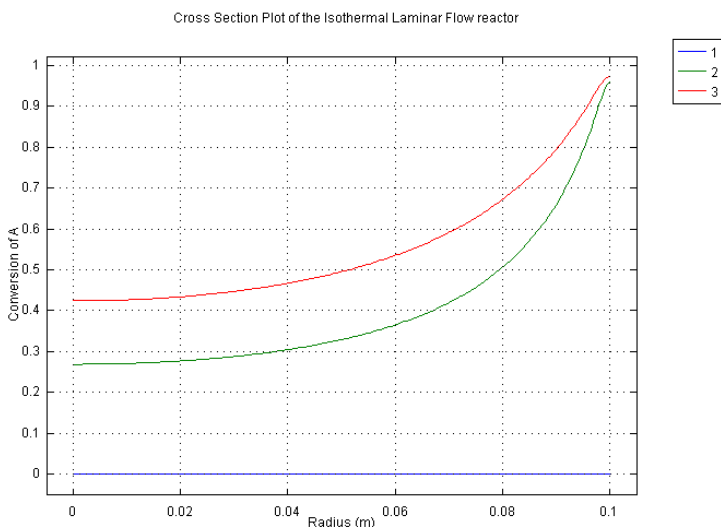
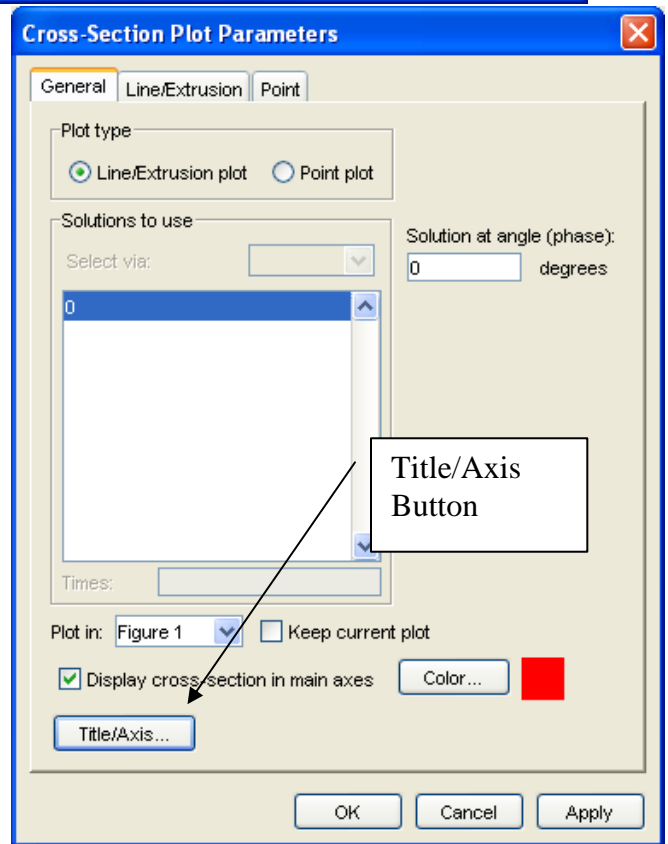
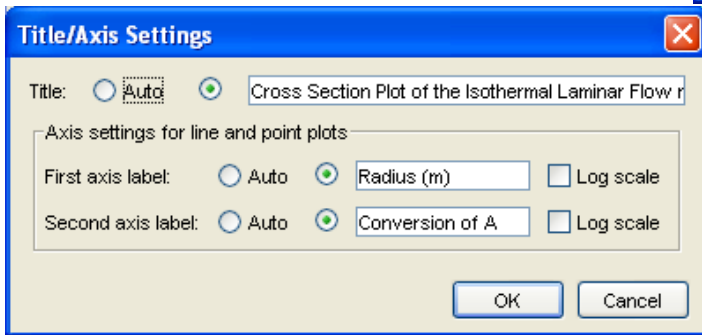
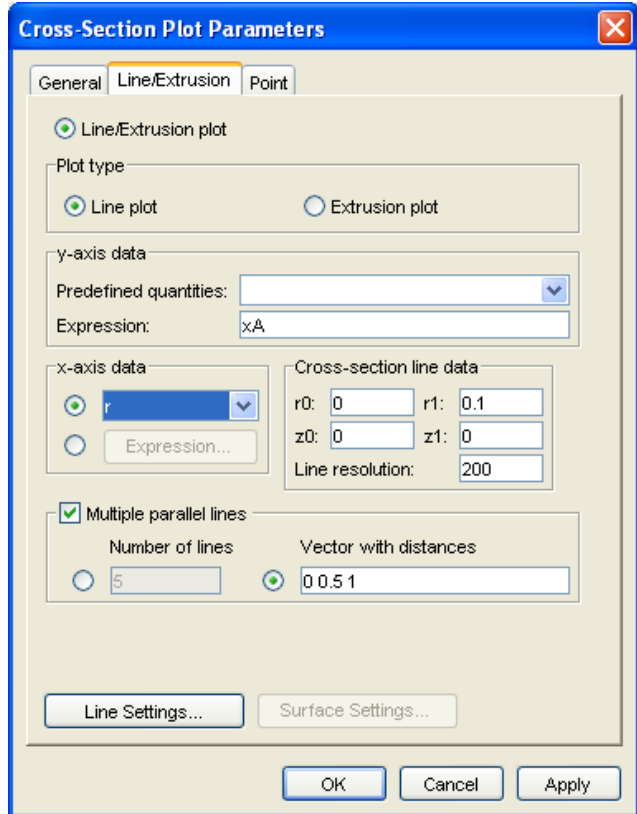
Figure 2-2: Radial conversion profiles at the inlet, outlet and halfway through an isothermal reactor.

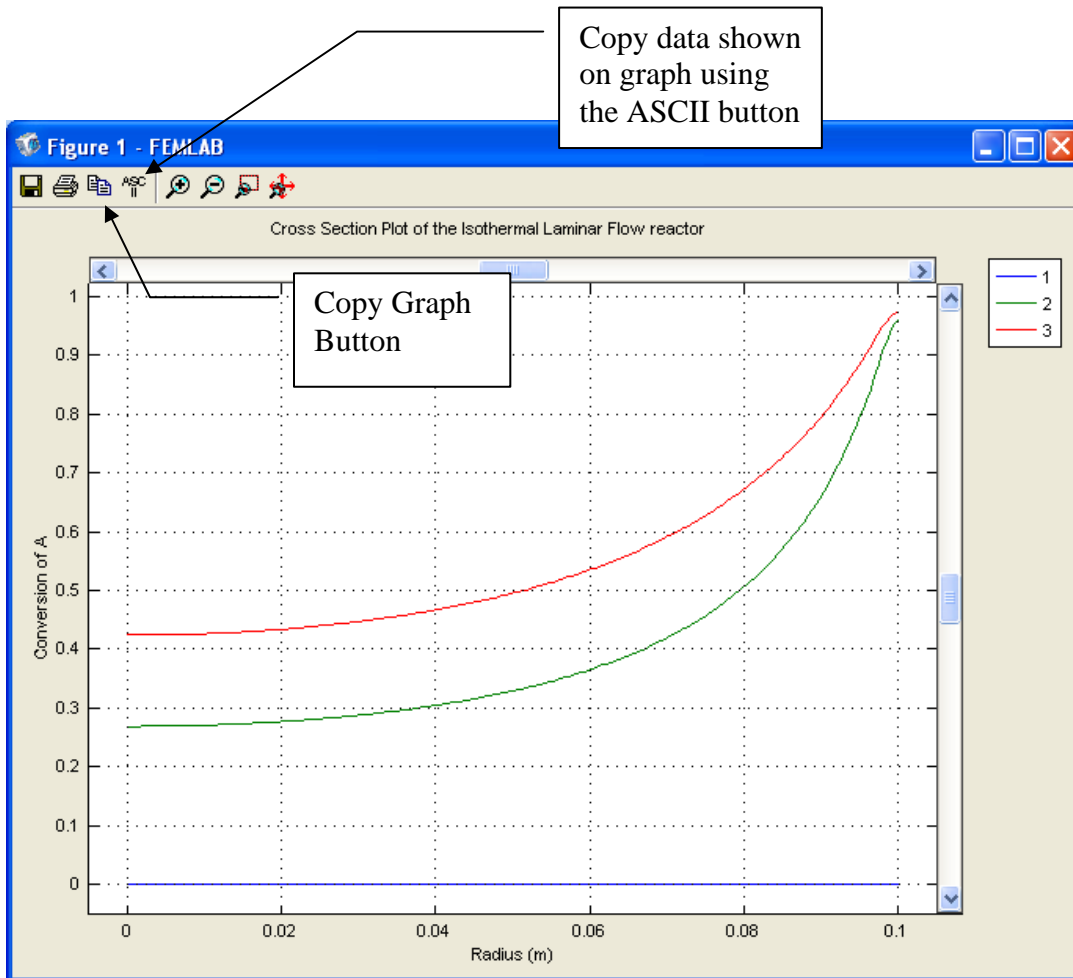
24. In Step 22 of the pdf file it asked you to make a Cross-Section plot. I prefer to use as the x-axis data the r coordinate. Also in the line Settings box I always request a legend.



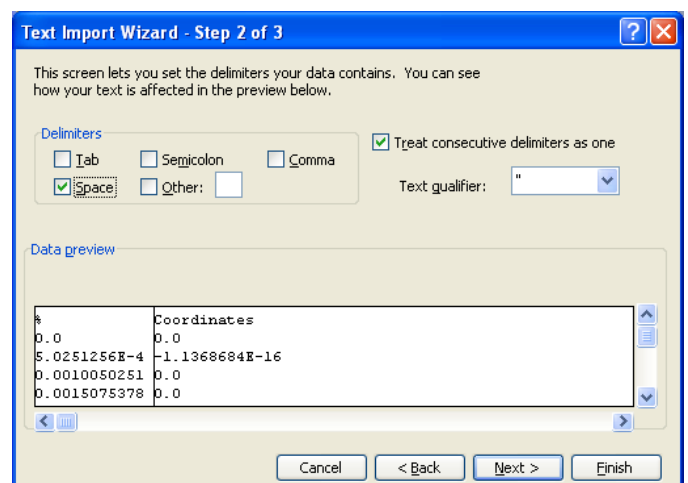
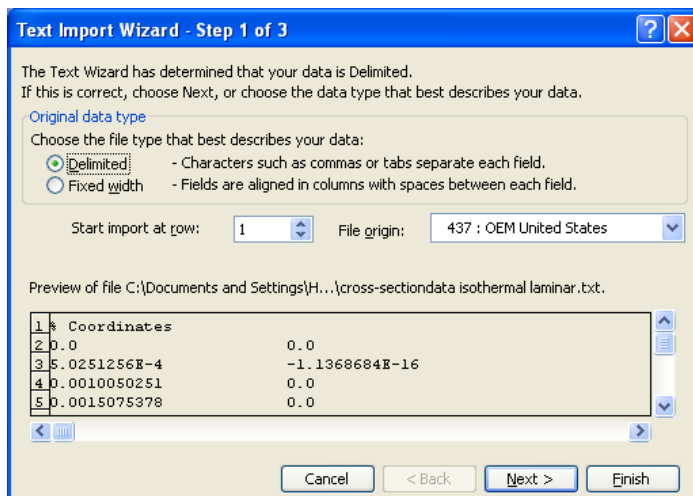
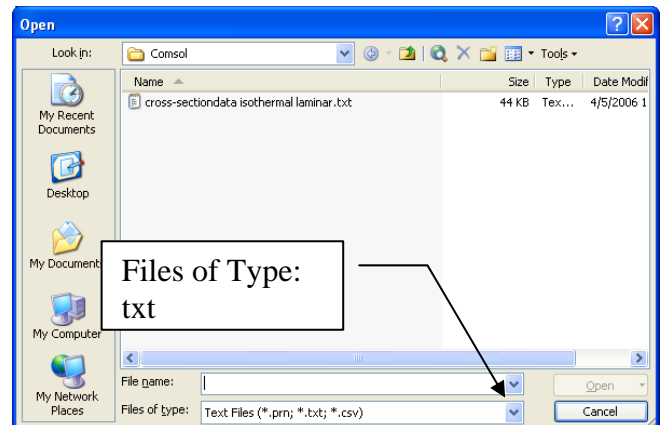
25. Also a title to the graph as well as axis labels can be specified. Select the General tab and the Title/Axis button.

26. This plot can now be pasted into a word document by selecting the MS windows copy icon.





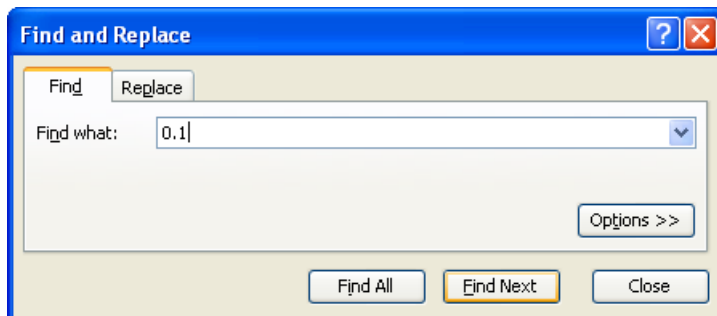
27. To obtain a table of data shown on the cross section plot then you must click on the ASCII button and then save this file.
28. The file will be a text file that can be opened by excel for further analysis. Open the txt file by having excel look for text files.
29. Then start the conversion of the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



30. The data is placed in two columns (x,y). The first cross-section at $z=0\text{m}$ is listed, followed by the second cross-section $z=0.5\text{m}$, followed by the third cross-section at $z=1.0\text{m}$. 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			



FEMLAB ECRE can also calculate integral expressions of the solution. One such entity is the mixing cup outlet concentration, which gives the average concentration in the liquid that exits the reactor. For species A, the average concentration is defined according to the equation

$$C_{A,av} = \frac{\int_{outlet} 2\pi r C_A u_z dr}{\int_{outlet} 2\pi r u_z dr}$$

along the outlet boundary. Start by calculating the integral of $C_A u_z$ over the outlet boundary.

- 23** Go to the **Postprocessing** menu and select **Boundary Integration**.
- 24** Select boundary 3 in the **Boundary selection** list.

25 Enter $2\pi r c_A u_z$ in the **Expression** edit field.

26 Click **Apply**.

The value of the integral appears in the status bar at the bottom and reads 0.114385. You can now calculate the integral of u_z .

27 Enter $2\pi r u_z$ in the **Expression** edit field and click **Apply**.

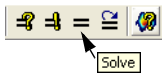
The value of this integral is $5e-4$, which gives an average concentration of $0.114385/5e-4$, which is approximately 230 mole m^{-3} .

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

Questions and Exercises

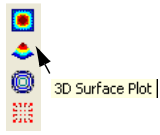
To answer the following questions you can either use the results in the model just described or you can solve it again with a new set of input data.

- 1** Why is the concentration of species A near the reactor wall lower than the concentration near the center?
- 2** Where in the reactor do you find the minimum and maximum reaction rates?
- 3** How much is the average conversion? (Hint: See the calculation of the average concentration in the previous section.)
- 4** This exercise requires that you change the activation energy for the reaction in the model. Do so by going to the **Options** menu and working with the **Constants** menu item (see item 5 in the section “Model Equations and Input Data” on page 21). We have already tabulated the notations in the section “Model Parameters” on page 15. After changing the input data, click the **Solve** button to solve the problem.



It is useful to take the graphs you obtain by changing the activation energy and examine them in both two and three dimensions. Once in the Postprocessing mode

you can toggle between a two- and three-dimensional plot by clicking the **2D Surface Plot** button or **3D Surface Plot** button.



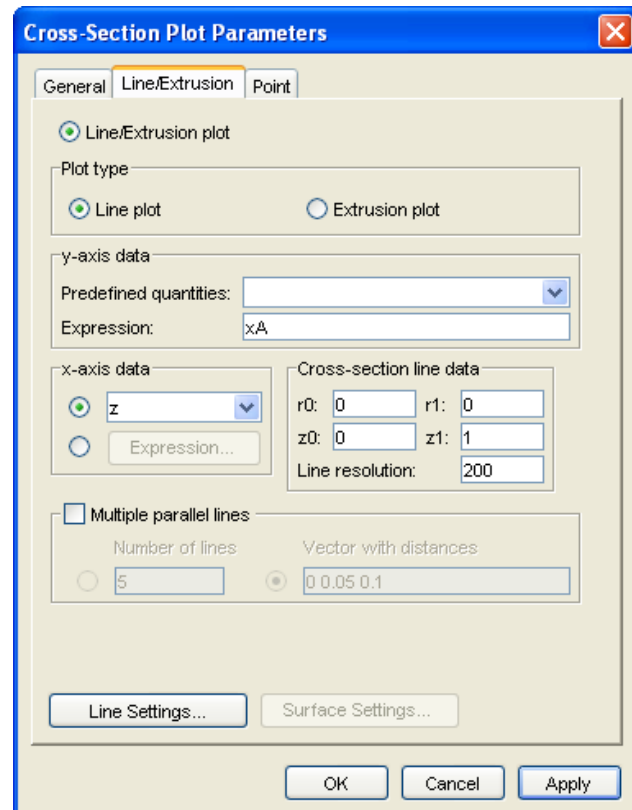
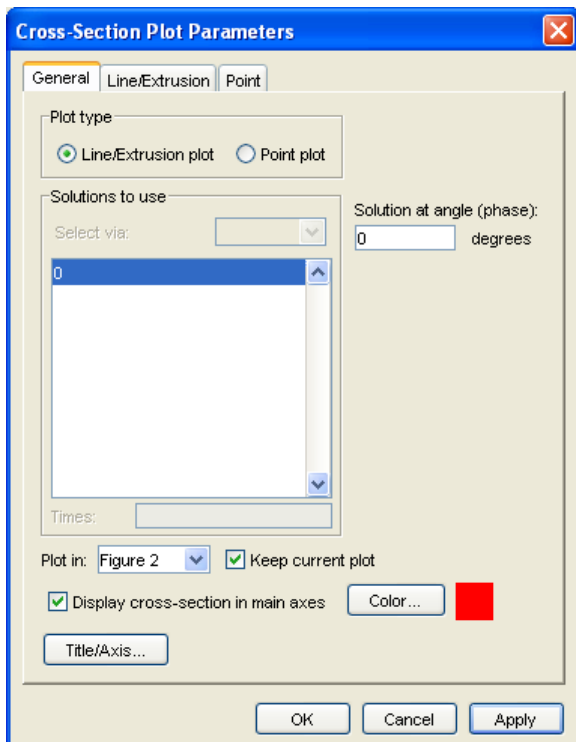
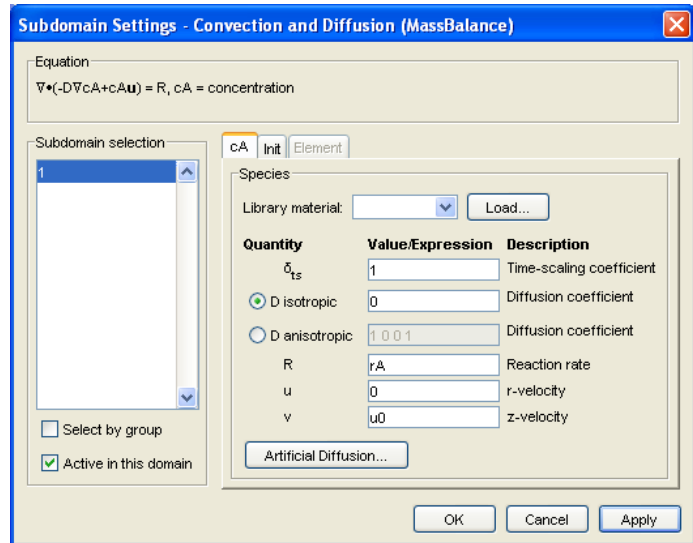
- a How do the conversion profiles and the average conversion change if you increase the activation energy by a factor of 1.5?
- b How do these same entities change if you decrease the activation energy by multiplying the original value by a factor of 0.95?

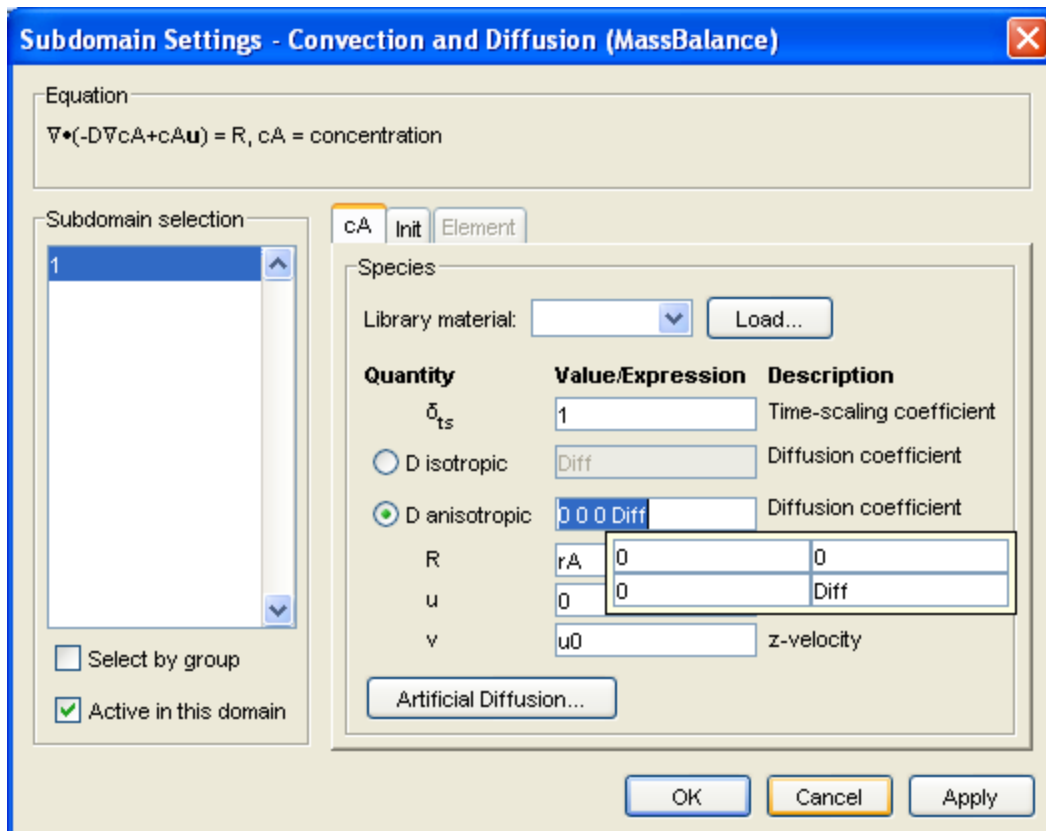
The reaction rate is very sensitive to changes in activation energy. Altering the activation energy to a lower value increases the reaction rate. A high reaction rate in combination with the low flow rate close to the wall results in very large concentration gradients. In order to capture an accurate concentration profile, you must apply a dens mesh in the inlet area near the wall.

You have now investigated the isothermal reactor example. Let's proceed by introducing the energy balance in the reactor.

To be Submitted:

- 1) POLYMATH model and requested plots
- 2) Reynolds number calculations
- 3) Answer Questions 1-4 on pages 29 and 30 of 32 in the pdf file (ECRE tutorial pages 31&32).
- 4) Reset your model to the base case conditions. Now run the COMSOL model with the diffusivity set to zero and remove the parabolic velocity profile by setting the z-velocity to the average velocity of u_0 .
 - a) Produce a surface plot and a cross-section plot to compare with the previous case of laminar flow. Compare the base case with the case of zero diffusivity and a uniform velocity profile.
 - b) Make a new cross section plot of conversion as a function of axial position. Choose to plot in a new figure and keep your old plot. You will need to change your titles. Make a plot in excel of this data compared to X_A vs L data obtained from your POLYMATH model.
 - c) Compare the average outlet conversion from the COMSOL laminar flow model (base case) with the conversions obtained from the POLYMATH PFR model and the COMSOL model with zero diffusivity and the uniform velocity profile. Write a statement on the comparison of the conversion of these two data sets.
- 5) Reset the base case to have only axial diffusion with value of $\text{Diff}=1\text{e-}2 \text{ m}^2/\text{s}$. See Figure on next page. Then repeat the analysis in steps a though c of question 4).





In the Table for anisotropic the Diffusivities are:

Dr (radial)	
	Dz (axial)