Unsteady-State Diffusion in a Slab

This simple example is based on Cutlip and Shacham Problem 7.13: Unsteady-State Mass Transfer in a Slab. We will start with a simple problem in which the slab has no A present at the start of the problem. Then we will move on to solve the Geankoplis/Cutlip and Shacham problem and compare the solutions between Comsol and Polymath. See the text for an explanation of the problem and the governing equations.

PROBLEM DEFINITION

We start with the following PDE to solve:

$$\frac{\partial C_A}{\partial t} = D_{AB} \frac{\partial^2 C_A}{\partial x^2}$$

with a slight modification of the boundary and initial conditions from problem C&S7.13:

$$t = 0 \qquad C_A = 0 \text{ for all } x$$

$$C_A = 4 \times 10^{-3} \text{ kmol/m}^3 \qquad x = 0$$

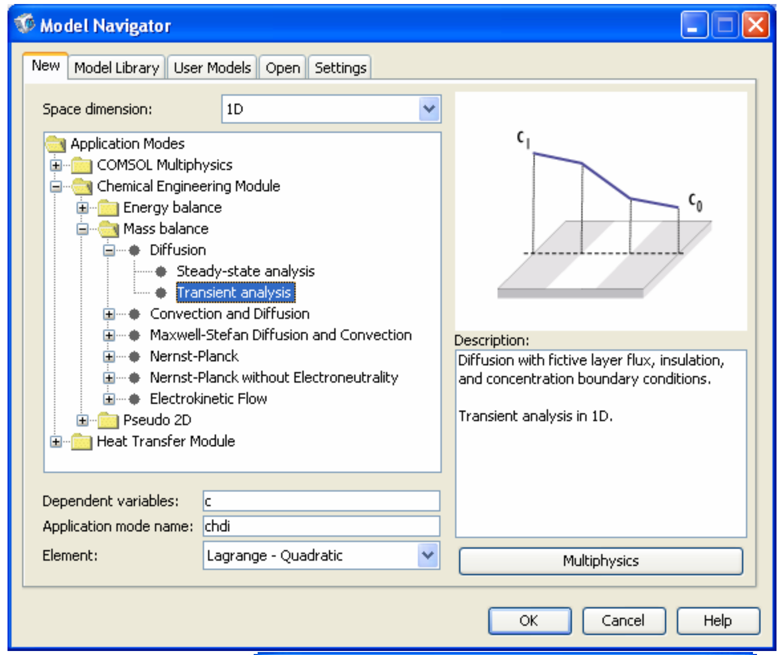
$$\text{Wall is insulated} \left(\left. \frac{\partial C_A}{dx} \right|_{x=0.004m} = 0 \right) \text{at } x = 0.004m$$

Later we will examine the initial condition in which there is a concentration profile in the slab. We are now ready to model our system in COMSOL.

The analytical solution to the above equation is given by an infinite Fourier series in which the slab thickness is x=h. This problem is referred to in texts as transient diffusion in a finite-dimensional medium.

SOLVINGTHE PROBLEM USING THE GRAPHICAL USER INTERFACE

Select the **1D** application mode **Mass Balance, Transient analysis**, in **Cartesian coordinates** from the **Chemical Engineering Module**. Then select OK.



Geometry Modeling

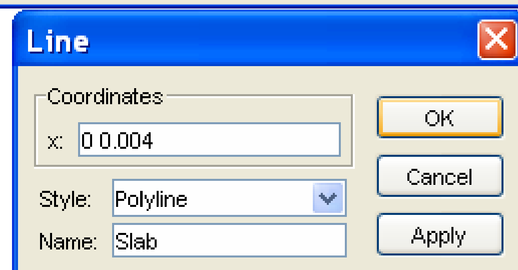
Select Line from the Specify objects menu item in the Draw menu.

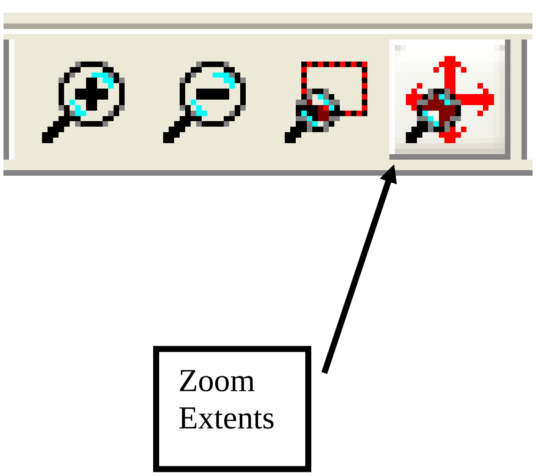
Specify 0 and 0.004 as **Start** and **Stop** and set the name slab.

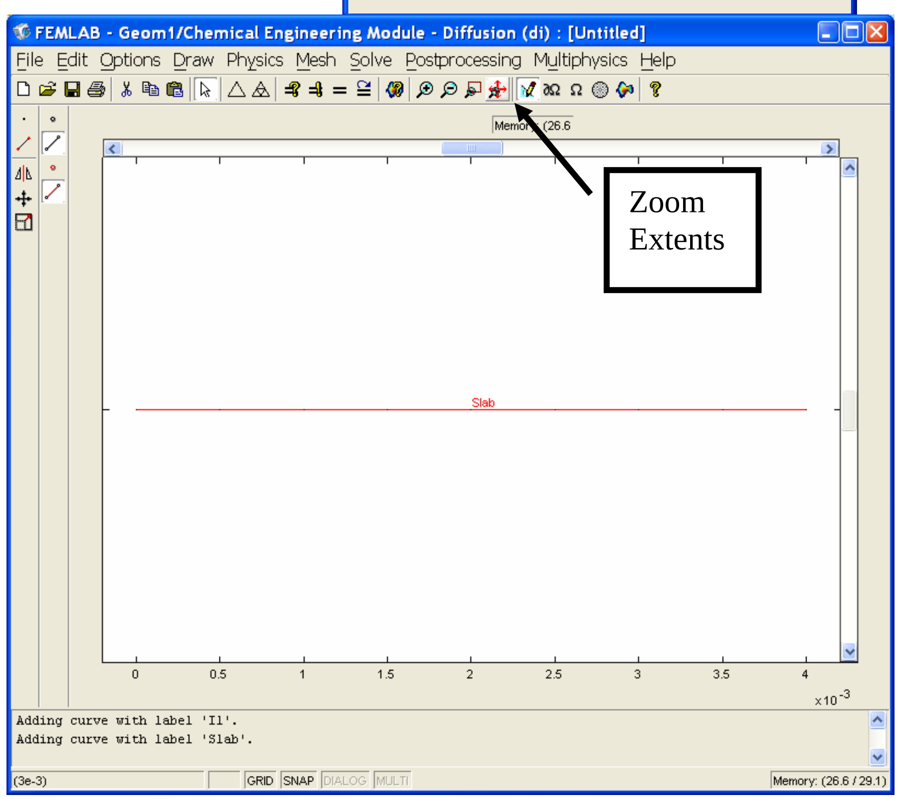
Type slab in the Name edit field.

Click OK.

Click the Zoom Extents button•

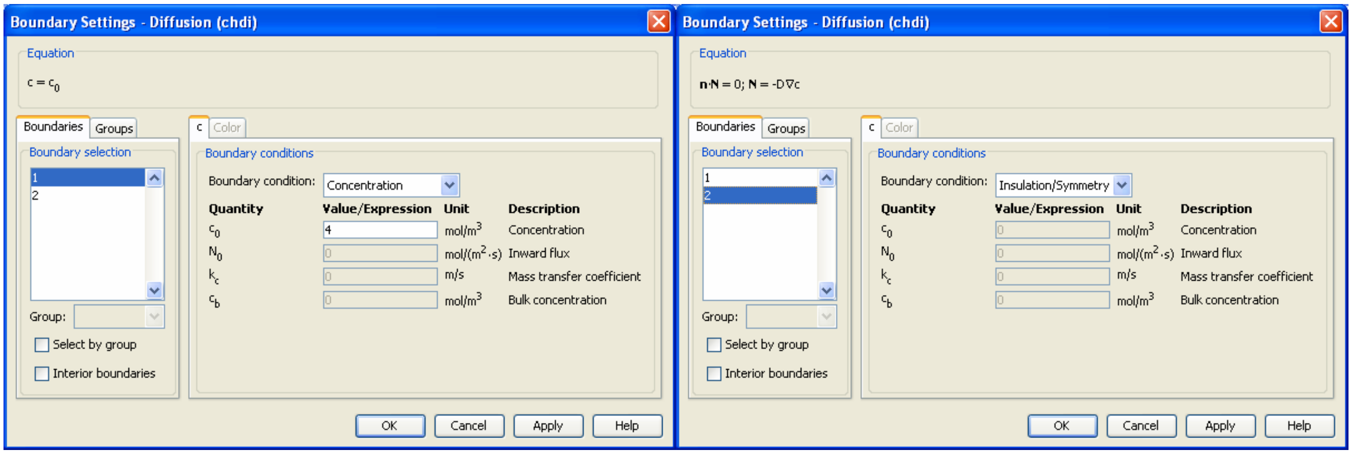






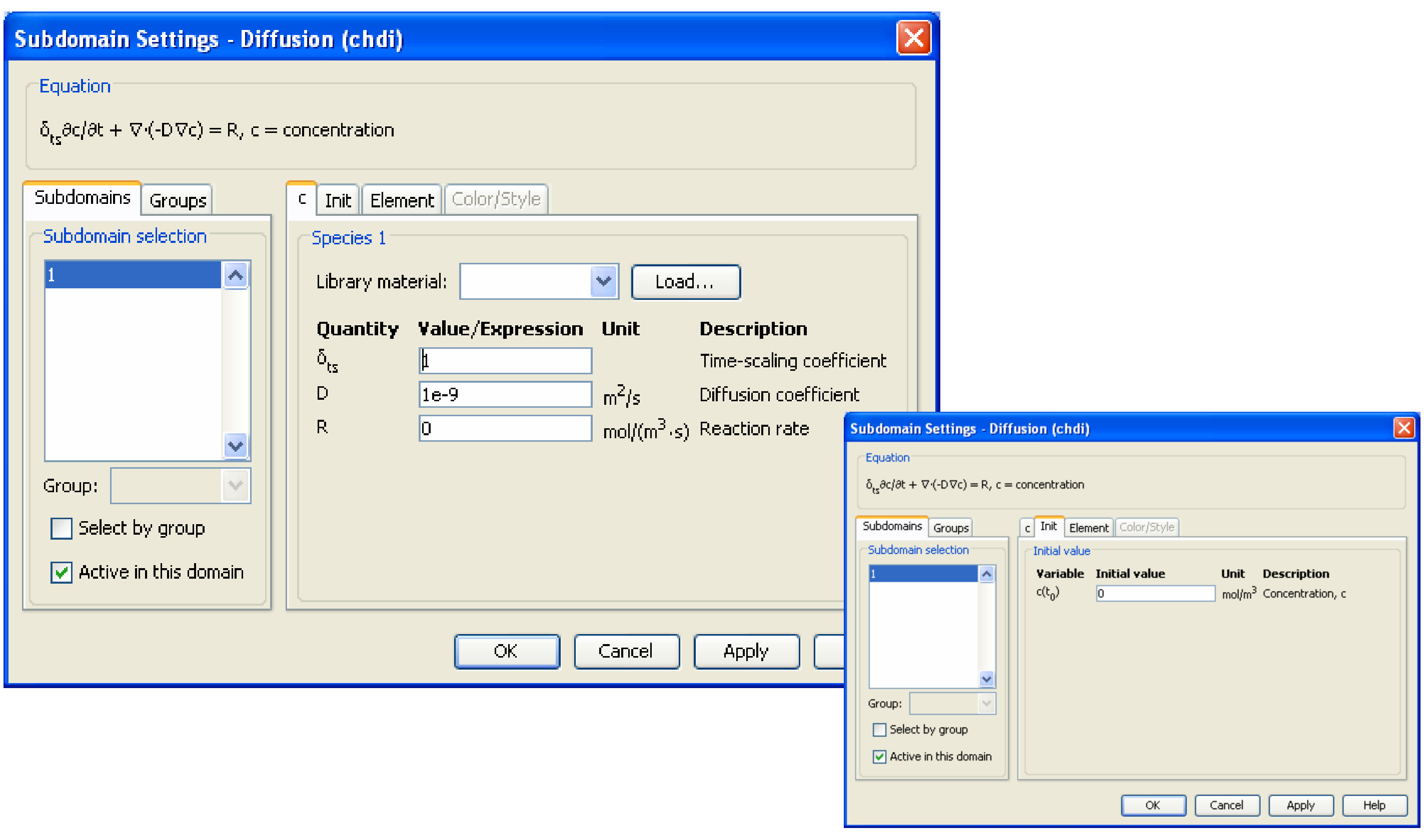
Boundary Conditions

1. Select **Boundary Settings** from the **Physics** menu.
2. Select boundary 1 and specify the concentration as 4 mol/m^3 and the second boundary condition as Insulation/symmetry.
3. Click **OK**.



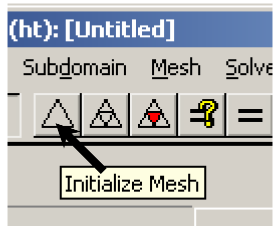
Subdomain Settings

1. Select **Subdomain Settings** from the **Physics** menu.
2. Select subdomain 1 and enter the Diffusion coefficient of $1X10^{-9}$ m^2/s. The default settings for the Initial conditions are set to zero concentration. The reaction rate is set to zero and we are not using any time scaling so the time-scaling coefficient is set to 1.

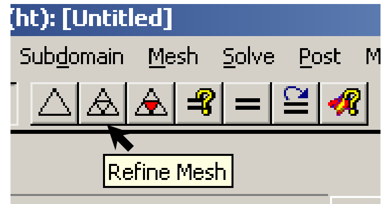


Mesh Generation

Initialize the mesh

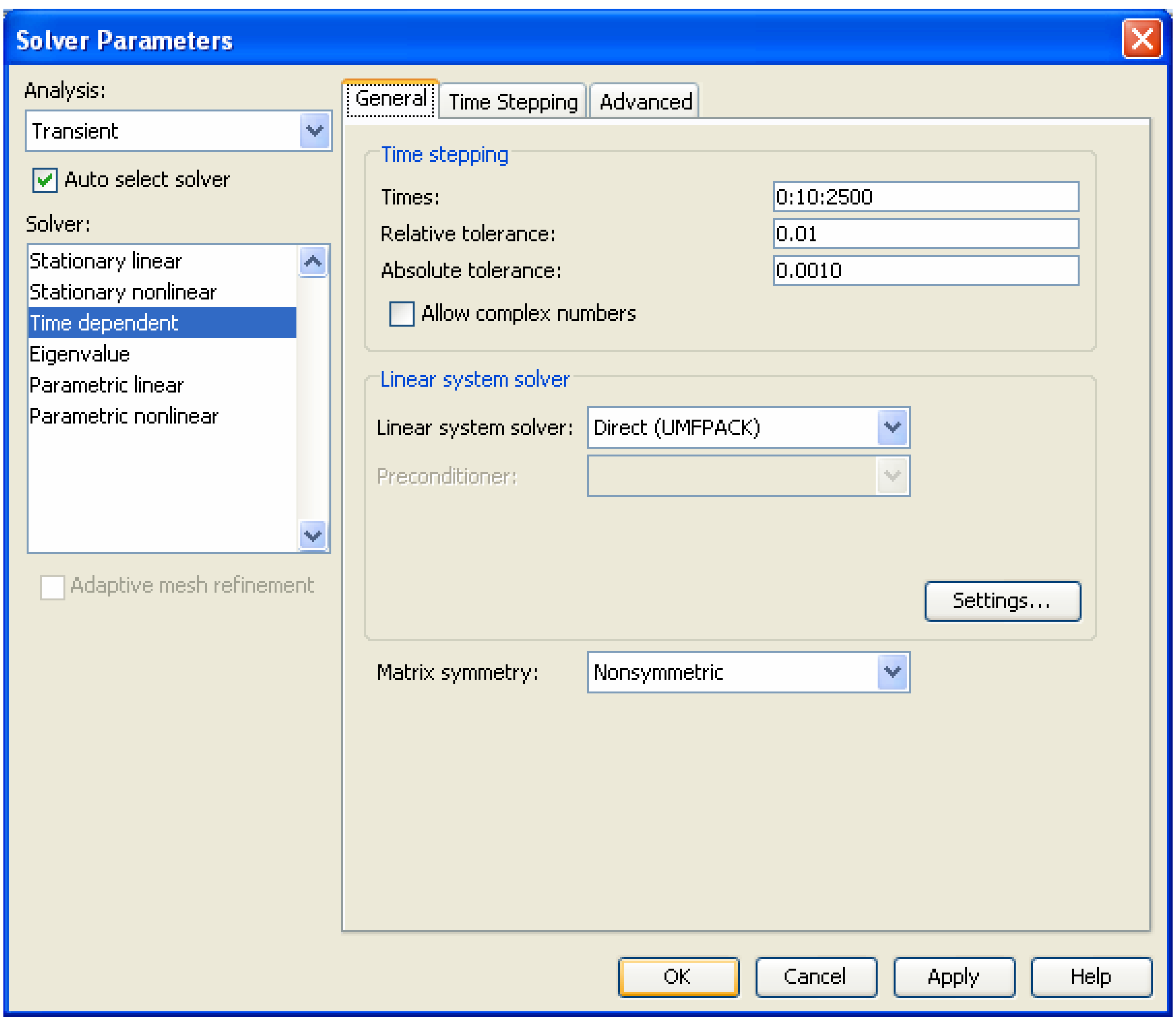


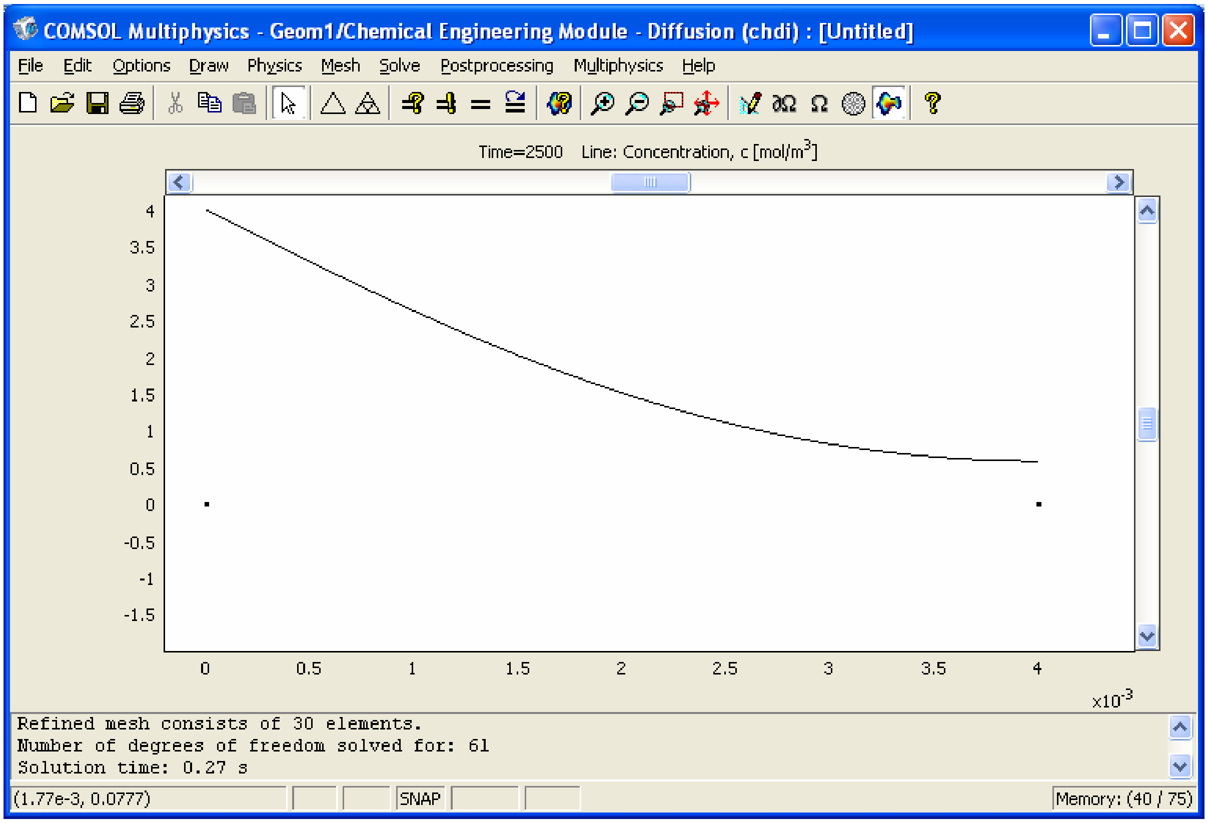
Refine the mesh once.



Computing the Solution

1. Select **Solver Parameters** in the **Solve** menu.
2. Type 0:10:2500 in the **Times** edit field in the **General** page. This stands for how you would like the output reported. This will report results starting at time t=0, stepping at intervals of 10 s and ending at 2500 s.
3. Click **OK**.
4. Click the **Solve** button in the Main toolbar





5. Now compare this to a polymath solution: Go to the course home page and click on the link POLYMATH CD (Rowan Students Only). Pull up problem 7.13a and change the initial conditions to be zero. You may also want to change the initial concentrations to have units of mol/m^3 instead of kmol/m^3. This is not necessary but will aid in making a comparison plot.
6. And then make a plot as shown in the following page.

POLYMATH Report 7.13 modified Unsteady-state Mass Transfer in a Slab (zero initial concentration)
Ordinary Differential Equations 29-Sep-2005

Calculated values of DEQ variables

	Variable	Initial value	Minimal value	Maximal value	Final value
1	t	0	0	2500.	2500.
2	CA2	0	0	0.0032935	0.0032935
3	CA3	0	0	0.0026235	0.0026235
4	CA4	0	0	0.0020219	0.0020219
5	CA5	0	0	0.0015126	0.0015126
6	CA6	0	0	0.0011105	0.0011105
7	CA7	0	0	0.0008223	0.0008223
8	CA8	0	0	0.0006498	0.0006498
9	DAB	1.0E-09	1.0E-09	1.0E-09	1.0E-09
10	deltax	0.0005	0.0005	0.0005	0.0005

11	CA9	0	-8.627E-07	0.0005922	0.0005922
12	CA0	0.006	0.006	0.006	0.006
13	K	1.5	1.5	1.5	1.5
14	CA1	0	0	0.004	0.004

Differential equations

1 d(CA2)/d(t) = DAB * (CA3 - 2 * CA2 + CA1) / deltax ^ 2

2 d(CA3)/d(t) = DAB * (CA4 - 2 * CA3 + CA2) / deltax ^ 2

3 d(CA4)/d(t) = DAB * (CA5 - 2 * CA4 + CA3) / deltax ^ 2

4 d(CA5)/d(t) = DAB * (CA6 - 2 * CA5 + CA4) / deltax ^ 2

5 d(CA6)/d(t) = DAB * (CA7 - 2 * CA6 + CA5) / deltax ^ 2

6 d(CA7)/d(t) = DAB * (CA8 - 2 * CA7 + CA6) / deltax ^ 2

7 d(CA8)/d(t) = DAB * (CA9 - 2 * CA8 + CA7) / deltax ^ 2

Explicit equations

1 DAB = 1.0e-9

2 deltax = 0.0005

3 CA9 = If (t == 0) Then (0) Else ((4 * CA8 - CA7) / 3)

4 CA0 = 6.0e-3

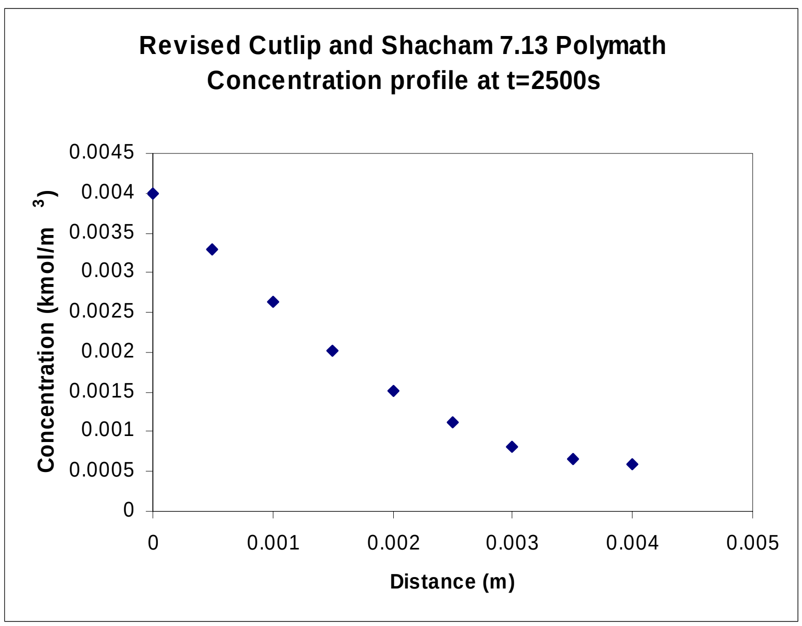
5 K = 1.5

6 CA1 = If (t == 0) Then (0) Else (CA0 / K)

General

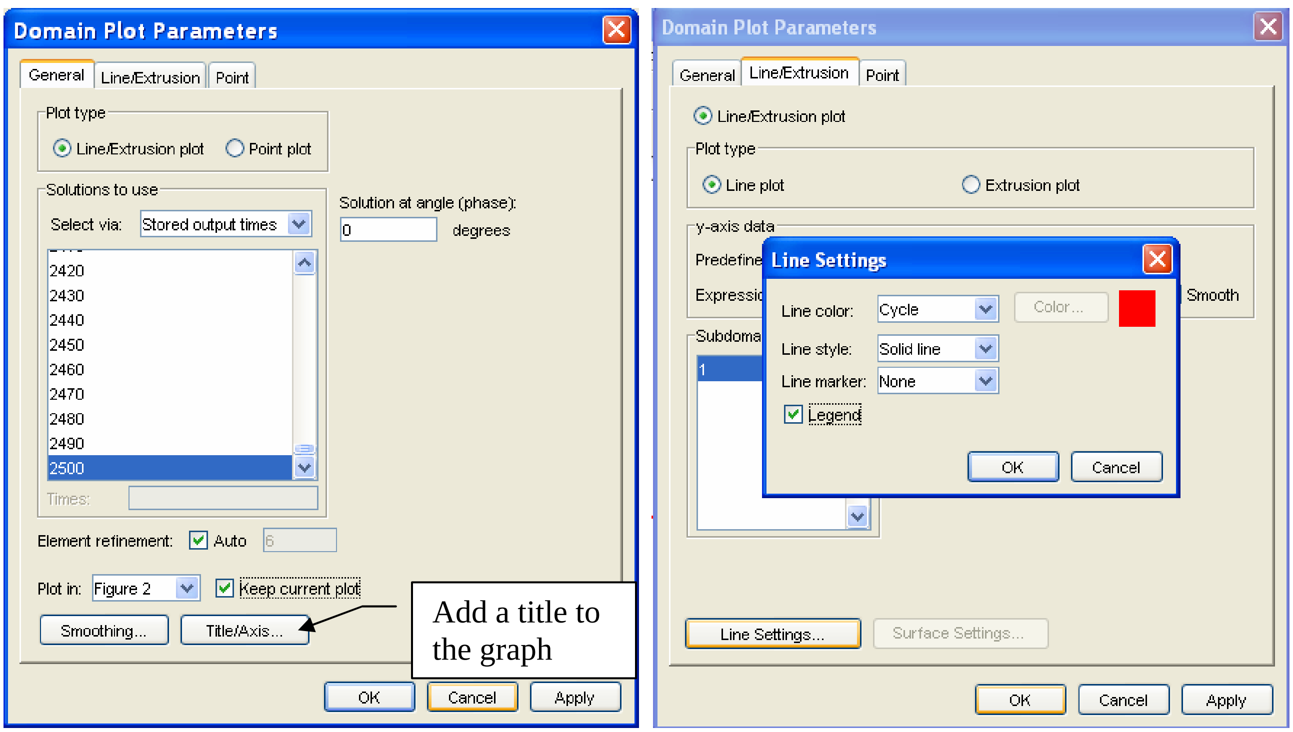
Total number of equations	13
Number of differential equations	7
Number of explicit equations	6
Elapsed time	0.000 sec
Solution method	RKF_45
Step size guess. h	0.000001
Truncation error tolerance. eps	0.000001

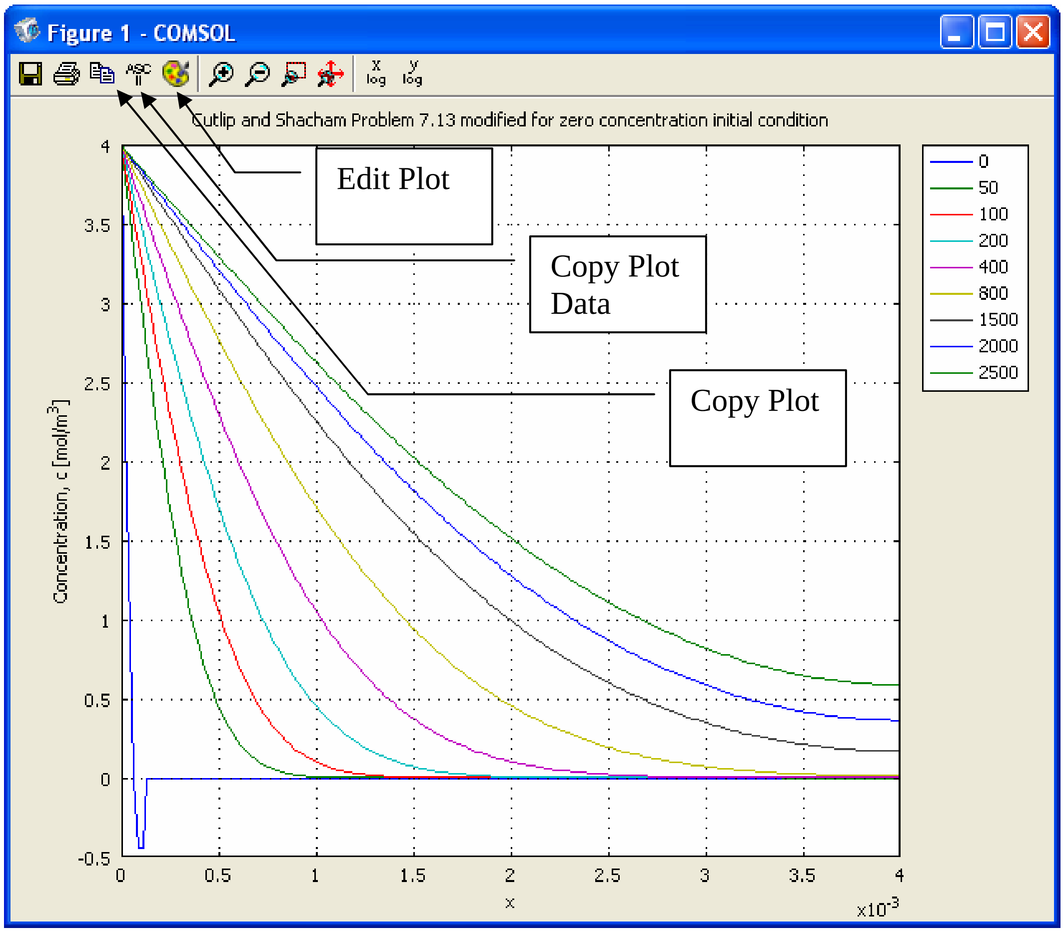
Save your polymath solution in a word document to be submitted at the end of the tutorial.



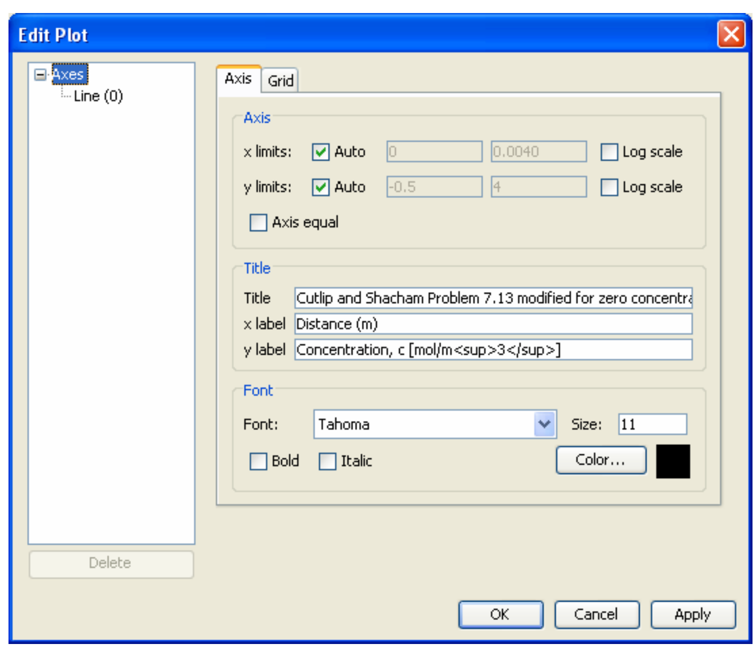
Post Mode

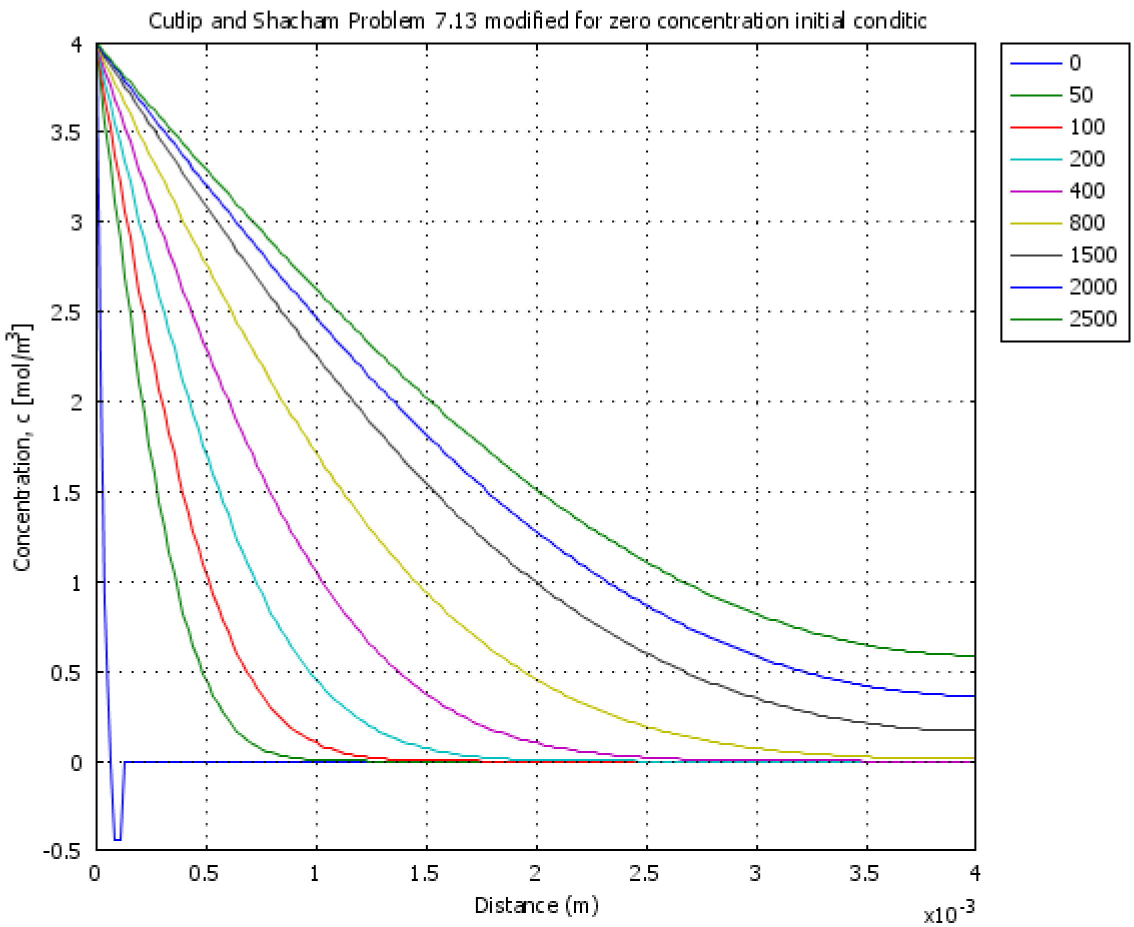
1. Select **Domain Plot Parameters** from the **Postprocessing** menu.
2. Select the **General** tab and select the **Line/extrusion plot** check box under **Plot type**.
3. Select the following time-steps, 0, 50, 100, 200, 400, 800, 1500, 2000, 2500 from the **Solutions to use** list by holding down the **Ctrl** key.
4. Click **OK**.
5. Add a title to the graph by pressing the Title/Axis button
6. Request a legend by choosing the Line/Extrusion tab and select the Line Settings button.
7. Select OK
8. You should now have a plot with a title as shown on the next page.





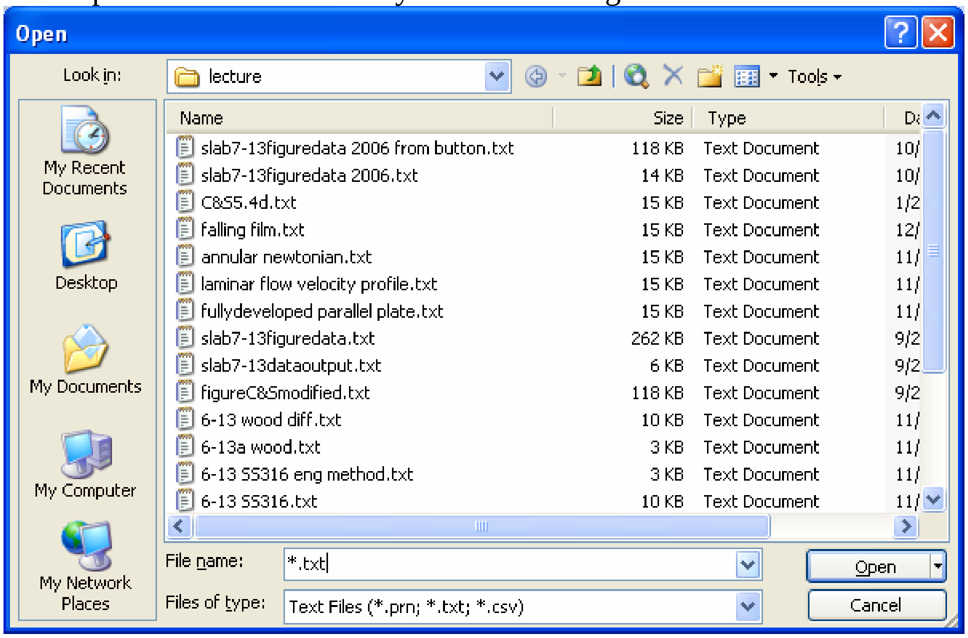
9. Change the x-axis description of this plot by selecting the painters pad to edit the plot. Change the x-axis description to be Distance (m).
10. Paste a copy of this plot into your word document by using the copy button. (See the location of this button in the figure on the previous page.)



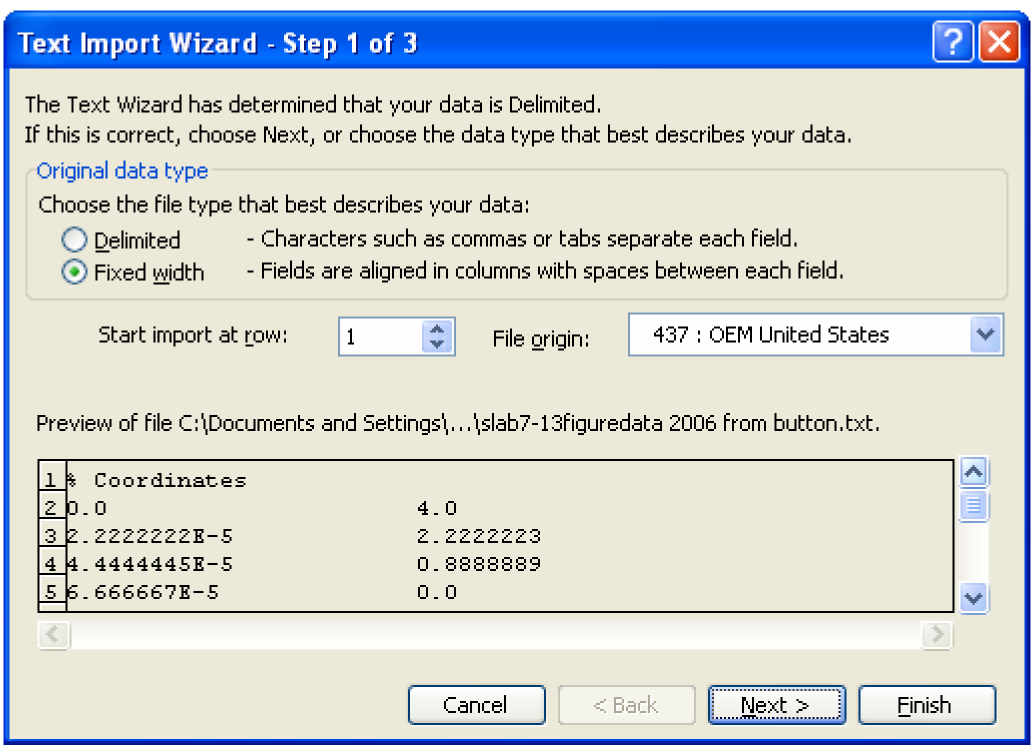


11. Compare this plot to a polymath plot. (To produce this polymath plot you will need to use the Edit Paste Special Transpose command.
12. Make an additional plot in excel comparing the two solutions. In this figure you will plot data from Polymath and Comsol on the same figure.
13. ***Exporting the Current COMSOL Plot to a File***
    There are several methods to export the data to a text file that can be imported into a spreadsheet. I recommend using the short cut button. The short cut button is located on the Figure 1 plot of Comsol. Select the ASCII button on your plot (Figure 1), which is shown in the previous page. Save this data as a text file and then import it into a spreadsheet.

14. Open the text file. The data will be in the following form: x,y coordinates for each time that is given in the legend of the Comsol Figure 1 plot. You will need to open this data with an excel spreadsheet. Make sure you are searching for a *.txt file in the Files of type: line.

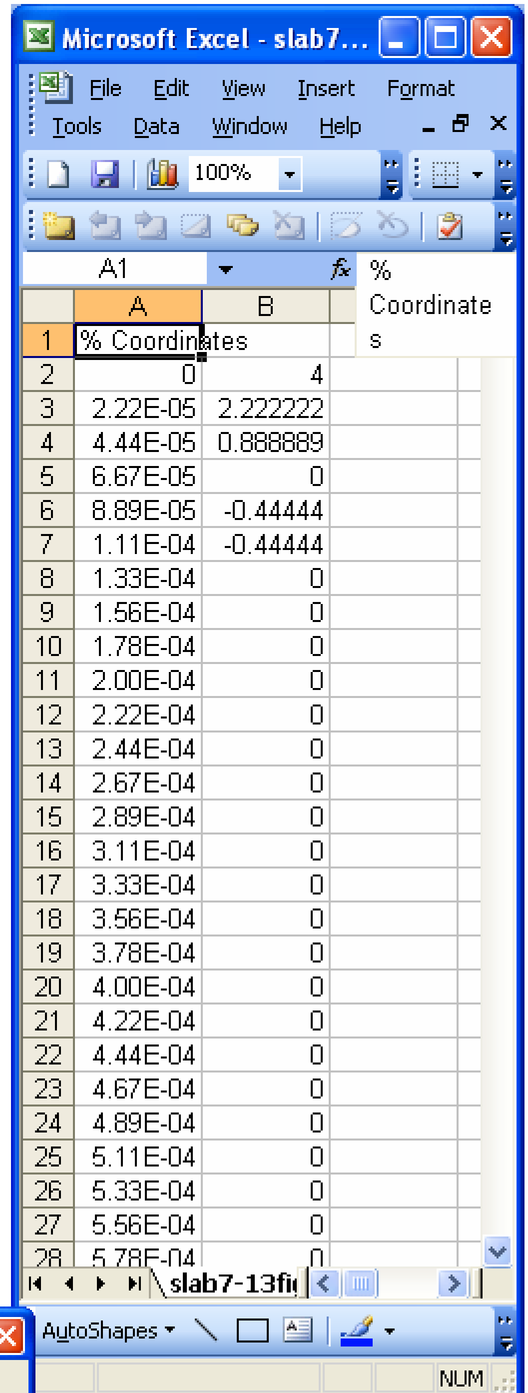


15. Next a Text Import Wizard will open. Select fixed width and then Next. Check to see that the data is being imported in two columns by scrolling down with the scroll bar and then press Finish.



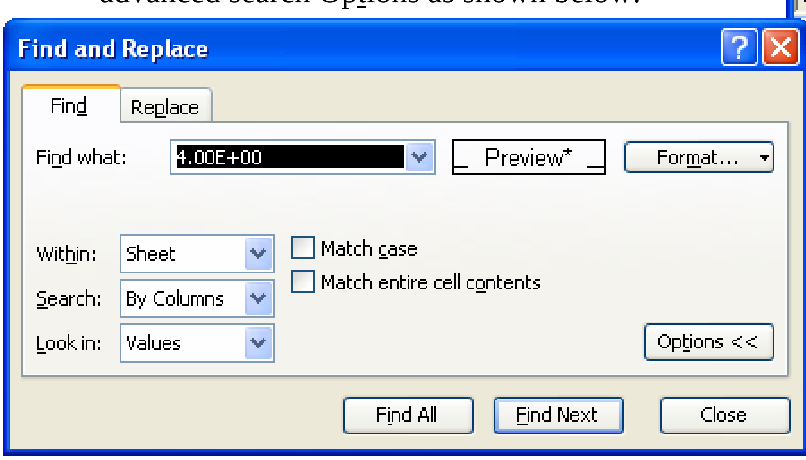
16. You should now have 2 columns of data in the spreadsheet. The data in the column A is the distance coordinate in meters and the data in column B is the concentration in mol/m3. Each data set corresponds to the time parameter of the plot in Comsol Figure 1.

	A	B
	Distance (m)	Concentration (mol/m^3)
2	The first data set corresponds to the time t=0s	
183	The second data set corresponds to the time t=50s	
364	The third data set corresponds to the time t=100s	
1450	The last data set corresponds to the time t=2500s	

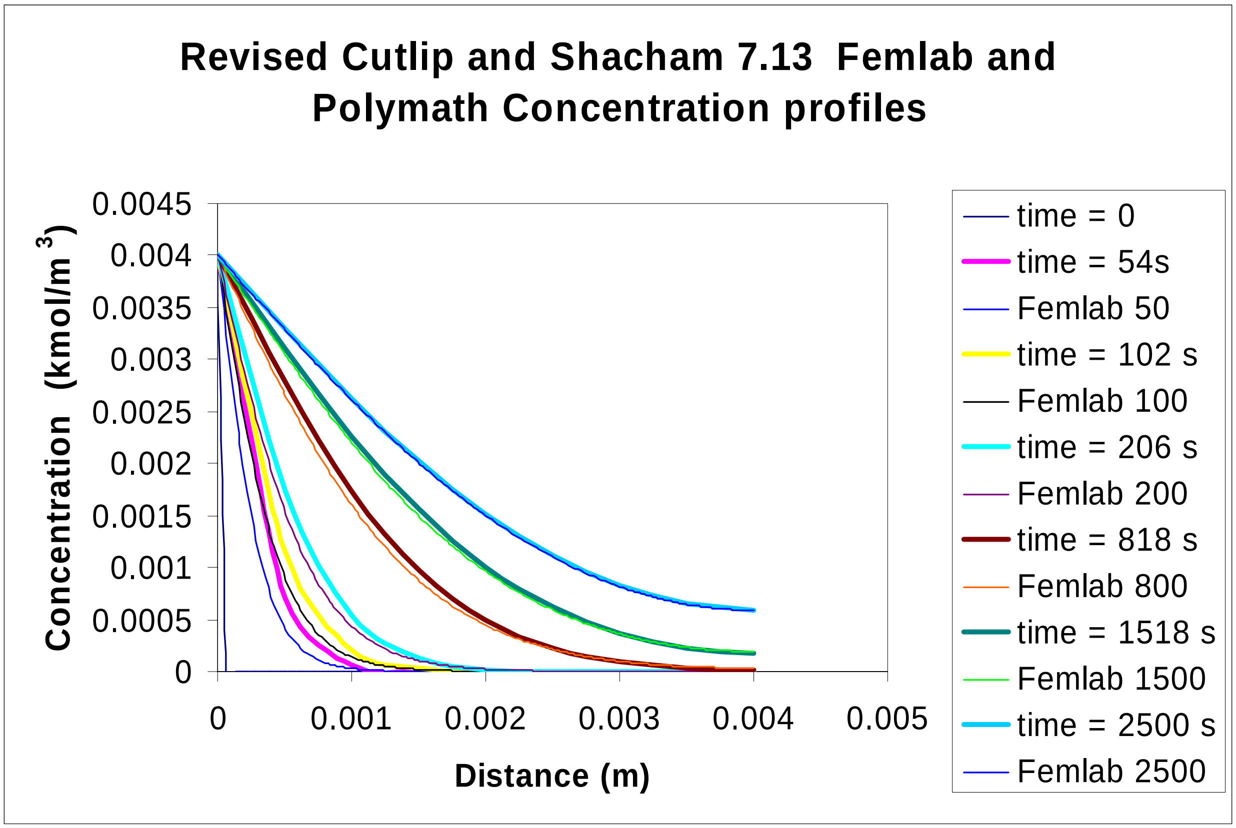


17. Notice that in the B column the data a $x = 0$ m is always set at the initial condition of $C_A = 4\ \text{mol/m}^3$.

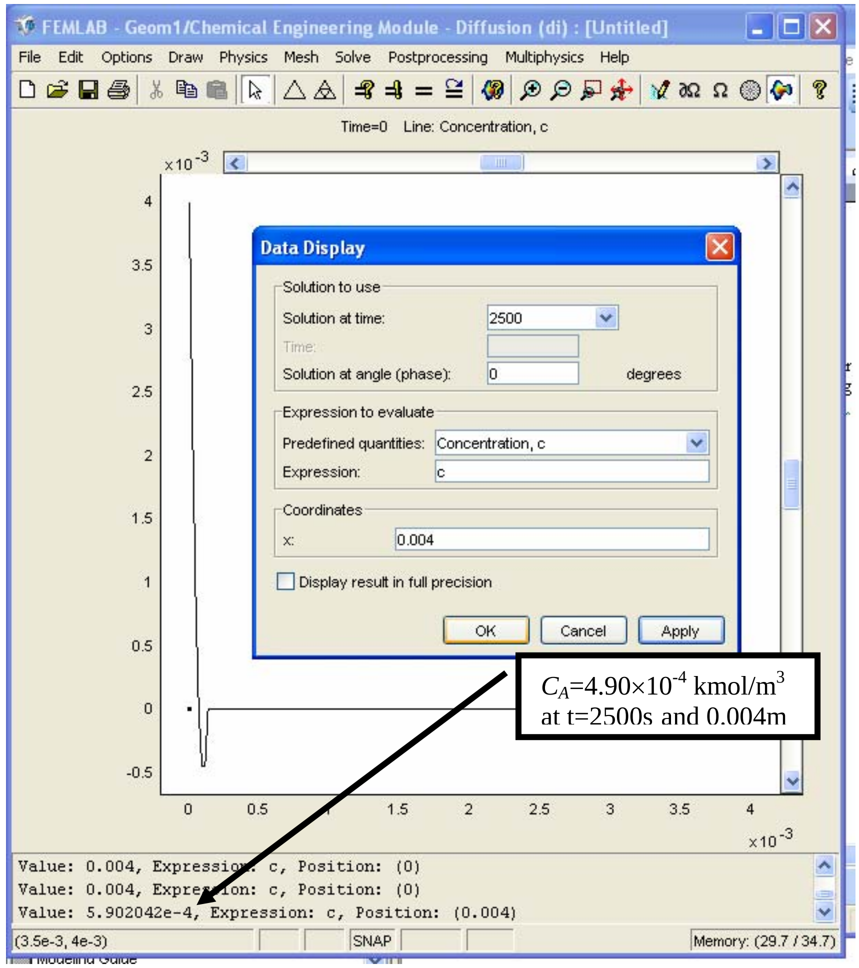
18. To quickly find the start of each data set you can utilize the edit find feature of excel. First format column B to be in scientific notation format. Then you can search for 4.00E00 and this will give you the start of each set of data. You will need to save the file as an excel spread sheet and use the advanced search Options as shown below:



19. Submit all 3 of the above plots at the end of the period or as specified by the instructor.

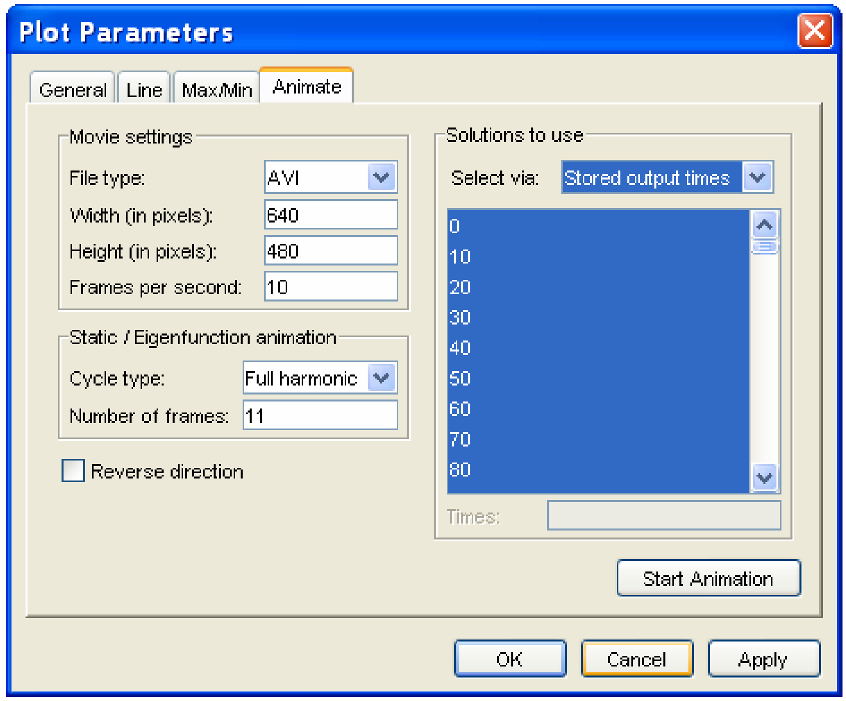


20. **Getting Numerical Results Directly** The postprocessing mode in 2D can display the numerical value of the current surface or contour plot. Get this value by clicking anywhere in the model domain. The message log shows the value of the plotted property. In 1D, click in the plot area to display the value of the currently plotted expression. If snapping is active, the selected points snap to the grid points.



21. Use the **Data Display** dialog box to evaluate an expression at a certain coordinate. If applicable select the solution to use and then select one of the predefined quantities or enter an arbitrary expression containing COMSOL variables. If you want to evaluate the expression at several coordinates you can enter them separated by spaces in the edit fields in the **Coordinates** frame.
22. Click **Apply** or **OK** to display the value of the expression in the message log at the bottom of the COMSOL user interface. Select the **Display result in full precision** check box to get the value with as many significant digits as possible. To control the setting of this check box for new models, use the corresponding check box on the **Postprocessing** tab in the **Preferences** dialog box.

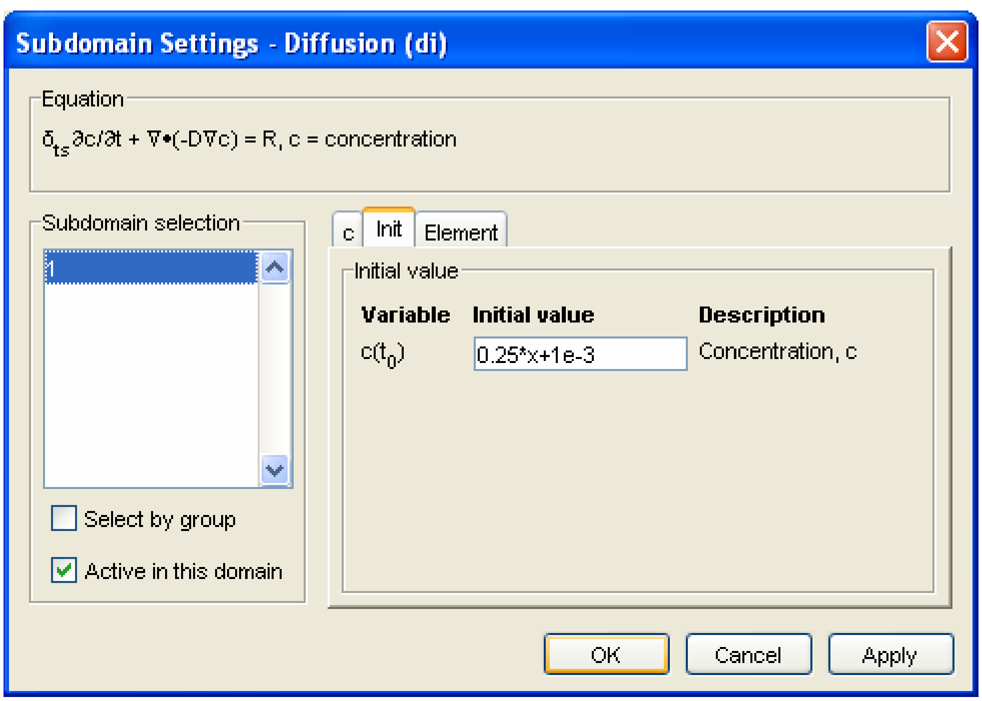
Create a Movie



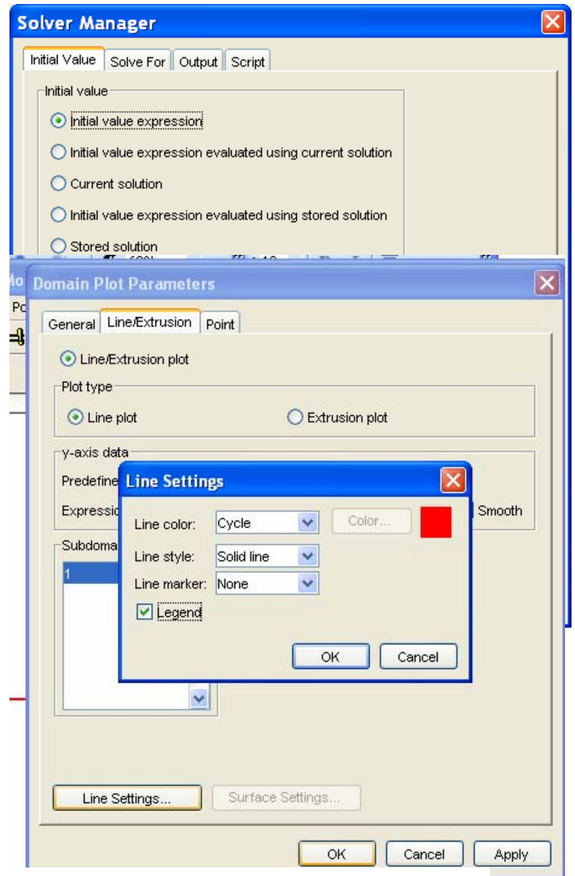
23. Select **Plot Parameters** from the **Postprocessing** menu.
24. Go to the Animate Tab
25. Select the times you want to show in the animation by clicking on the numbers while holding down the animate key. (don't select too many or your will have a very long movie)
26. We can now view how the Concentration varies in time by selecting **Animate** in the **Plot Parameters** menu.

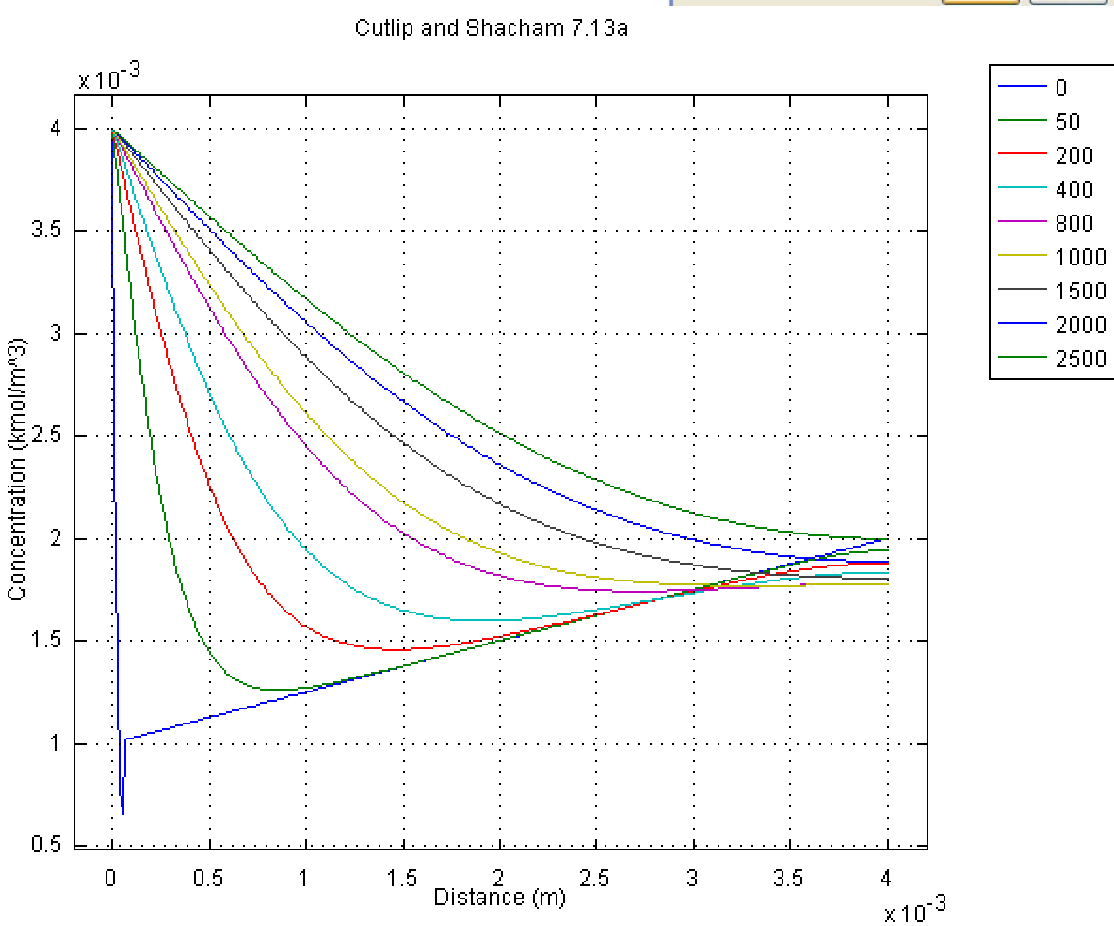
Cutlip and Shacham Problem 7.13a

27. Now we will solve the original problem 7.13a (Given originally as Geankoplis Example 7.7C) Go to the initial condition specifications of the slab and change them to have a linear variation from 1×10^{-3} to 2×10^{-3} kmol/m^3 over the distance of 0.004 m. This is done by entering the following equation in the Physics, Subdomain Settings,



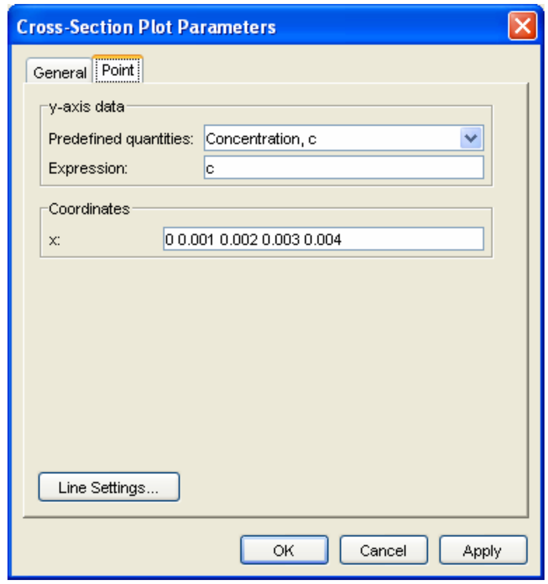
28. Make sure that you are solving from the initial conditions and not restarting the problem. Chose Solver, Solver Manager and select Initial value expression.
29. Now you will obtain the following result after specifying the times to be plotted and request a legend (choose the Line/Extrusion tab and select the Line Settings button).
30. Notice that the below plot did not use the refined mesh.

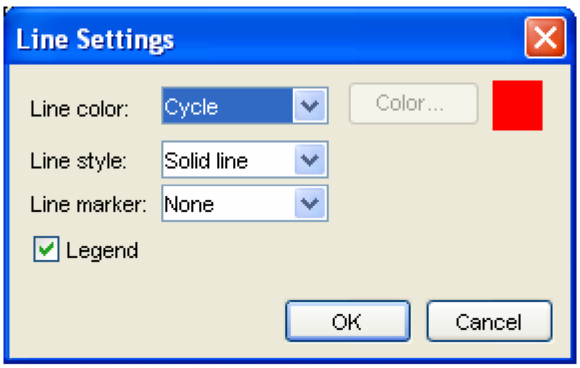


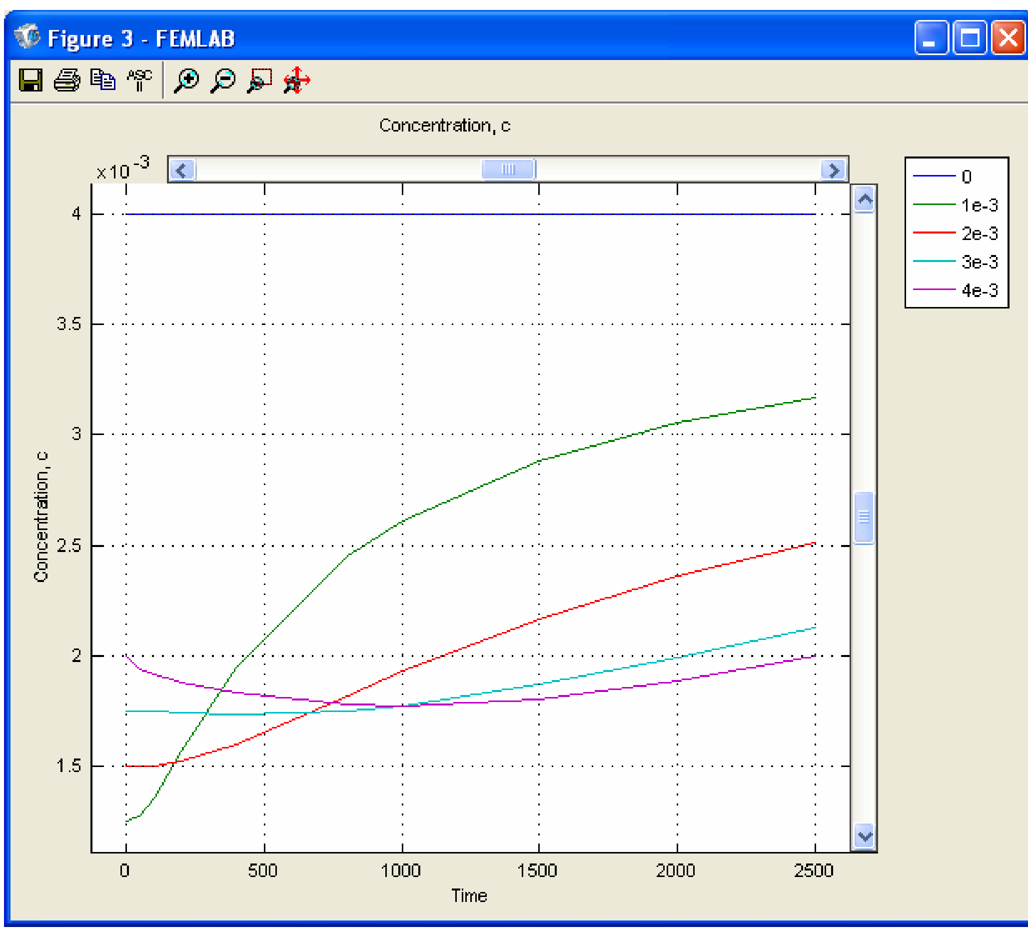


Other types of plots

31. Cross-Section Plot – this is the default plot produced by POLYMATH. You can plot the concentration as a function of time at specific distances. In this mode once again select the desired times and then specify the distances you would like ploted as parameters. In the following plot I have selected 0, 0.001, 0.002, 0.003 and 0.004 m. Also go into line settings option of the Cross-Section Plot Parameters and request a legend.







Culip & Shacham 7.13e – Flux boundary condition

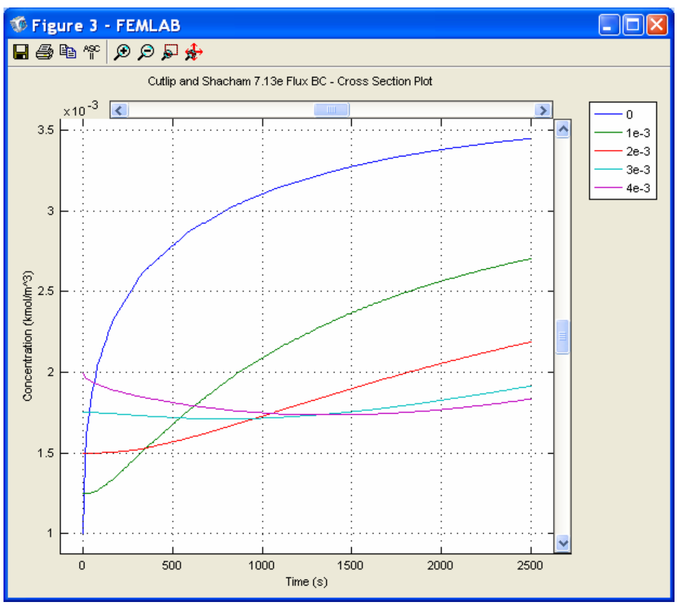
32. In this part of the problem you need to use the flux boundary condition with a mass transfer coefficient. The boundary condition is given as

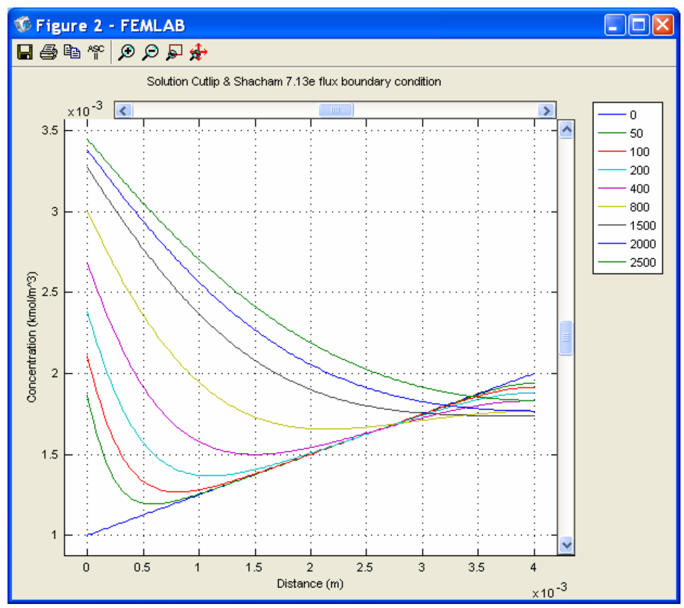
$$N_A = k_c\left(C_{A0} - C_{Ai}\right) = k_c\left(C_{A0} - KC_A\big|_{x=0}\right)$$

33. To modify this for the COMSOL boundary conditions

$$N_A = k_c\left(C_{A0} - KC_A\big|_{x=0}\right) = Kk_c\left(\frac{C_{A0}}{K} - C_A\big|_{x=0}\right)$$

34. Produce plots similar to the last two given below.





Submit after completing this Tutorial in a word document containing the following. This should be emailed to Hesketh@rowan.edu.

1. Modified 7.13 (Initial condition of zero concentration of A in slab)
    a. Polymath solution
    b. Plot of concentration as a function of distance with the parameter of time.
        i. Polymath
        ii. COMSOL
        iii. Both COMSOL and Polymath results on same plot
    c. Comment on the comparison between COMSOL and Polymath results
2. Cutlip & Shacham Problem 7.13a
    a. Polymath Solution
    b. COMSOL Plot of concentration as a function of distance with the parameter of time
    c. COMSOL Cross Section plot similar to the output from Polymath (See Figure 3-COMSOL above)
    d. Comment on the difference between the initial conditions of the solid (subdomain) as zero concentration and linear concentration.
3. Cutlip & Shacham Problem 7.13e
    a. COMSOL Plot of concentration as a function of distance with the parameter of time
    b. COMSOL Cross Section plot similar to the output from Polymath (See Figure 3-COMSOL above
    c. Comment on the difference between a constant surface boundary condition and a flux boundary condition.