

Unsteady-State Diffusion in a Slab

This simple example is based on Cutlip and Shacham Problem 10.13: Unsteady-State Mass Transfer in a Slab. We will start with a simple problem in which the slab has no species 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&S10.13:

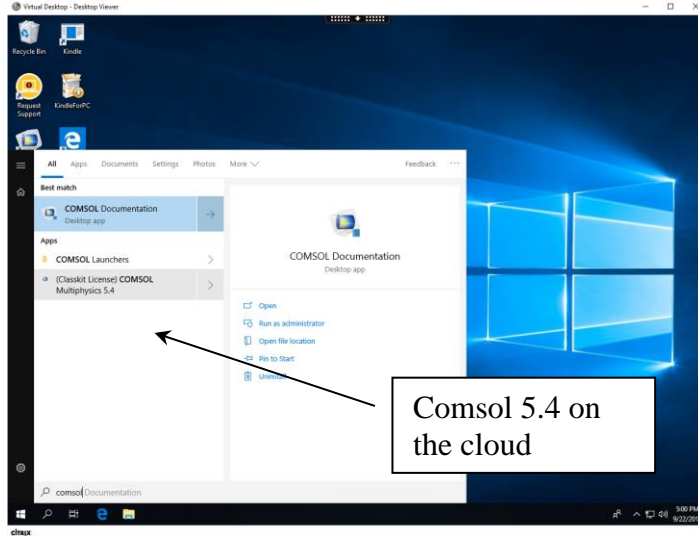
$$\begin{aligned} t = 0 \quad C_A &= 0 \text{ for all } x \\ C_A &= 4 \times 10^{-3} \text{ kmol/m}^3 \quad x = 0 \\ \text{Wall is insulated} \quad \left(\frac{\partial C_A}{\partial x} \right)_{x=0.004m} &= 0 \end{aligned}$$

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.

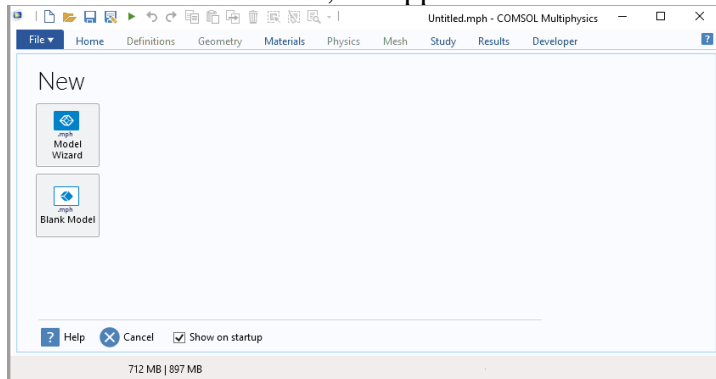
The analytical solution to the above equation is given by an infinite Fourier series in which the slab thickness is $x=h$. This problem is referred to in texts as transient diffusion in a finite-dimensional medium.

Unsteady-State Diffusion through a slab

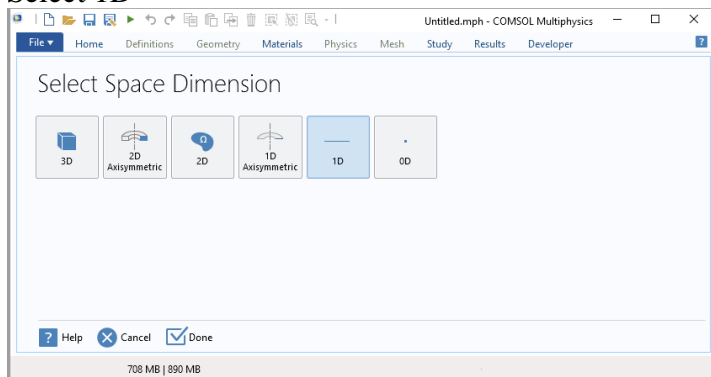
1. Use the Rowan Cloud by opening the Citrix Desktop and then open Comsol: Start COMSOL Multiphysics 5.4 Classkit License not the Documentation.



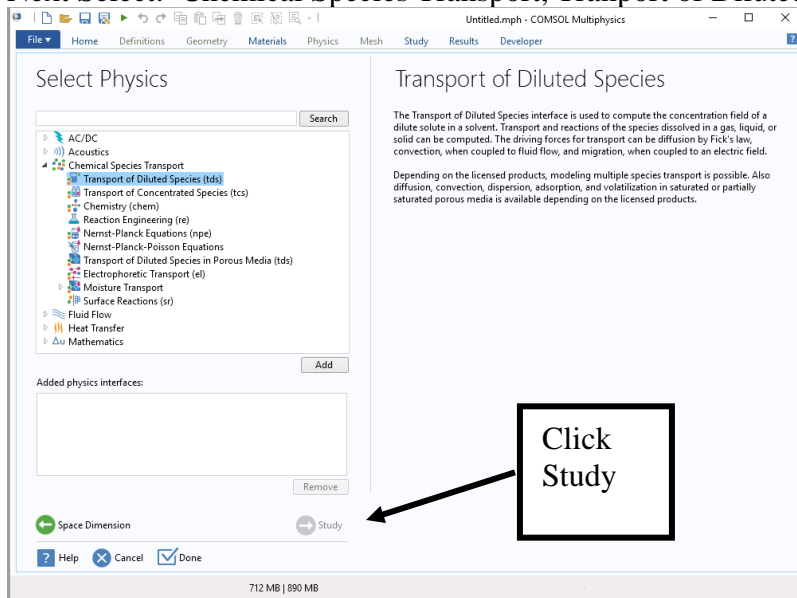
Select the Model Wizard, 1D application mode



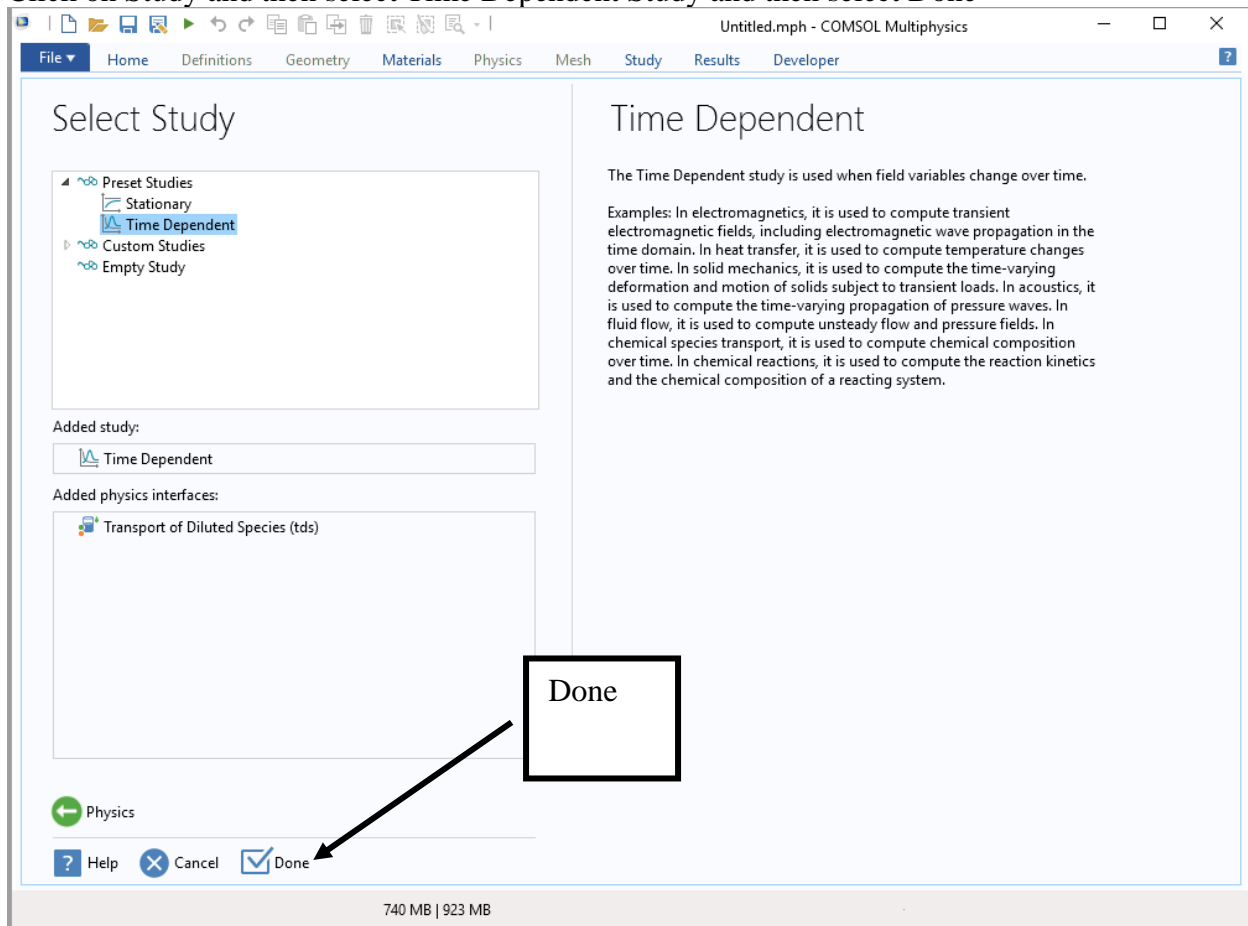
Select 1D



Next Select: Chemical Species Transport, Transport of Diluted Species and press Add.

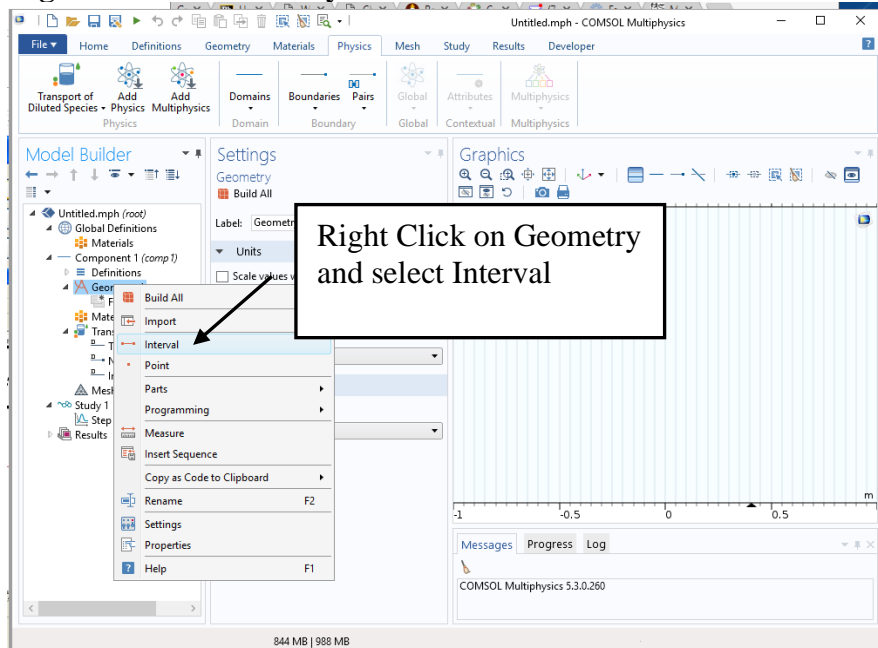


Click on Study and then select Time Dependent Study and then select Done

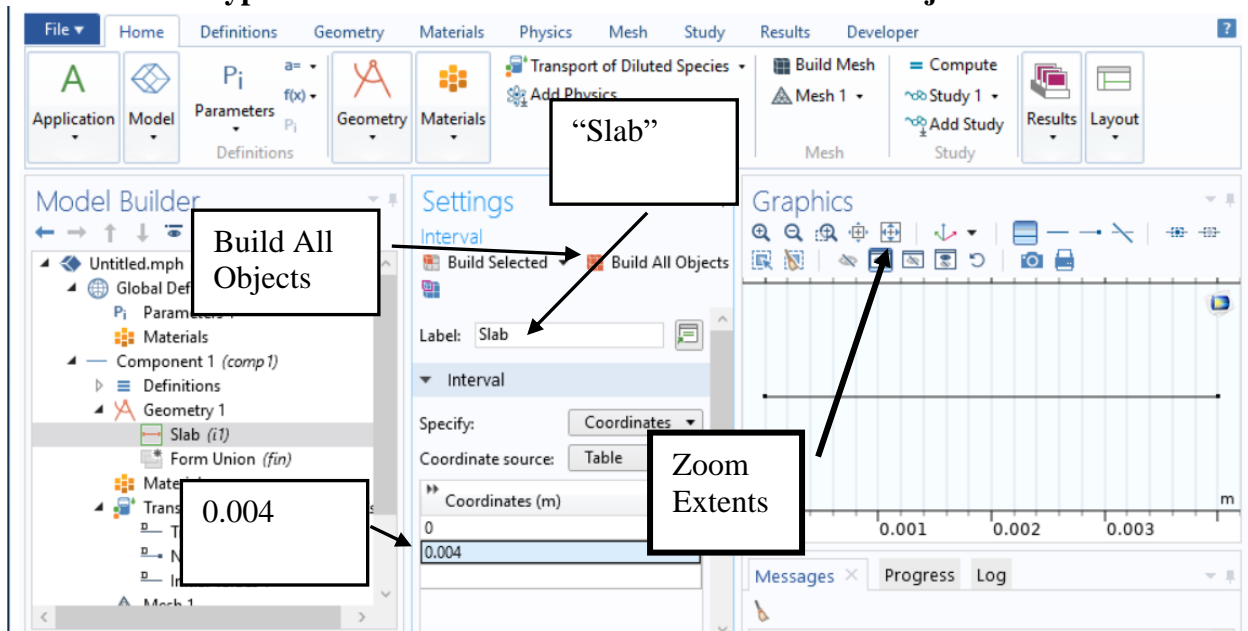


Geometry Modeling

Right click on Geometry and select Interval

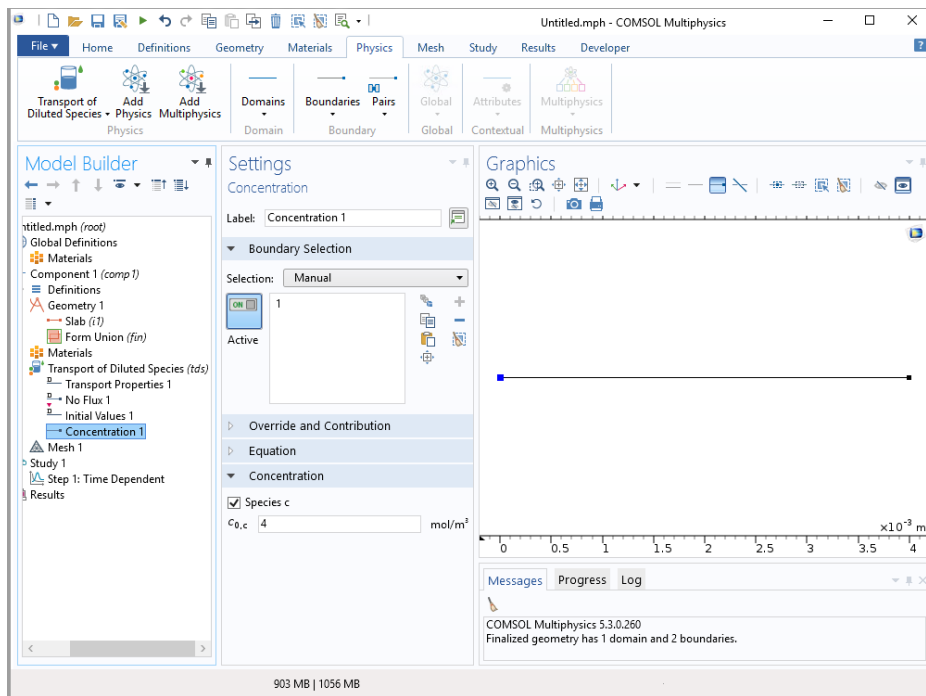
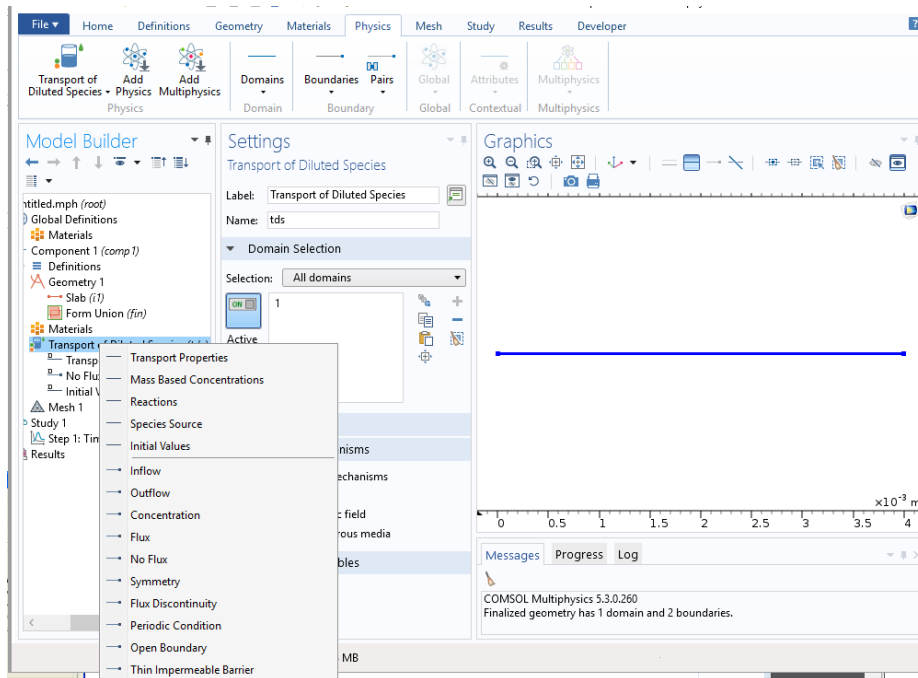


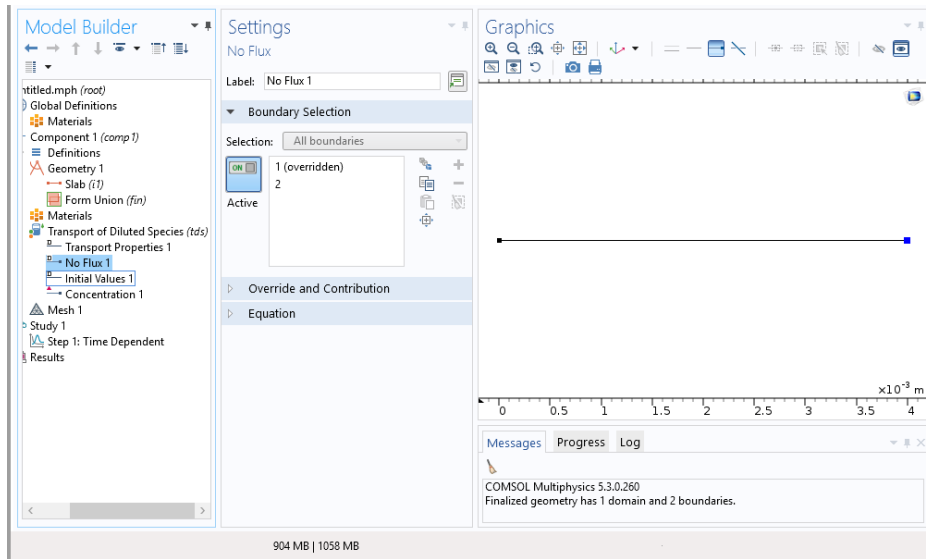
Specify 0 and 0.004 as **Coordinates of the line segment** and type over the word slab over the word interval. **Type slab in the Label field. Now select Build All Objects**



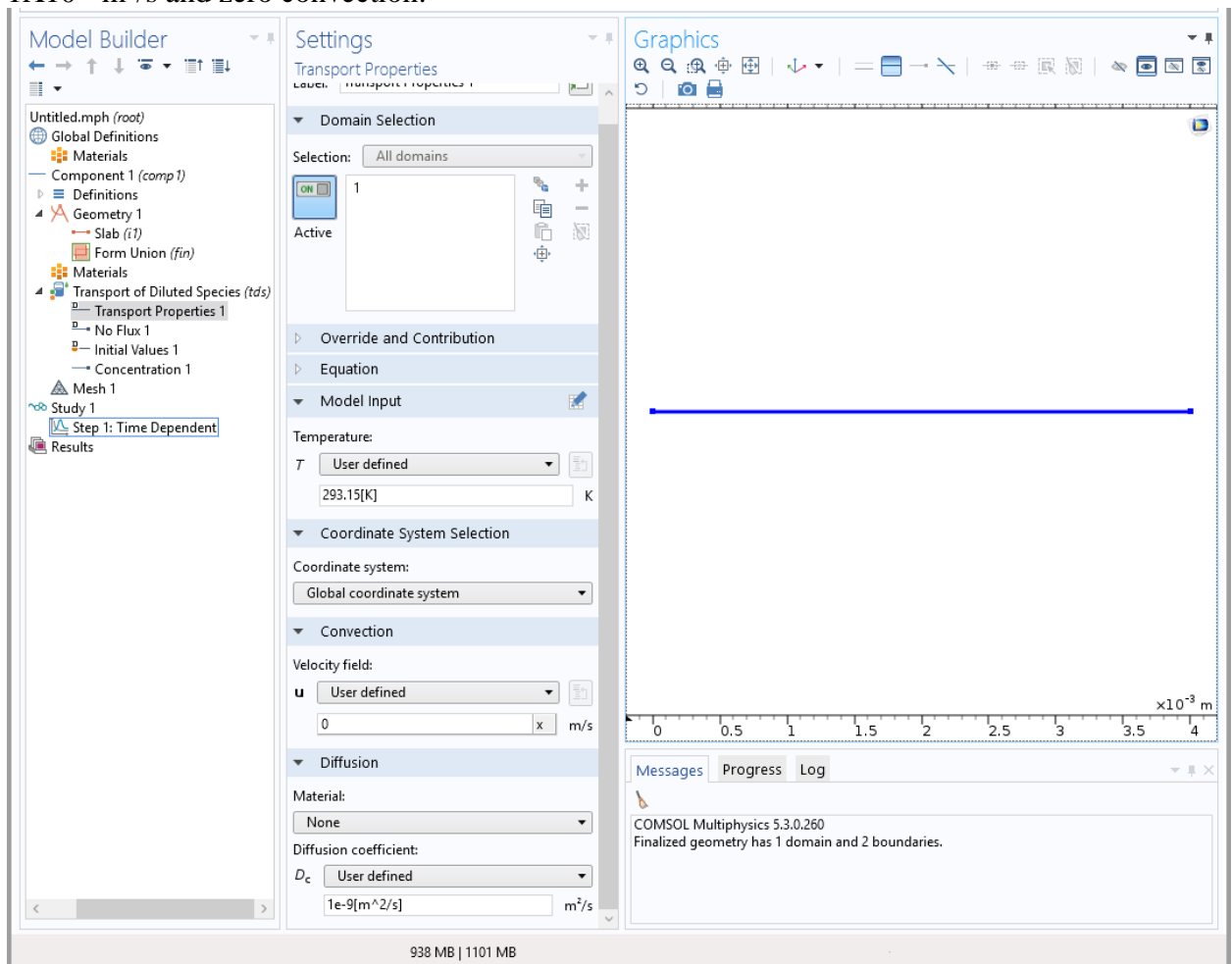
Boundary Conditions

1. Right click on Transport of Diluted Species and select the Concentration boundary condition. Click on the left end of the interval to select the boundary and then specify the concentration as 4 mol/m^3 (Picture shown below)
2. Click on the second boundary point and check that this is the no Flux 1 boundary condition. This shows that the other boundary has no flux or is insulated.

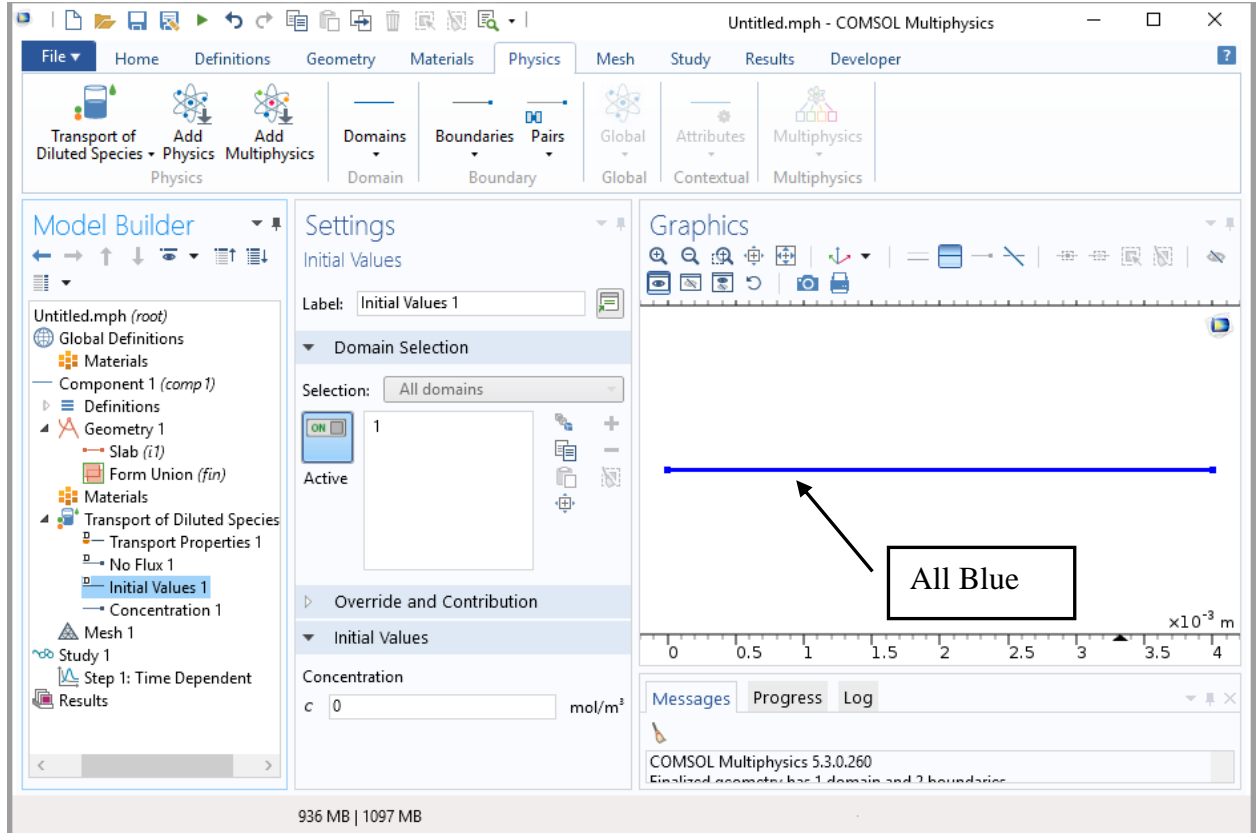




3. Select Transport Properties 1 and use the default values of the Diffusion coefficient of $1 \times 10^{-9} \text{ m}^2/\text{s}$ and zero convection.

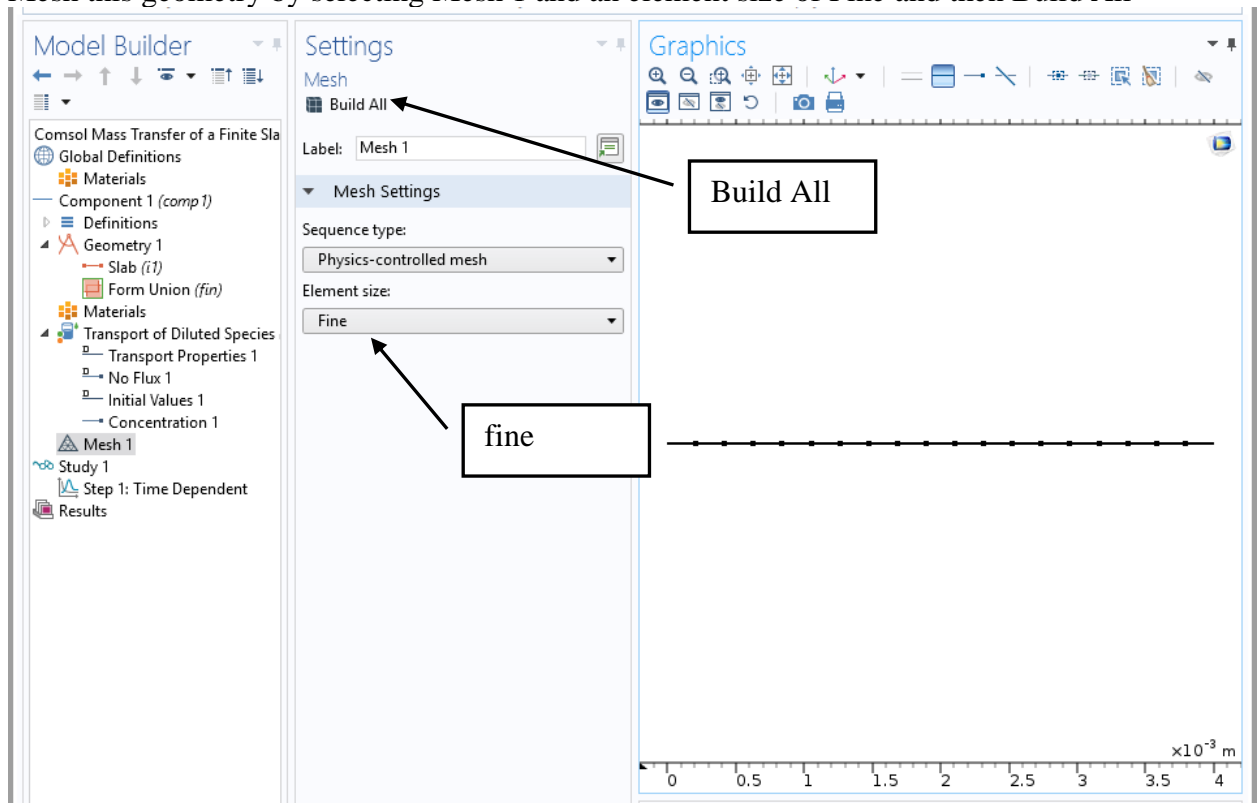


4. Also Click on Initial Values 1 to see that they are zero concentration for the entire interval. The line is now blue.



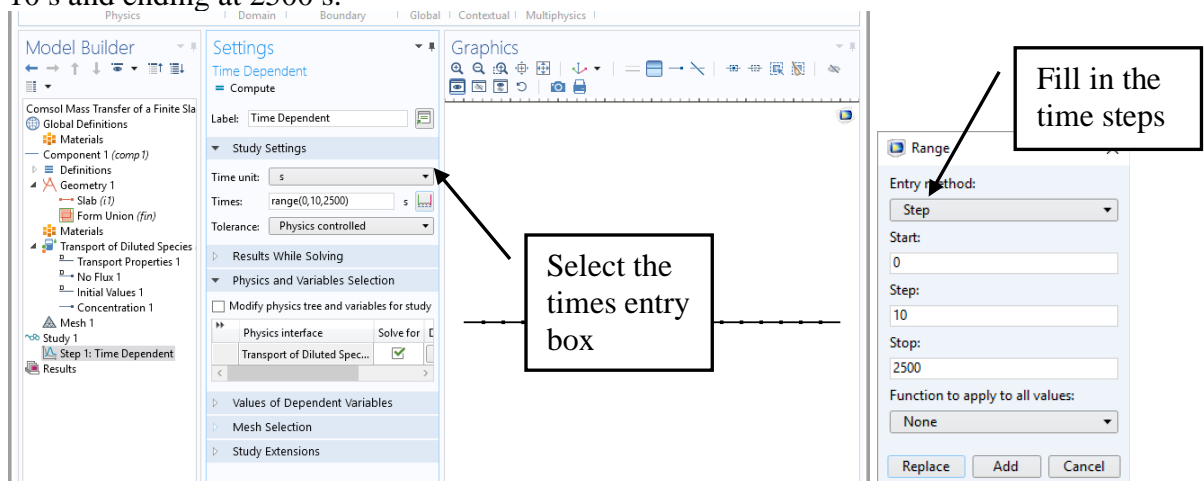
5. Perhaps now is a good time to save your file

- Mesh this geometry by selecting Mesh 1 and an element size of Fine and then Build All

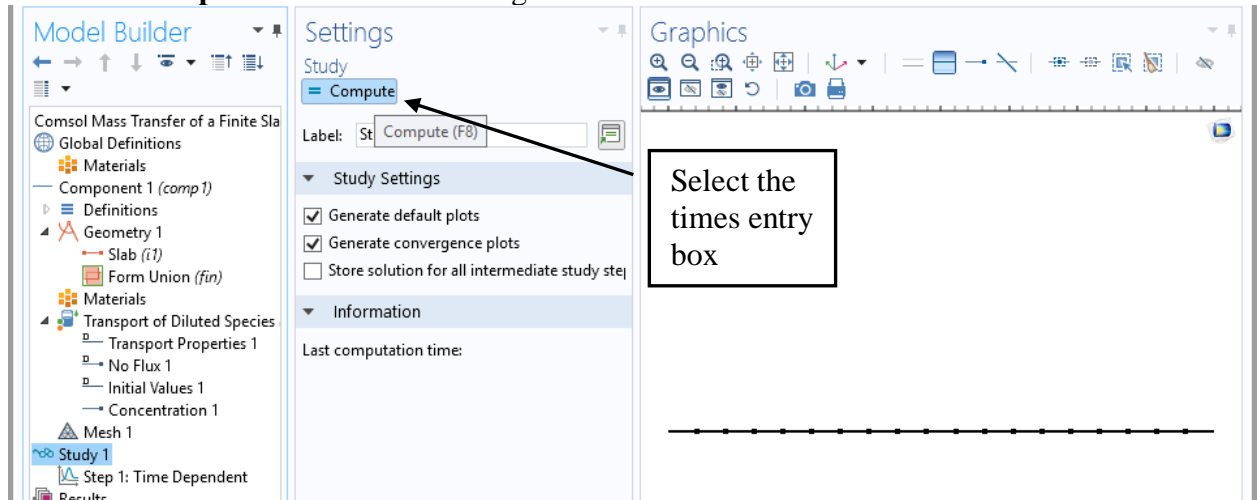


Computing the Solution

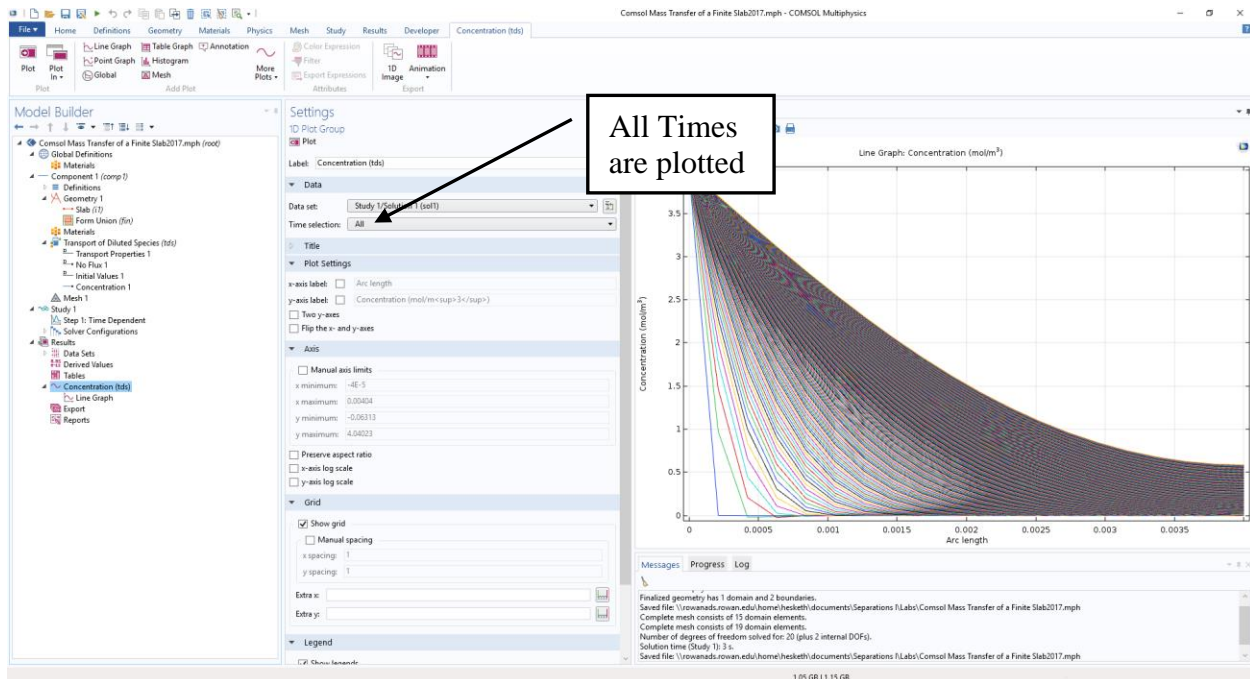
- Select **Step 1: Time Dependent** under Study 1.
- Select the times entry box and start at 0 s, Step 10 s and end at 2500 s and then select Replace. or you can type 0:10:2500 directly in the box. This stands for how you would like the output reported. This will report results starting at time $t=0$, stepping at intervals of 10 s and ending at 2500 s.



- Click the **Compute** button in the Settings Window



- WOW it plotted all of the times!



- Now compare this to a polymath solution: Pull up problem C&S10.13a from Blackboard and change the initial conditions to be zero. You may also want to change the initial concentration of CA0 to 4 mol/m³ instead of kmol/m³. This is not necessary but will aid in making a comparison plot.
- And then make a plot as shown in the following page of Concentration vs distance at 2500s. So for this plot you only need the final concentrations at t=2500s. Don't use Markers for simulated data!!

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 $d(CA2)/dt = DAB * (CA3 - 2 * CA2 + CA1) / \text{deltax}^2$
- 2 $d(CA3)/dt = DAB * (CA4 - 2 * CA3 + CA2) / \text{deltax}^2$
- 3 $d(CA4)/dt = DAB * (CA5 - 2 * CA4 + CA3) / \text{deltax}^2$
- 4 $d(CA5)/dt = DAB * (CA6 - 2 * CA5 + CA4) / \text{deltax}^2$
- 5 $d(CA6)/dt = DAB * (CA7 - 2 * CA6 + CA5) / \text{deltax}^2$
- 6 $d(CA7)/dt = DAB * (CA8 - 2 * CA7 + CA6) / \text{deltax}^2$
- 7 $d(CA8)/dt = DAB * (CA9 - 2 * CA8 + CA7) / \text{deltax}^2$

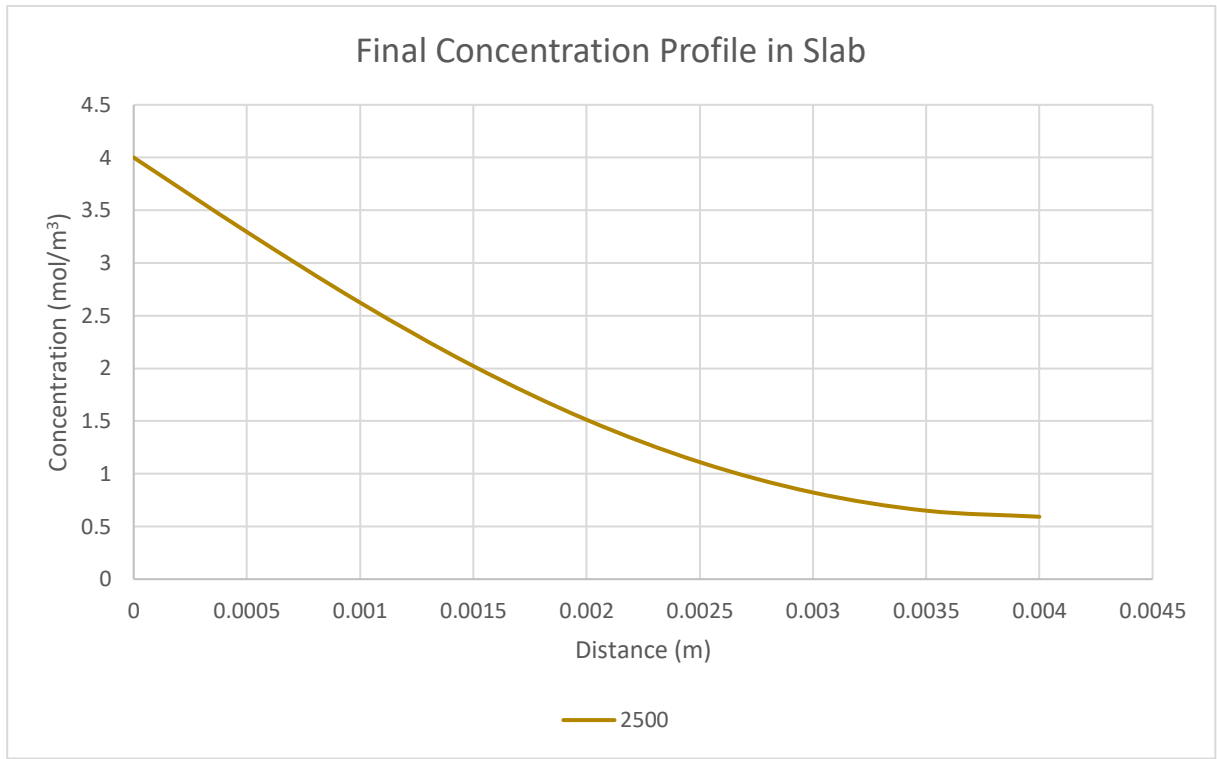
Explicit equations

- 1 $DAB = 1.0e-9$
- 2 $\text{deltax} = 0.0005$
- 3 $CA9 = \text{If } (t == 0) \text{ Then } (0) \text{ Else } ((4 * CA8 - CA7) / 3)$
- 4 $CA0 = 6.0e-3$
- 5 $K = 1.5$
- 6 $CA1 = \text{If } (t == 0) \text{ Then } (0) \text{ Else } (CA0 / K)$

General

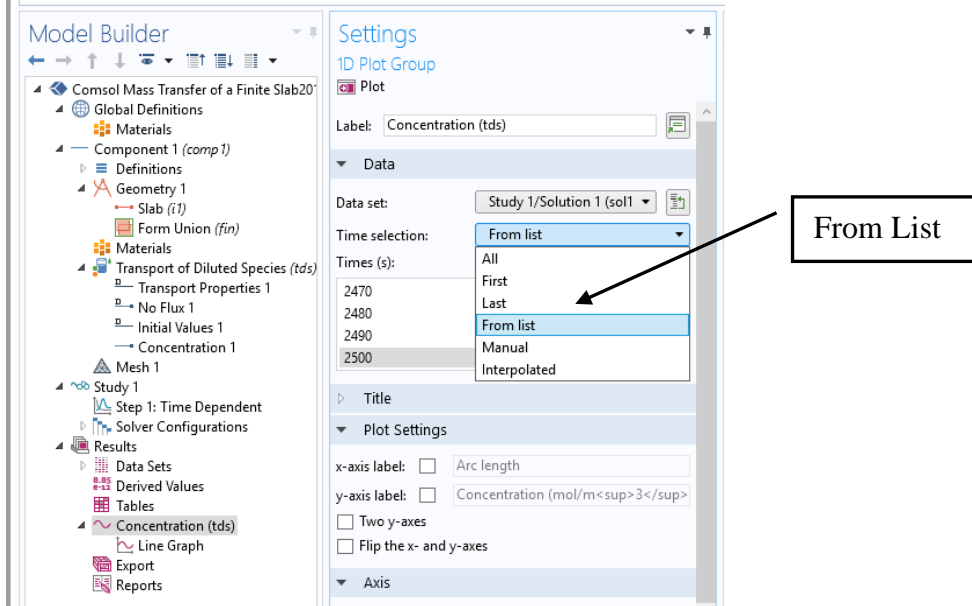
Total number of equations	13
Number of differential equations	7
Number of explicit equations	6
Elapsed time	0.000 sec
Solution method	RKF_45
Step size guess. h	0.000001
Truncation error tolerance. eps	0.000001

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

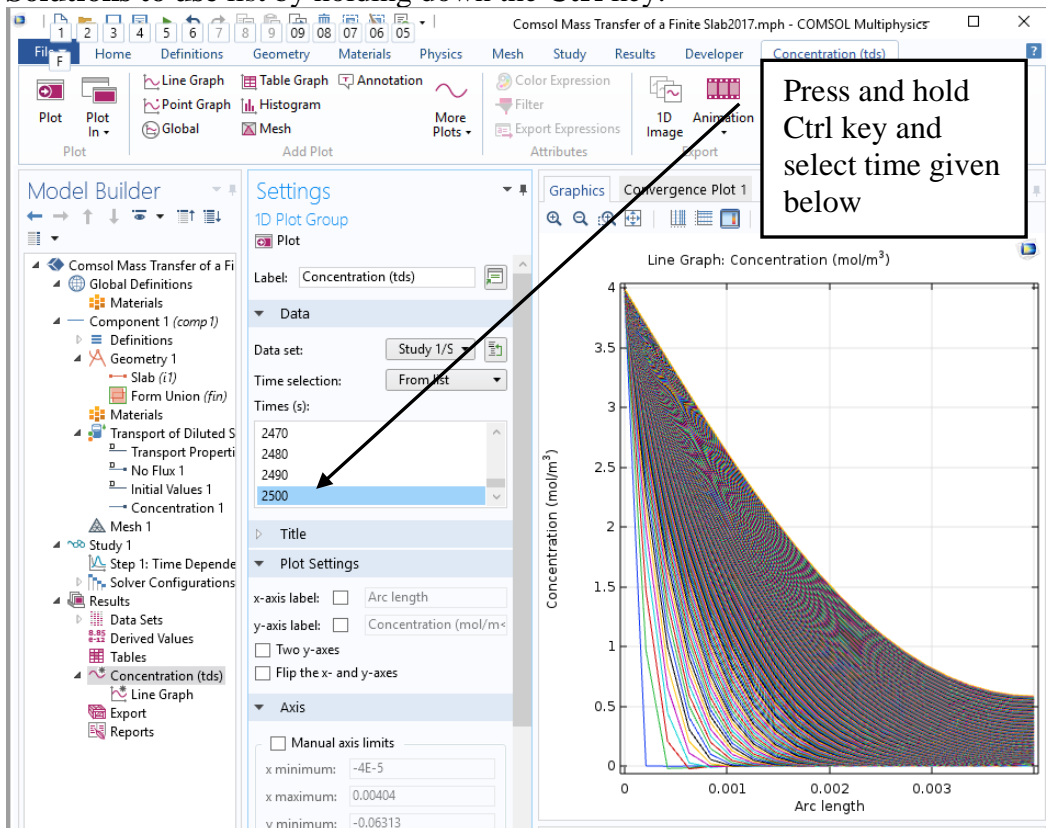


Post Mode

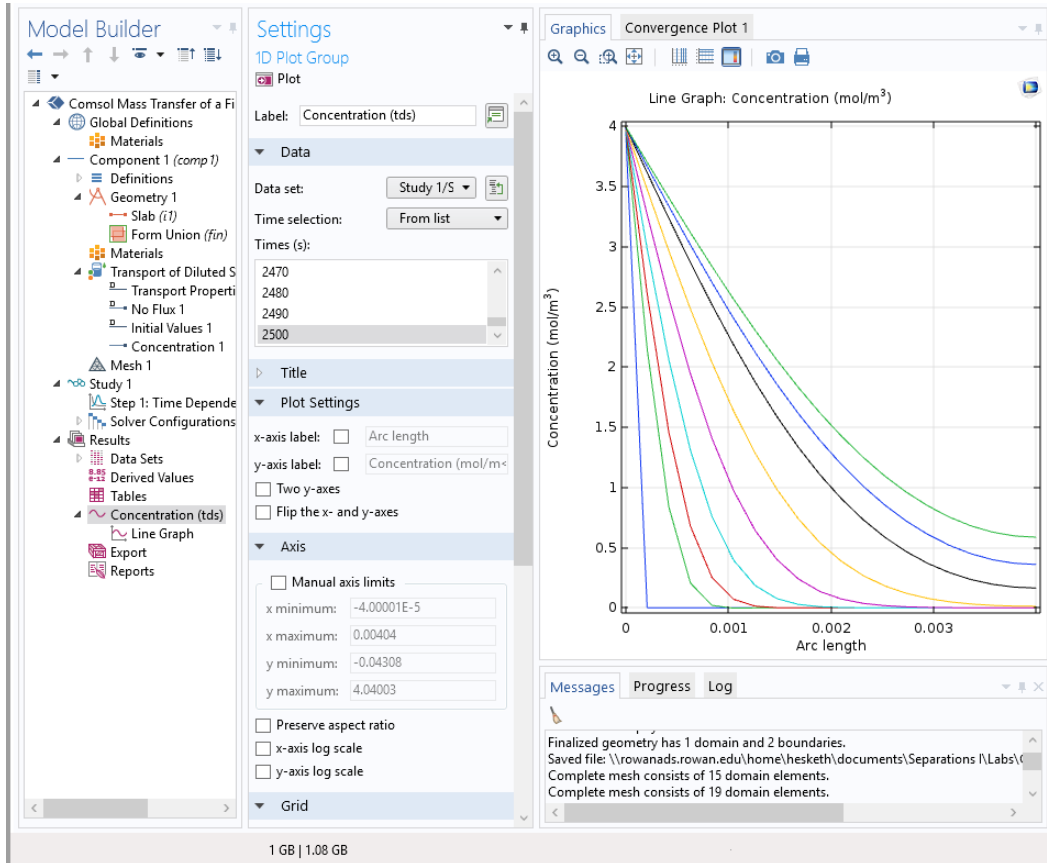
1. Select the Concentration Plot and then in the Time Selection choose **From list**.



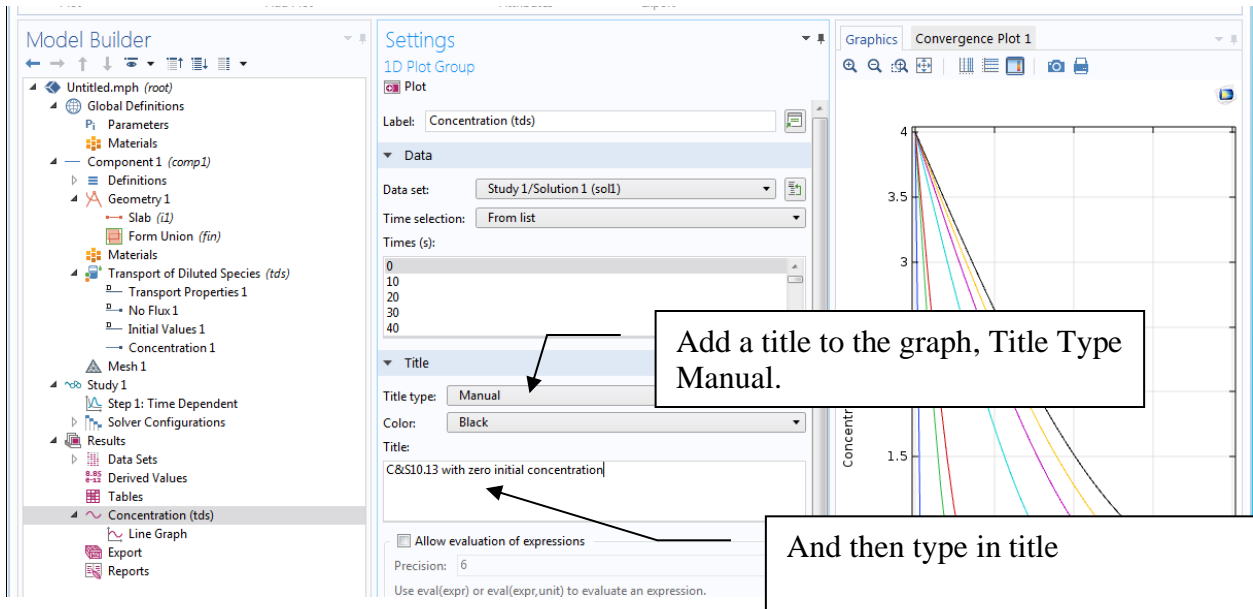
2. Select the following time-steps, 0, 50, 100, 200, 400, 800, 1500, 2000, 2500 from the **Solutions to use list** by holding down the **Ctrl** key.



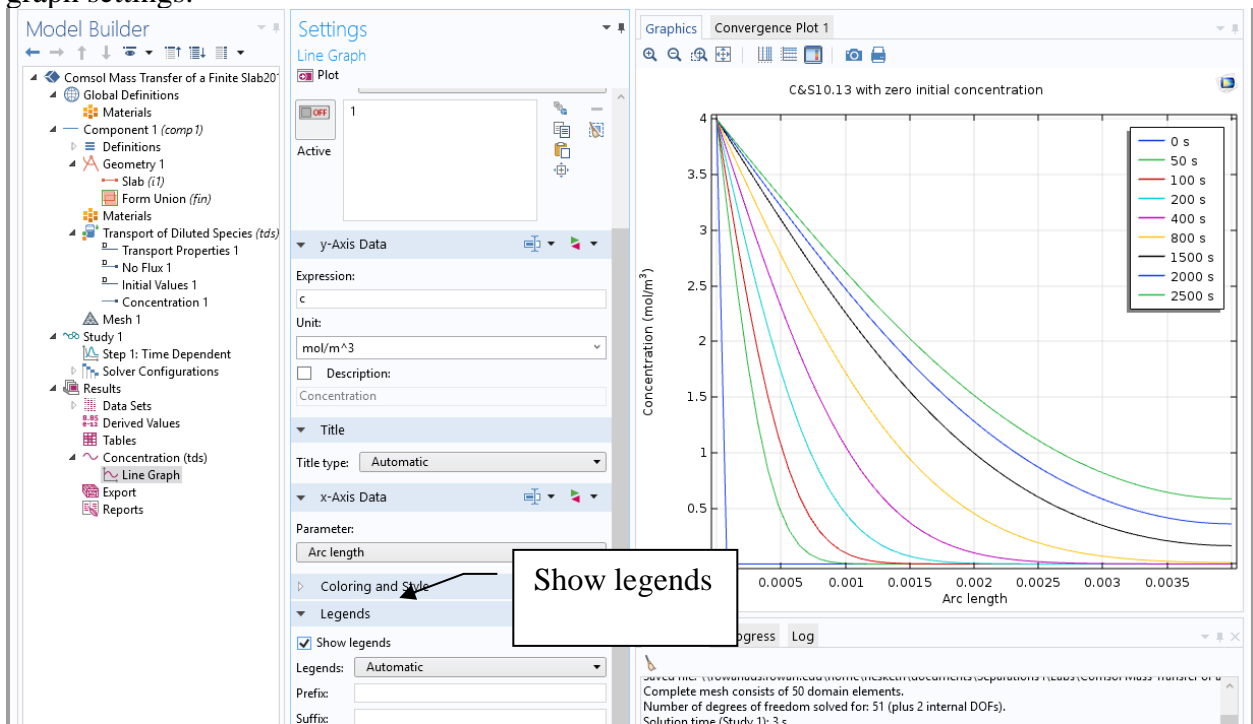
- Click on the plot button.



- Notice the kinks in the green, red and blue lines. Go back and create a finer mesh and resolve the problem. (but not too fine or you will have too many points in your graph you will make later!
- Add a title to the graph by pressing the Title/Axis button: C&S10.13 with zero initial concentration.

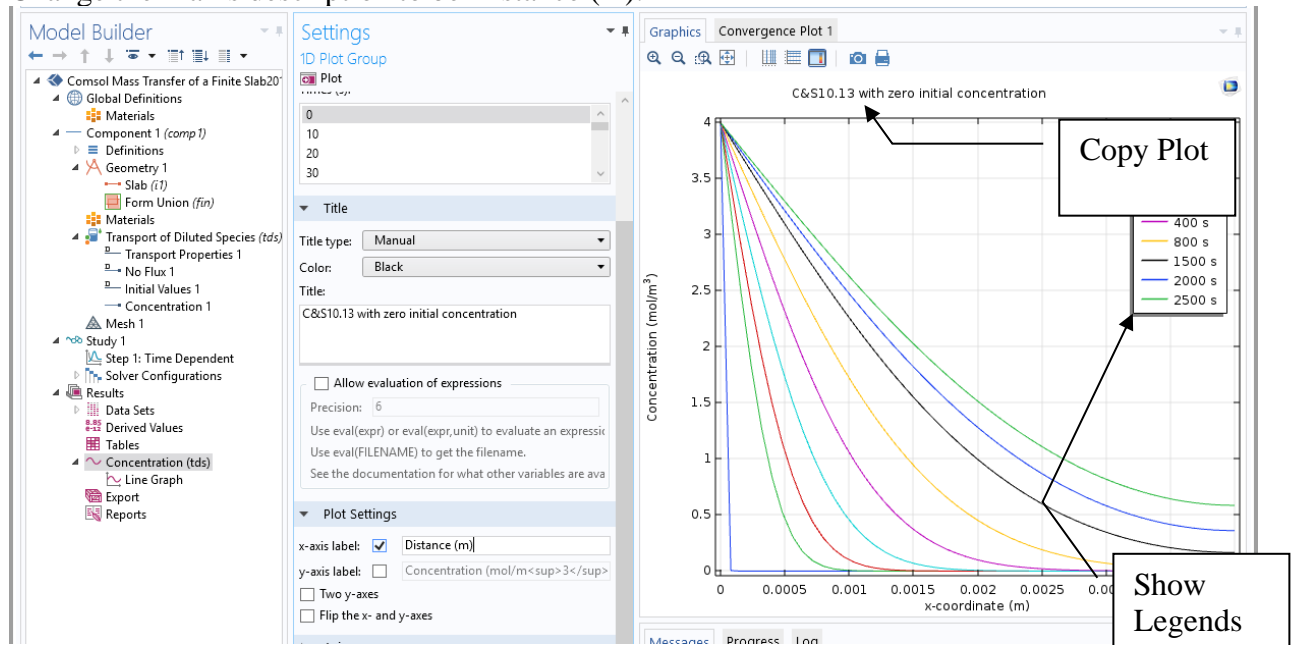


6. Select Line Graph, and then Legends to give a legend by choosing Show legends in the line graph settings.



7. You should now have a plot with a title as shown above.

8. 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).



9. 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 above.)

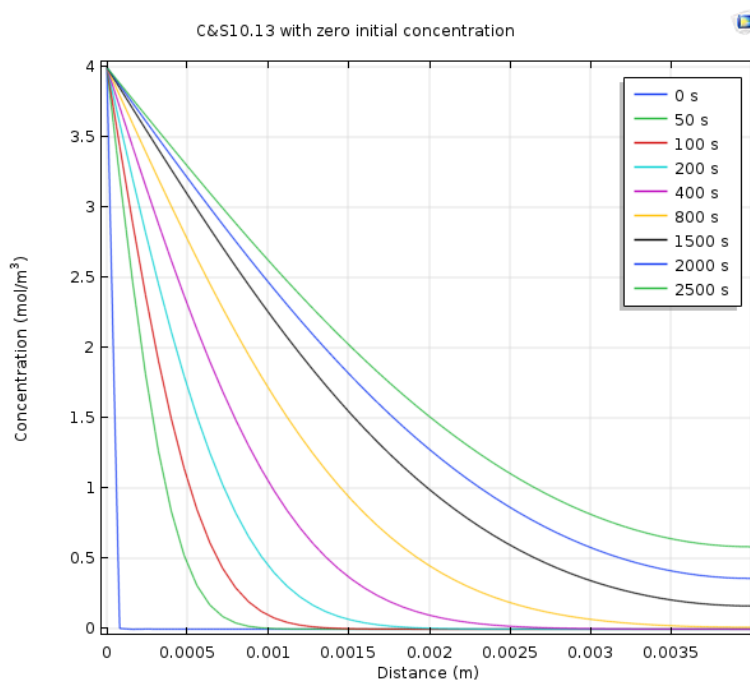


Figure 1: Problem C&S10.13 with initial concentrations of zero

10. You will now compare this plot to a plot of the polymath output. You will first make the Polymath plot and then copy this and make an additional plot in excel comparing the two

11. *Exporting the Current COMSOL Plot to your excel File*

The figure displays a 2D plot of concentration (mol/m³) versus distance (m) for a diffusion problem. The plot shows several curves representing different time steps (0 s, 50 s, 100 s, 200 s, 400 s, 800 s, 1500 s, 2000 s, 2500 s). The concentration decreases from approximately 4.0 mol/m³ at x=0 to 0 mol/m³ at x=0.0035 m. The plot is titled "C6510.13 with zero initial concentration". The software interface includes a menu bar, a toolbar, and a list of models on the left.



Book2 - Excel -> File Home Insert Page Layout Formulas DATA REVIEW VIEW Aspen Properties Aspen Simulation Workbook ADD-INS

From Access From Web From Text From Other Sources -> Existing Connections Refresh All -> Connections Properties Edit Links

Sort Filter Reapply Advanced Sort & Filter

Text to Columns Flash Fill Remove Duplicates Data Validation -> Consolidate What-If Analysis -> Data Tools

Columns

1785 0.0033600 0000000003 0.6816339613293493

1786 0.0033800 0000000003 0.6760383216265209

1787 0.0034000 0000000003 0.6704426819236564

1788 0.0034200 0000000003 0.6648470422208099

1789 0.0034400 0000000003 0.6592514025179635

1790 0.0034600 0000000003 0.654032807709502

1791 0.0034800 0000000003 0.6495551590239369

1792 0.0035000 0000000003 0.6447070372769236

1793 0.0035200 0000000003 0.6398589155299103

1794 0.0035400 0000000003 0.6357578080748274

1795 0.0035600 0000000003 0.6316567006197445

1796 0.0035800 0000000003 0.6275555931646617

1797 0.0036000 0000000003 0.6234544857095788

1798 0.0036200 0000000003 0.6200998820541279

1799 0.0036400 0000000003 0.6167452783986771

Text to Columns

Split a single column of text into multiple columns.

For example, you can separate a column of full names into separate first and last name columns.

You can choose how to split it up: fixed width or split at each comma, period, or other character.

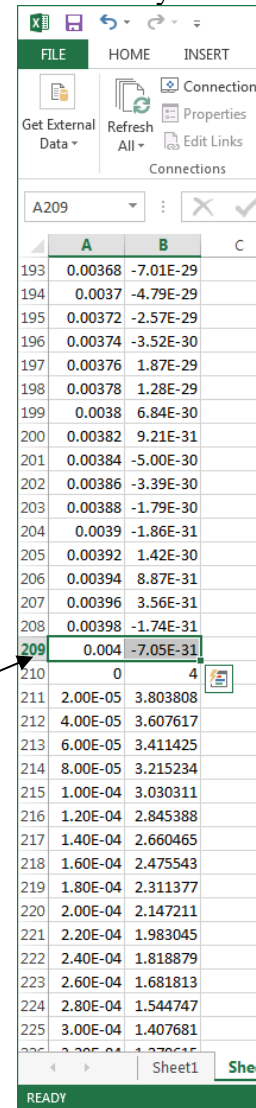
Tell me more

The screenshot shows an Excel spreadsheet with a data table. The table has columns labeled A through AC. The data in column A consists of numerical values, likely representing a time series or simulation results. A dialog box titled 'Convert Text to Columns - Step 2 of 3' is open, showing the 'Delimiters' tab. The dialog box contains a list of delimiters (Tab, Semicolon, Comma, Space, Other) and a preview of the data being converted. The data is a list of numerical values, likely representing a time series or simulation results. The status bar at the bottom indicates 'COUNT: 1809'.

18

problem is that all of the data is in these 2 columns! To locate each set you could search for

Depending on how fine your meshing is will determine how many data points you have for the first time step.

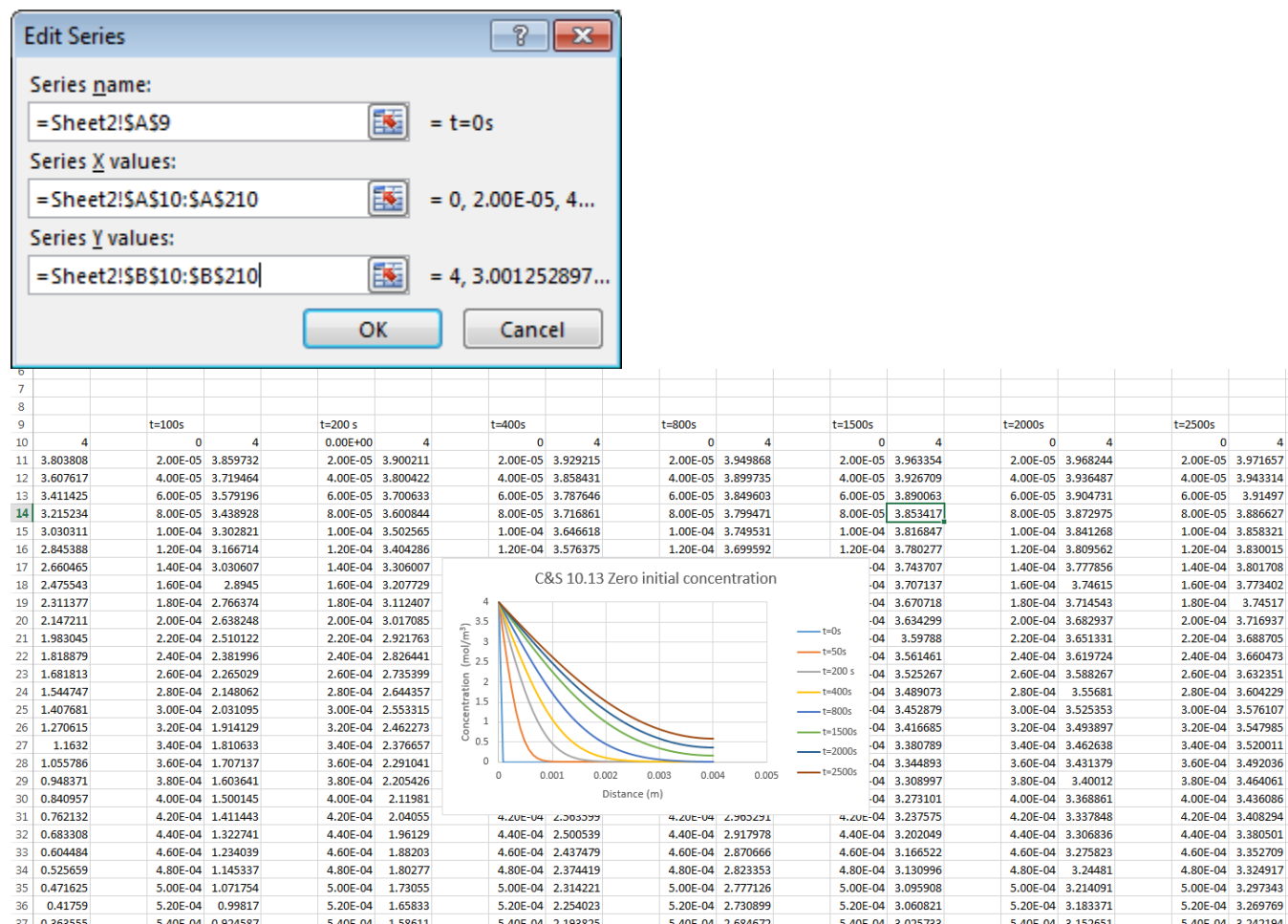


	A	B	C
193	0.00368	-7.01E-29	
194	0.0037	-4.79E-29	
195	0.00372	-2.57E-29	
196	0.00374	-3.52E-30	
197	0.00376	1.87E-29	
198	0.00378	1.28E-29	
199	0.0038	6.84E-30	
200	0.00382	9.21E-31	
201	0.00384	-5.00E-30	
202	0.00386	-3.39E-30	
203	0.00388	-1.79E-30	
204	0.0039	-1.86E-31	
205	0.00392	1.42E-30	
206	0.00394	8.87E-31	
207	0.00396	3.56E-31	
208	0.00398	-1.74E-31	
209	0.004	-7.05E-31	
210	0	4	
211	2.00E-05	3.803808	
212	4.00E-05	3.607617	
213	6.00E-05	3.411425	
214	8.00E-05	3.215234	
215	1.00E-04	3.030311	
216	1.20E-04	2.845388	
217	1.40E-04	2.660465	
218	1.60E-04	2.475543	
219	1.80E-04	2.311377	
220	2.00E-04	2.147211	
221	2.20E-04	1.983045	
222	2.40E-04	1.818879	
223	2.60E-04	1.681813	
224	2.80E-04	1.544747	
225	3.00E-04	1.407681	

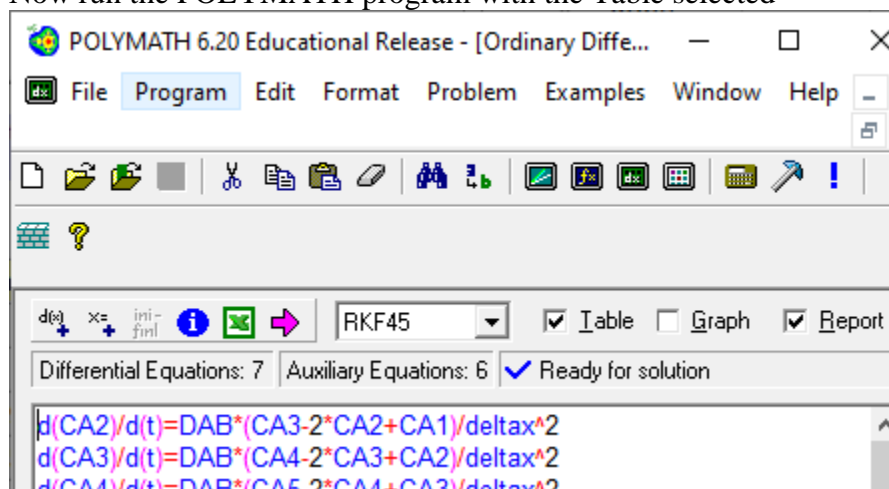
0.004 that will appear as the last data point of each data set.

15. Its now that you wish that you didn't make the mesh so fine! I use the End key and the arrow buttons to quickly navigate through excel.

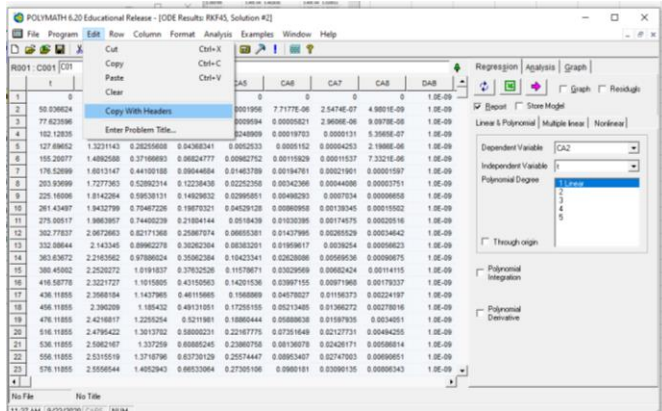
16. Now make the same plot as Figure 1 using excel. (In excel add a scatter plot and bring in each set of data. Remember to use the End key and arrow to avoid scrolling for long times!)



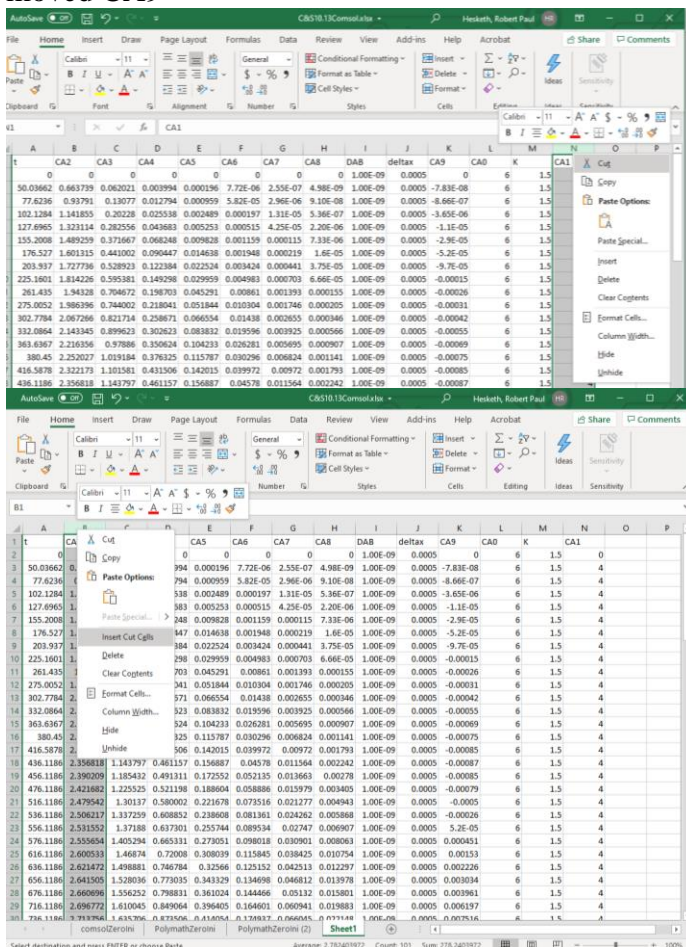
17. Now run the POLYMATH program with the Table selected



18. Copy the data using Edit, Copy with Headers

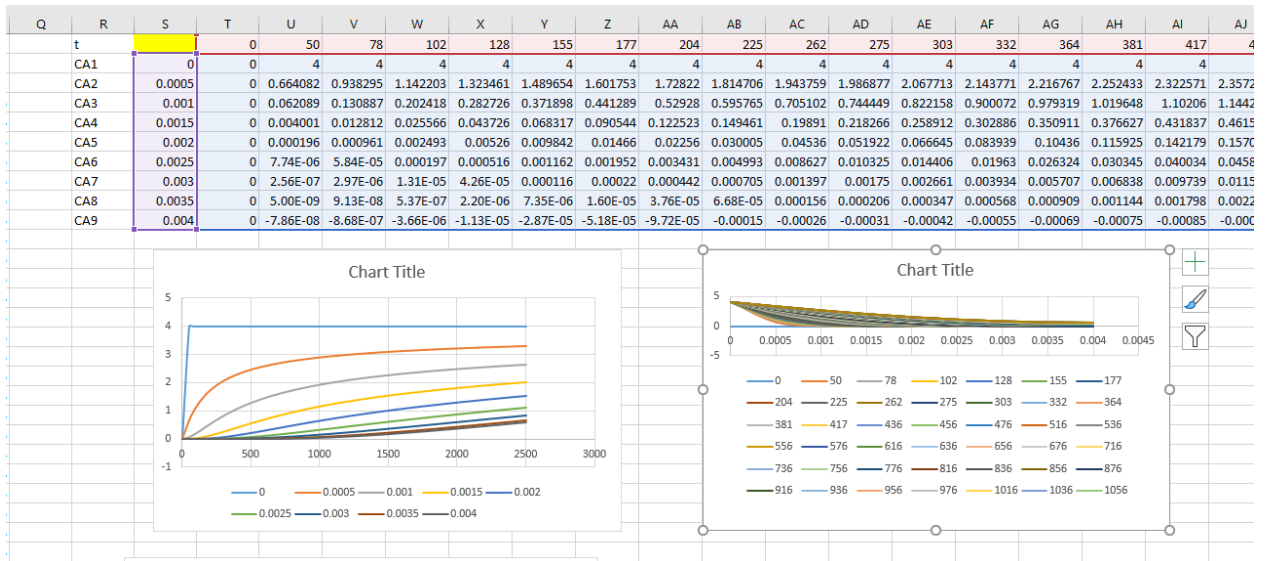


19. Now transform your Polymath output to match what is given in comsol. In other words make a plot of concentration as a function of distance at various times. First put all the concentrations in order(CA1, CA2 etc). To do this select the entire column and Cut and then click on the column letter and insert Cut Cells. I had to move CA1 before CA2. Then I moved CA9



	A	B	C	D	E	F	G	H	I	J	K
1	t	CA1	CA2	CA3	CA4	CA5	CA6	CA7	CA8	CA9	DAB
2	0	0	0	0	0	0	0	0	0	0	1.00E-05
3	50.03662	4	0.663739	0.062021	0.003994	0.000196	7.72E-06	2.55E-07	4.98E-09	-7.83E-08	1.00E-05
4	77.6236	4	0.93791	0.13077	0.012794	0.000959	5.82E-05	2.96E-06	9.10E-08	-8.66E-07	1.00E-05
5	102.1284	4	1.141855	0.20228	0.025538	0.002489	0.000197	1.31E-05	5.36E-07	-3.65E-06	1.00E-05
6	127.6965	4	1.323114	0.282556	0.043683	0.005253	0.000515	4.25E-05	2.20E-06	-1.1E-05	1.00E-05
7	155.2008	4	1.489259	0.371667	0.068248	0.009828	0.001159	0.000115	7.33E-06	-2.9E-05	1.00E-05
8	176.527	4	1.601315	0.441002	0.090447	0.014638	0.001948	0.000219	1.6E-05	-5.2E-05	1.00E-05
9	203.937	4	1.727736	0.528923	0.122384	0.022524	0.003424	0.000441	3.75E-05	-9.7E-05	1.00E-05
10	225.1601	4	1.814226	0.595381	0.149298	0.029959	0.004983	0.000703	6.66E-05	-0.00015	1.00E-05

20. Next add a row that gives distances since these are hidden in the use of the lines for CA1, CA2 etc.



21. Next add a row for the distance. I inserted two columns and then a new row under row 2. In this way I can add a label in cell B3. Next I typed in D2 a zero and in E2 0.0005. Next I selected these two cells and moved my mouse to the solid green square (the cursor turns to a black + sign when it is over the green square) to repeat this series to get values starting at 0 and ending at 0.004m with increment of 0.0005m.

The top screenshot shows a Microsoft Excel spreadsheet with the following data in the visible range:

	CA2	CA3	CA4	CA5	CA6	CA7	CA8	CA9	DAB	deltax	CA0	K
2	0	0	0	0	0	0	0	0	1.00E-09	0.0005	6	1
3	50.03662	4	0.663739	0.062021	0.003994	0.000196	7.72E-06	2.55E-07	4.98E-09	-7.83E-08	1.00E-09	0.0005
4	77.6236	4	0.93791	0.13077	0.012794	0.000959	5.82E-05	2.96E-06	9.10E-08	-8.66E-07	1.00E-09	0.0005
5	102.1284	4	1.141855	0.20228	0.025538	0.002489	0.000197	1.31E-05	5.36E-07	-3.65E-06	1.00E-09	0.0005
6	127.6965	4	1.323114	0.282556	0.043683	0.005253	0.000515	4.25E-05	2.20E-06	-1.1E-05	1.00E-09	0.0005
7	155.2008	4	1.489259	0.371667	0.068248	0.009828	0.001159	0.000115	7.33E-06	-2.9E-05	1.00E-09	0.0005
8	176.527	4	1.601315	0.441002	0.090447	0.014638	0.001948	0.000219	1.6E-05	-5.2E-05	1.00E-09	0.0005
9	203.937	4	1.727736	0.528923	0.122384	0.022524	0.003424	0.000441	3.75E-05	-9.7E-05	1.00E-09	0.0005
10	225.1601	4	1.814226	0.595381	0.149298	0.029959	0.004983	0.000703	6.66E-05	-0.00015	1.00E-09	0.0005
11	261.435	4	1.94328	0.704672	0.198703	0.045291	0.00861	0.001393	0.000155	-0.00026	1.00E-09	0.0005
12	275.0052	4	1.986396	0.744002	0.218041	0.051844	0.010304	0.001746	0.000205	-0.00031	1.00E-09	0.0005
13	302.7784	4	2.067266	0.821714	0.258671	0.066554	0.01438	0.002655	0.000346	-0.00042	1.00E-09	0.0005

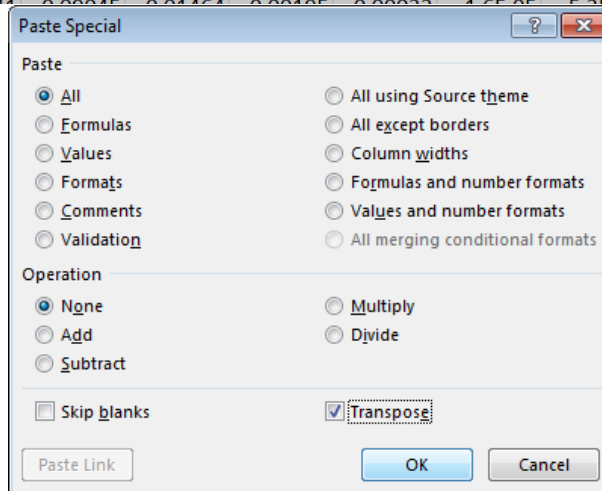
The bottom screenshot shows a zoomed-in view of a smaller spreadsheet with the following data in the visible range:

	CA1	CA2	CA3	CA4
1	t	CA1	CA2	CA3
2	x (m)	0	0.0005	
3		0	0	0
4		50.03662	4	0.663739
5		77.6236	4	0.93791
6		102.1284	4	1.141855
7		127.6965	4	1.323114

22. Select the data and copy (put mouse on the t, then press and hold Shift and then the down arrow twice (or until you reach the end of the column) and then similarly to get all of the C's.

B	C	D	E	F	G	H	I	J	K	L	M
	t	CA1	CA2	CA3	CA4	CA5	CA6	CA7	CA8	CA9	DAB
x (m)		0	0.0005	0.001	0.0015	0.002	0.0025	0.003	0.0035	0.004	
	0	0	0	0	0	0	0	0	0	0	1.00E-09
	50.0366	4	0.66374	0.06202	0.00399	0.0002	7.72E-06	2.55E-07	4.98E-09	-7.83E-08	1.00E-09
	77.6236	4	0.93791	0.13077	0.01279	0.00096	5.8E-05	2.96E-06	9.10E-08	-8.66E-07	1.00E-09
	102.128	4	1.14186	0.20228	0.02554	0.00249	0.0002	1.3E-05	5.36E-07	-3.65E-06	1.00E-09
	127.697	4	1.32311	0.28256	0.04368	0.00525	0.00052	4.3E-05	2.20E-06	-1.1E-05	1.00E-09
	155.201	4	1.48926	0.37167	0.06825	0.00983	0.00116	0.00012	7.33E-06	-2.9E-05	1.00E-09

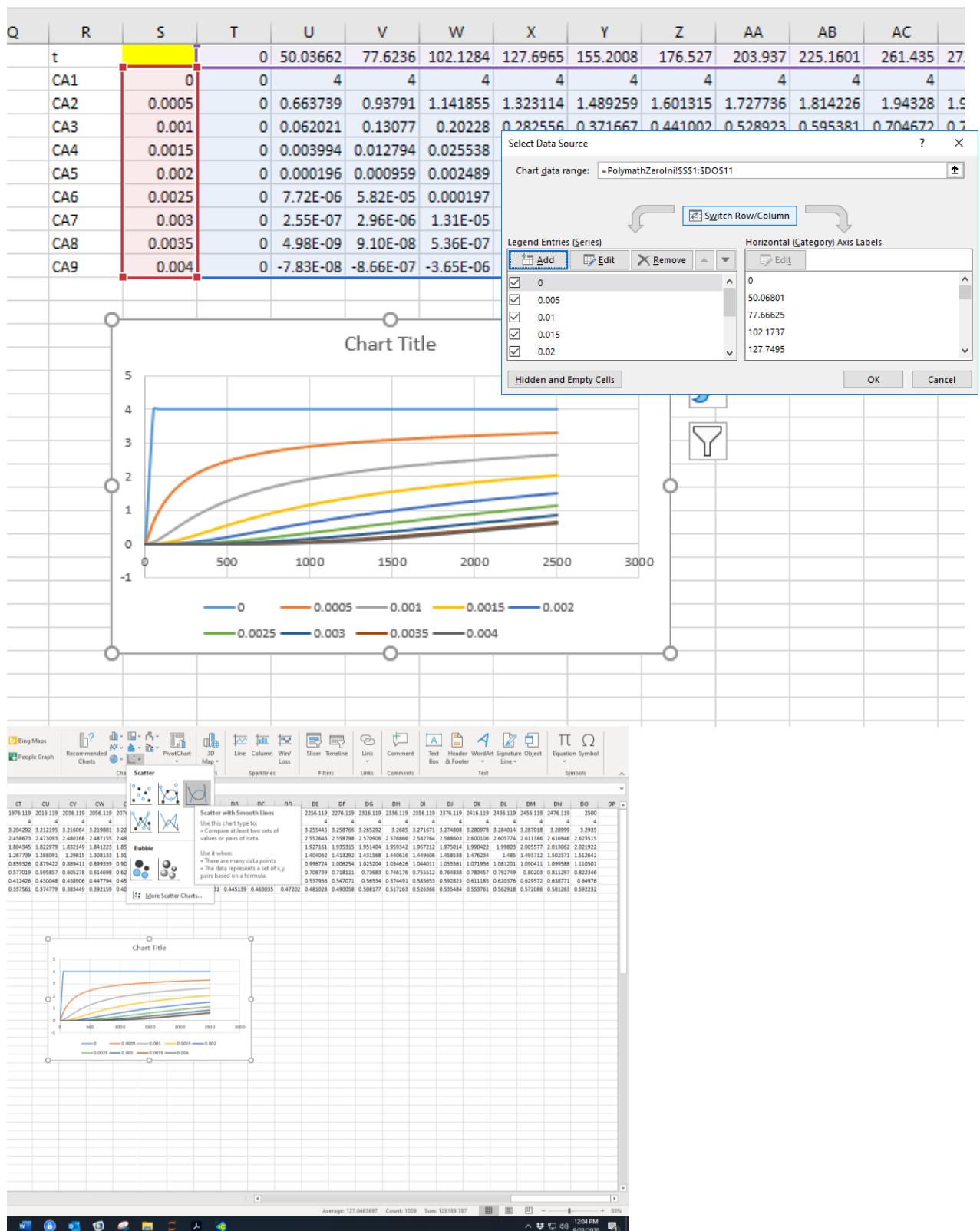
23. Then Paste Special, Transpose

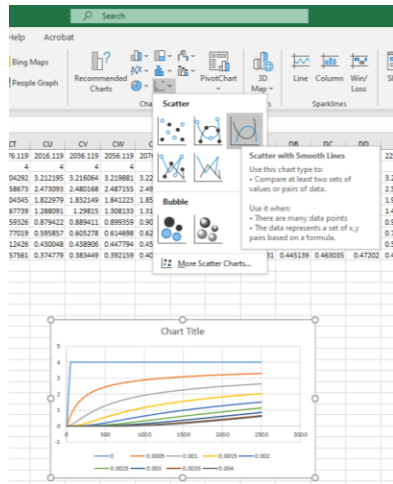


The result of the Transpose is that column S (In the image below) contains the distance entries. Row 1 contains the time entries. And the rest are concentrations in mol/m³

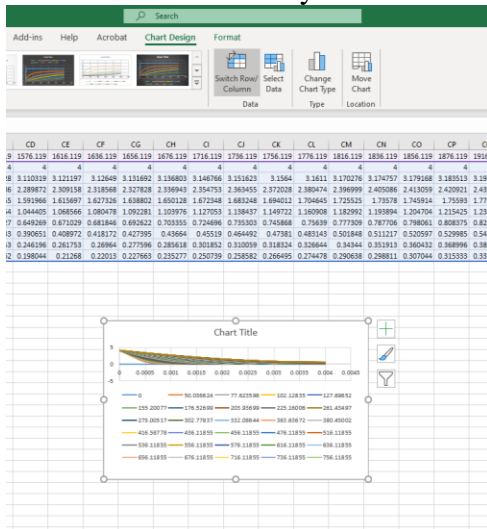
R	S	T	U	V	W	X
t		0	50.03662	77.6236	102.1284	127.69
CA1	0	0	4	4	4	
CA2	0.0005	0	0.663739	0.93791	1.141855	1.3231
CA3	0.001	0	0.062021	0.13077	0.20228	0.2825
CA4	0.0015	0	0.003994	0.012794	0.025538	0.0436
CA5	0.002	0	0.000196	0.000959	0.002489	0.0052
CA6	0.0025	0	7.72E-06	5.82E-05	0.000197	0.0005
CA7	0.003	0	2.55E-07	2.96E-06	1.31E-05	4.25E-
CA8	0.0035	0	4.98E-09	9.10E-08	5.36E-07	2.20E-
CA9	0.004	0	-7.83E-08	-8.66E-07	-3.65E-06	-1.1E-

24. Highlighting all the simulation results and time labels (In the above figure it was from S1 to DO10). Then inserting a scatter graph with smoothed lines results in a backward graph with time on the x-axis and distance as the labels.

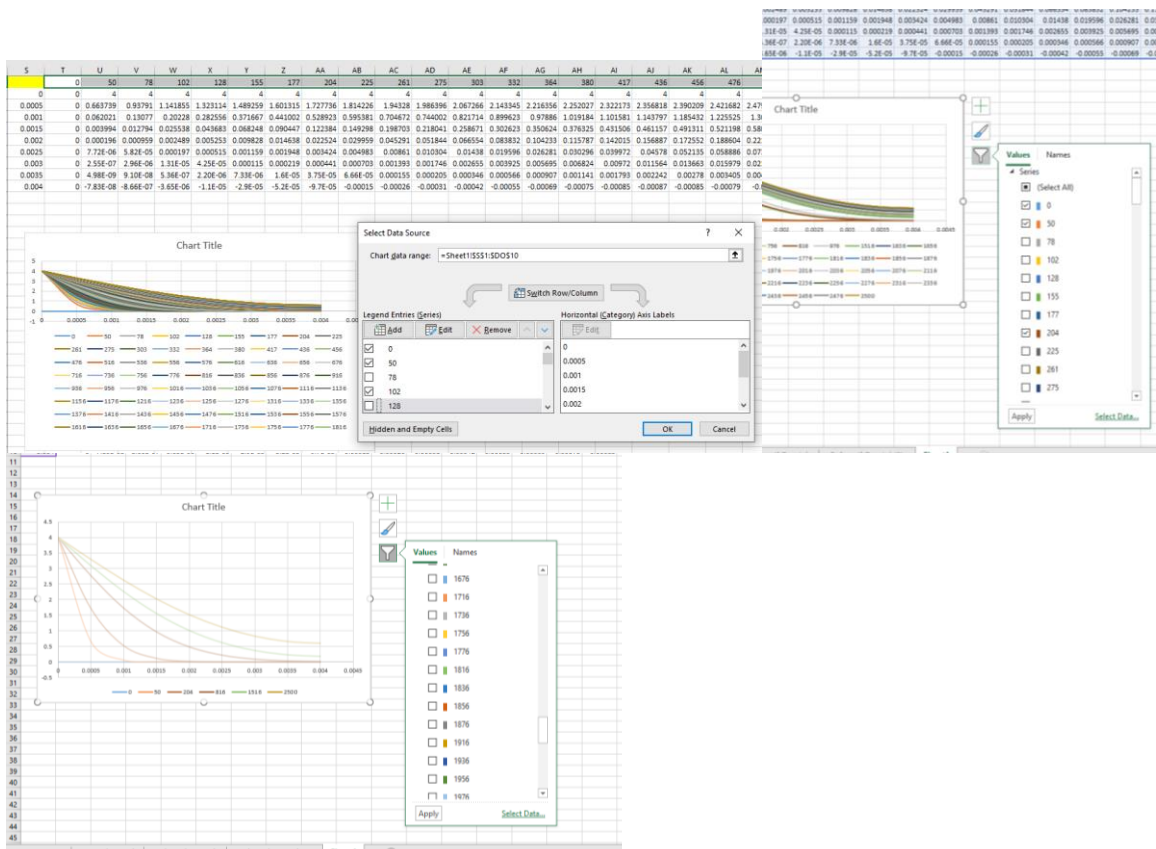




25. This can be switched by Switch Row/Column

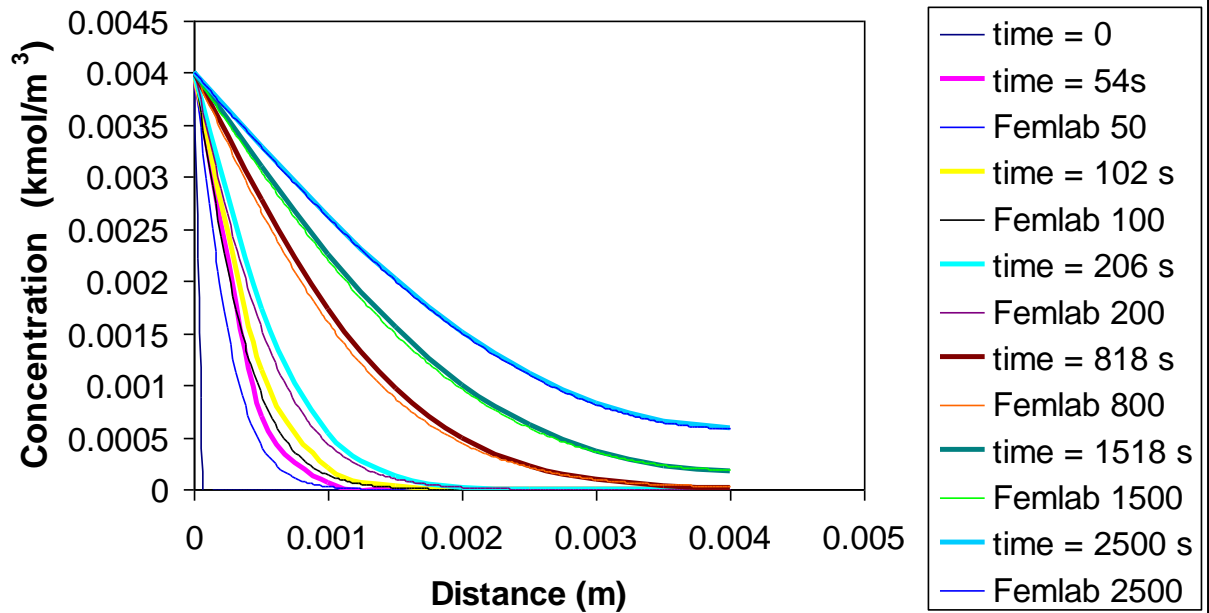


26. This is too many lines and the labels for the lines have too many digits. Format the times to show no decimal places and use then use the Format Select Data or the Funnel to the Right of the chart to only show a limited number of times on the plot



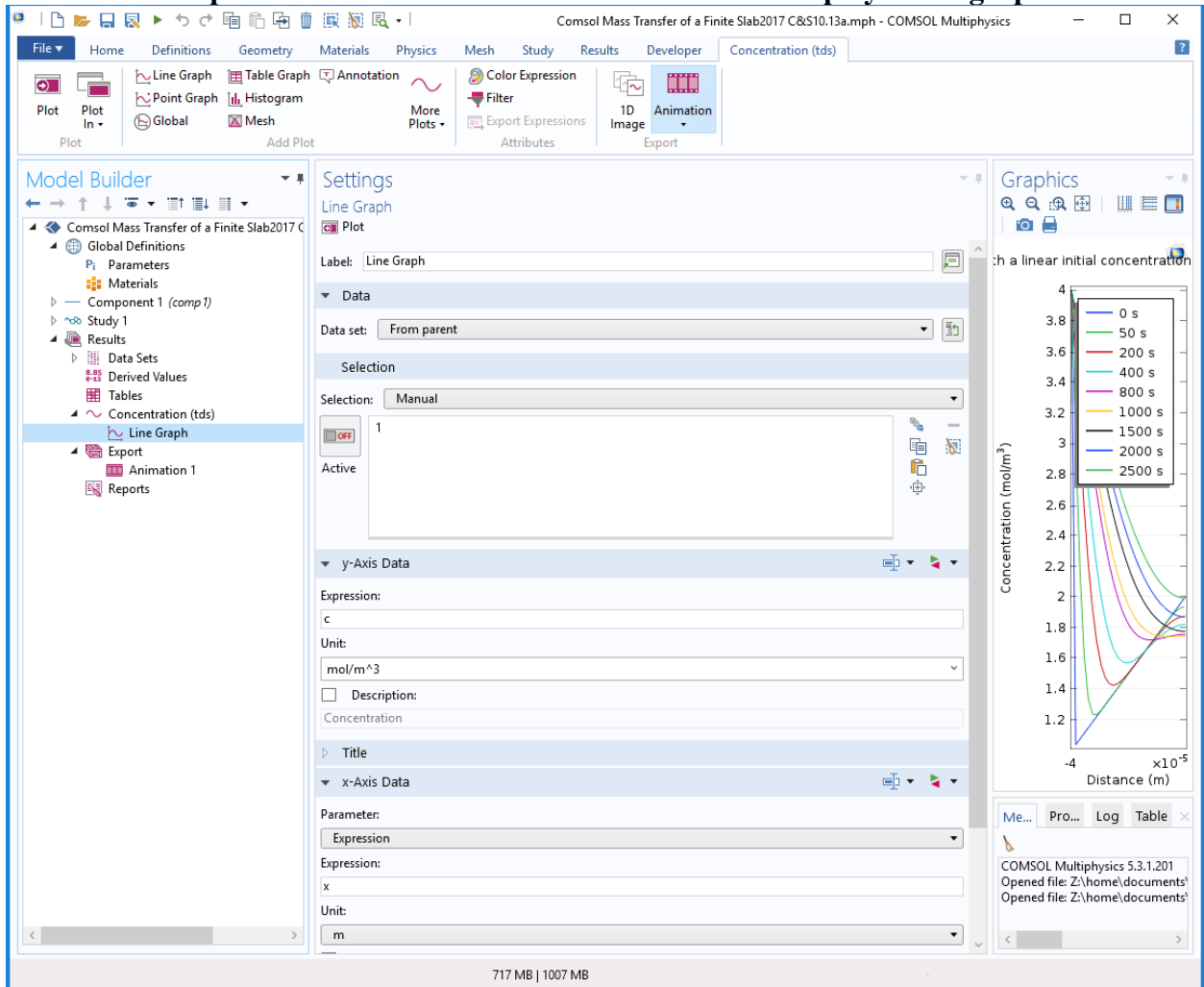
27. Next add axis labels, adjust axis limits (don't need negative numbers) and show the legend to the right of the graph.
28. Paste all 3 of the above plots into a word file.

Revised Cutlip and Shacham 7.13 Femlab and Polymath Concentration profiles

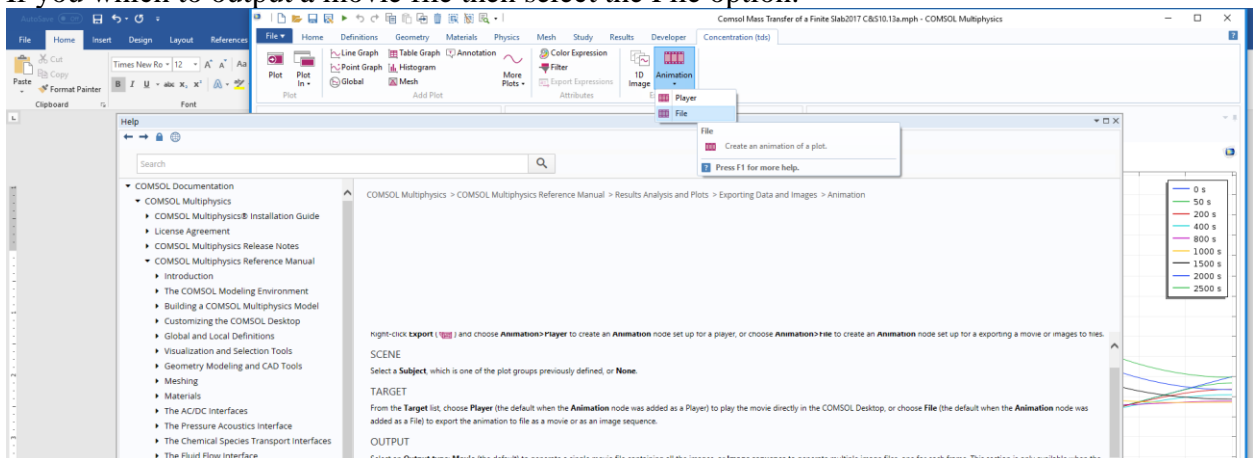


Create a Movie

29. Select **Line Graph** and then select **Animation** and a movie will play in the graph.

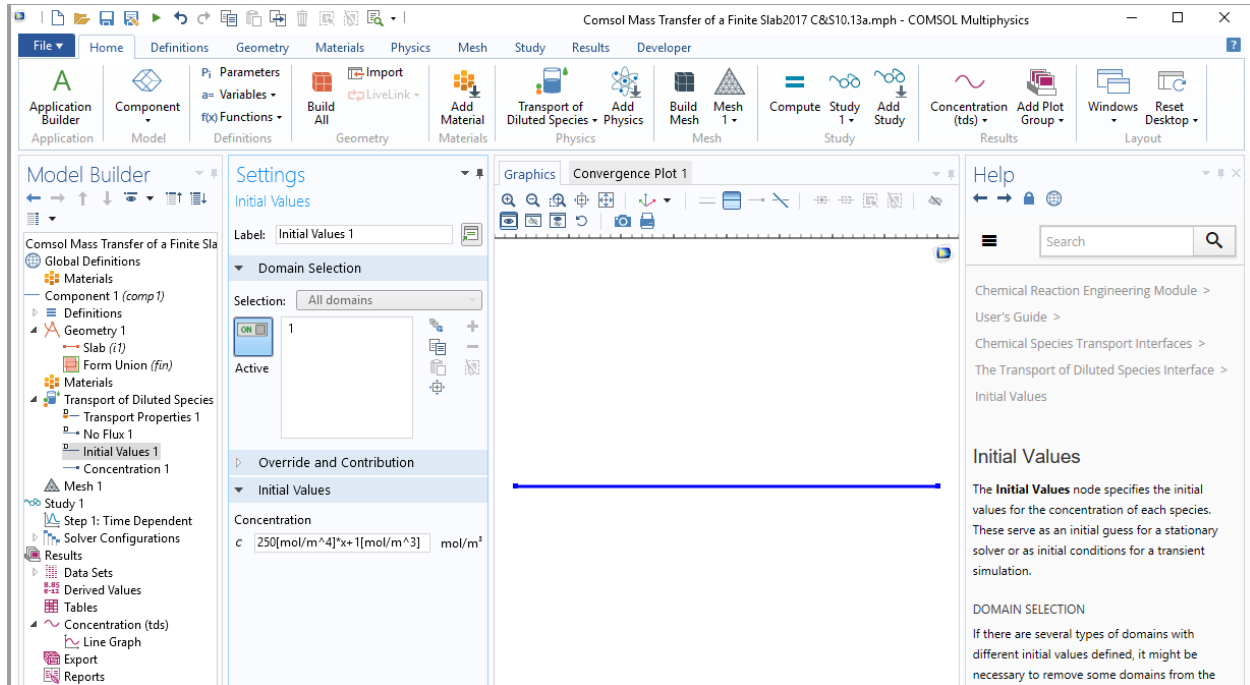


30. If you wish to output a movie file then select the File option:

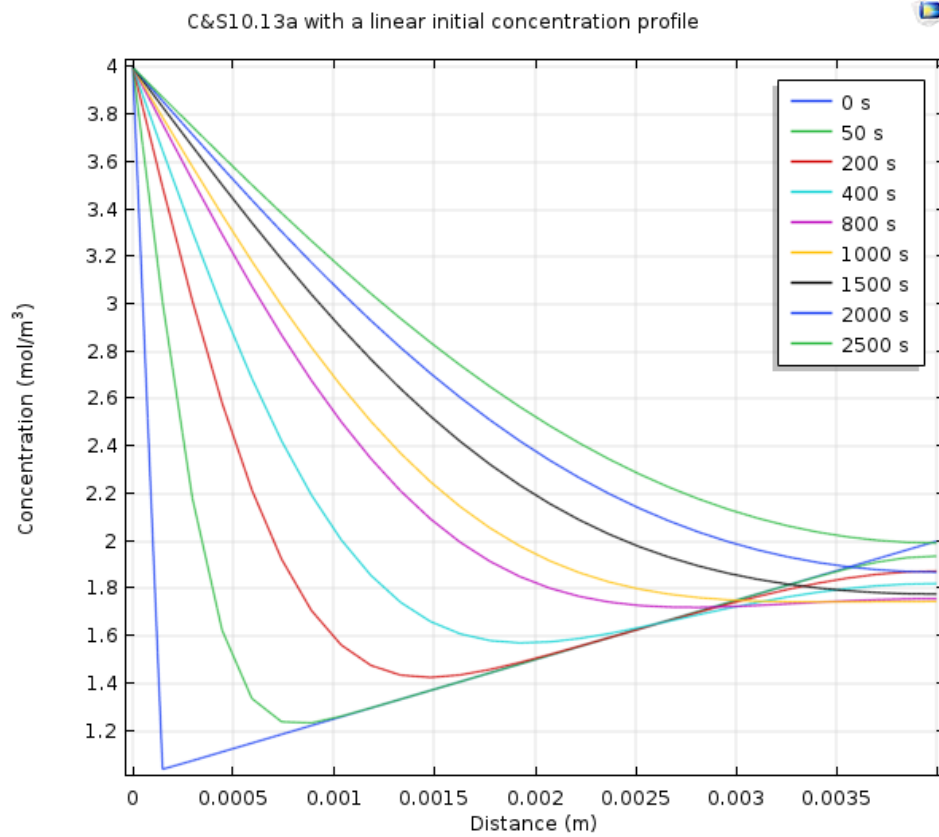


Cutlip and Shacham Problem 10.13a

31. Now we will solve the original problem 10.13a (Given originally as Geankoplis Example 7.7-1) 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/m³ over the distance of 0.004 m. This is done by entering the following equation in the Physics, Subdomain Settings,



32. 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).



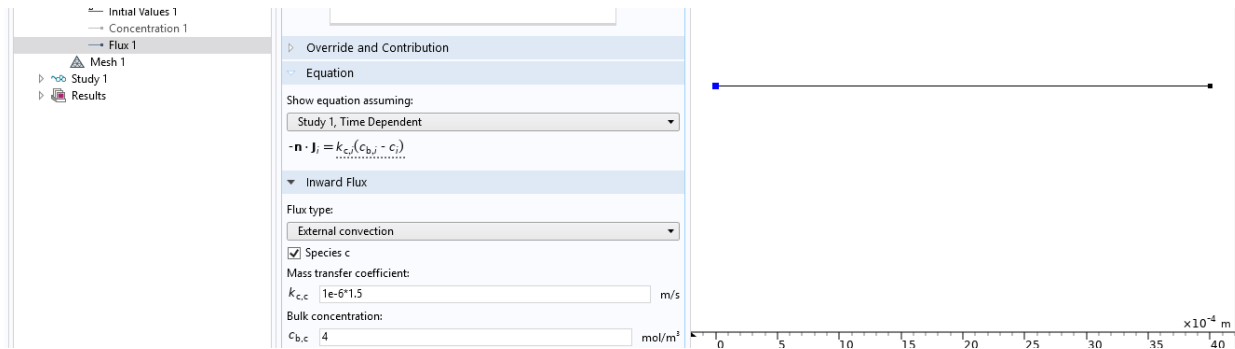
Cutlip & Shacham 10.13e – Flux boundary condition

33. In this part of the problem you need to use the flux boundary condition instead of the concentration boundary condition. The flux boundary condition uses a mass transfer coefficient. The boundary condition that you are using is based on the liquid phase concentrations:

$$N_A = k_c (C_A^{liq\ bulk} - C_A^{liq}|_{x=0}) = k_c (C_{A0}^{liq} - C_A^{liq}|_{x=0})$$

34. The comsol boundary condition is based on the solid concentration so you will need to modify the above equation as follows:

$$N_A = k_c (C_{A0}^{liq} - C_A^{liq}|_{x=0}) = k_c (C_{A0}^{liq} - K C_{A1}^{solid}) = k_c K (C_{A0}^{liq} / K - C_{A1}^{solid})$$



Submit files for Polymath and Comsol of parts 2 and 3

Submit after completing this Tutorial in a pdf document containing the following. .

1. Modified 10.13 (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 10.13a
 - a. Polymath Solution
 - b. COMSOL Plot of concentration as a function of distance with the parameter of time (default plot)
 - c. A comparison plot of POLYMATH and COMSOL in which Concentration is a function of distance with parameter of time.
 - d. Comment on the difference between the initial conditions of the solid (subdomain) as zero concentration and linear concentration.

3. (We will do this later!) Cutlip & Shacham Problem 10.13e
 - a. Polymath Solution
 - b. COMSOL Plot of concentration as a function of distance with the parameter of time (default plot)
 - c. A comparison plot of POLYMATH and COMSOL in which Concentration is a function of distance with parameter of time.
 - d. Comment on the difference between the initial conditions of the solid (subdomain) as zero concentration and linear concentration.