Unsteady-State Diffusion in a Slab

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:

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

$$C_A = 4 \times 10^{-3} \text{ kmol/m}^3 \qquad x = 0$$
Wall is insulated $\left(\frac{\partial C_A}{dx}\right|_{x=0.004m} = 0$ 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



Boundary Conditions

- 1. Select **Boundary Settings** from the **Physics** menu.
- 2. Select boundary 1 and specify the concentration as 4 mol/m³ and the second boundary condition as Insulation/symmetry.
- 3. Click OK.

I	Boundary Settings - Diffus	ion (chdi)				×	Boundary Settings - Diffu	sion (chdi)			
L	Equation					h	Equation				
	$c = c_0$						$\mathbf{n}{\cdot}\mathbf{N}=0;\mathbf{N}=-\mathbf{D}\nabla\mathbf{c}$				
	Boundaries Groups Boundary selection	c Color Boundary conditions				י ק	Boundaries Groups Boundary selection	C Color Boundary conditions			
L	1	Boundary condition:	Concentration	~			1	Boundary condition:	Insulation/Symmetry	~	
	2	Quantity	Value/Expression	Unit	Description		2	Quantity	Value/Expression	Unit	Description
		с ₀	4	mol/m ³	Concentration			с ₀	0	mol/m ³	Concentration
		N ₀	0	mol/(m ² ·	s) Inward flux			No	0	mol/(m ² ·s) Inward flux
		k _c	0	m/s	Mass transfer coefficient			k _c	0	m/s	Mass transfer coefficient
		G.	0	mol/m ³	Bulk concentration			сь	0	mol/m ³	Bulk concentration
	Group: 🗠 👻						Group: 🗠				
	Select by group						Select by group				
	Totorior boundarios						Totorior boundarios				
	Equation c = c_0 Boundaries Boundary selection 2 Boundary selection 2 Boundary selection Concentration No Select by group Interior boundaries OK Cancel				Ц						
			ОК	Cancel	Apply Help	5			ОК	Cancel	Apply Help

Subdomain Settings

- 1. Select Subdomain Settings from the Physics menu.
- 2. Select subdomain 1 and enter the Diffusion coefficient of $1X10^{-9}$ m²/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.

Subdomain Settings - Diffu	usion (chdi) 🛛 🔀	
Equation $\delta_{ts}\partial c/\partial t + \nabla \cdot (-D\nabla c) = R, c = c$	concentration	
Subdomains Groups	C Init Element Color/Style	
Subdomain selection	Species 1 Library material: Load Quantity Value/Expression Unit Description δ_{ts} Image: Comparison of the second sec	ettings - Diffusion (chdi) (-D \nabla c) = R, c = concentration Groups c Initial value Initial value Unit Description c(t_0) mol/m ³ Concentration, c
	OK Cancel Apply C Group: _ Select by V Active in	y group this domain
		OK Cancel Apply Help

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

Solver Parameters	
Analysis:	General Time Stepping Advanced
Iransient Image: Auto select solver Solver: Stationary linear Stationary nonlinear Time dependent Eigenvalue Parametric linear Parametric nonlinear	Time stepping Times: 0:10:2500 Relative tolerance: 0.01 Absolute tolerance: 0.0010 Allow complex numbers Linear system solver Linear system solver: Direct (UMFPACK) Preconditioner:
Adaptive mesh refinement	Settings
	Matrix symmetry: Nonsymmetric
	OK Cancel Apply Help





- 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/m³. This is not necessary but will aid in making a comparison plot.
- 6. And then make a plot as shown in the following page.

PC Ord	POLYMATH Report Ordinary Differential Equations			modified Unsteady-s	tate Mass Transf	er in a Slab (zero initial concentration) 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	К	1.5	1.5	1.5	1.5
14	CA1	0	0	0.004	0.004

Differential equations

1 $d(CA2)/d(t) = DAB * (CA3 - 2 * CA2 + CA1) / deltax ^ 2$ $2 <math>d(CA3)/d(t) = DAB * (CA4 - 2 * CA3 + CA2) / deltax ^ 2$ $3 <math>d(CA4)/d(t) = DAB * (CA5 - 2 * CA4 + CA3) / deltax ^ 2$ $4 <math>d(CA5)/d(t) = DAB * (CA6 - 2 * CA5 + CA4) / deltax ^ 2$ $5 <math>d(CA6)/d(t) = DAB * (CA7 - 2 * CA6 + CA5) / deltax ^ 2$ $6 <math>d(CA7)/d(t) = DAB * (CA8 - 2 * CA7 + CA6) / deltax ^ 2$ $7 <math>d(CA8)/d(t) = DAB * (CA9 - 2 * CA8 + CA7) / deltax ^ 2$

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.

Domain Plot Parameters 🛛 🛛 🔀	Domain Plot Parameters
General Line/Extrusion Point Plot type • Line/Extrusion plot Solutions to use Select via: Stored output times 2420 2430 2440 2450 2460 2480 2490 Plot in: Figure 2 Y Keep current plot Add a title to	General Line/Extrusion plot • Line/Extrusion plot Plot type • Line plot • Line settings Line color: Cycle Color Subdoma Line style: Solid line Color Subdoma Line style: Solid line Color Color Subdoma Line style: Solid line Color Color Line marker: None Color Color Line Settings



- 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.)

Edit Plot		X
Eves	Axis Axis x limits: ✓ Auto y limits: ✓ Auto → Auto → 0.5 ↓ Log scale ↓ Auto ↓<	
Delete		
	OK Cancel App	ly



- 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.

Open			? 🔀
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	Name	Size Type	Di 🔼
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My Recent	🗐 slab7-13figuredata 2006.txt	14 KB Text Document	10/
Documents	🗐 C&S5.4d.txt	15 KB Text Document	1/2
	🗐 falling film.txt	15 KB Text Document	12/
	🗐 annular newtonian.txt	15 KB Text Document	11/
Desktop	📃 laminar flow velocity profile.txt	15 KB Text Document	11/
	🗐 fullydeveloped parallel plate.txt	15 KB Text Document	11/
	🗐 slab7-13figuredata.txt	262 KB Text Document	9/2
	📃 slab7-13dataoutput.txt	6 KB Text Document	9/2
My Documents	🗐 figureC&Smodified.txt	118 KB Text Document	9/2
	📃 6-13 wood diff.txt	10 KB Text Document	11/
	📃 6-13a wood.txt	3 KB Text Document	11/
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My Computer	🗐 6-13 SS316.txt	10 KB Text Document	11/ 🚩
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Places	Files of type: Text Files (*.prn; *.txt; *.csv)	▼	Cancel

15. Next a Text Import Wizard will open. Select fixed width and then <u>N</u>ext. Check to see that the data is being imported in two columns by scrolling down with the scroll bar and then press <u>F</u>inish.

Text Import Wizard - Step 1 of	3		? 🗙
The Text Wizard has determined that y If this is correct, choose Next, or choose Original data type Choose the file type that best describ O Delimited - Characters suc O Fixed width - Fields are align	our data is Delimited. te the data type that b es your data: th as commas or tabs se ed in columns with space	est describes your data. eparate each field. ces between each field.	
Start import at <u>r</u> ow: 1 Preview of file C:\Documents and Sett	File <u>o</u> rigin:	437 : OEM United States	*
1 % Coordinates 2 0.0 3 2.2222228-5 4 4.4444458-5 5 6.6666678-5	4.0 2.2222223 0.8888889 0.0		
	Cancel < B	ack <u>Next ></u> <u>Fi</u> n	ish

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.

	Δ	D
	A	D
	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:

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	2	0	4		
	3	2.22E-05	2.222222		
	4	4.44E-05	0.888889		
	5	6.67E-05	0		
	6	8.89E-05	-0.44444		
	7	1.11E-04	-0.44444		
	8	1.33E-04	0		
	9	1.56E-04	0		
	10	1.78E-04	0		
	11	2.00E-04	0		
	12	2.22E-04	0		
	13	2.44E-04	0		
	14	2.67E-04	0		
	15	2.89E-04	0		
	16	3.11E-04	0		
	17	3.33E-04	0		
l	18	3.56E-04	0		
5	19	3.78E-04	0		
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	25	5.11E-04	0		
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NUM

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.

Plot Parameters	X
Plot Parameters General Line Max/Min Animate Movie settings File type: AVI Width (in pixels): 640 Height (in pixels): 480 Frames per second: 10 Static / Eigenfunction animation Cycle type: Cycle type: Full harmonic	Solutions to use Select via: Stored output times V 0 10 20 30 40 50
Number of frames: 11	60 70 80 Times:
	OK Cancel Apply

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/m³ over the distance of 0.004 m. This is done by entering the following equation in the Physics, Subdomain Settings,

Subdomain Settings - Dif	fusion (di)		×		
Equation δ _{ts} ∂c/∂t + ∇∙(-D∇c) = R, c = concentration					
Subdomain selection	c Init Elen	nent			
	Variable	Initial value	Description		
 ✓ Select by group ✓ Active in this domain 	c(t ₀)	0.25*x+1e-3	Concentration, c		
		ОК	Cancel Apply		

- 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.

	Solver Manager	
	Solver weiteBet	
	Initial Value Solve For Output Script	1
ving from the initial	Initial value	
a the second large	Initial value expression	
ig the problem.	Initial value expression evaluated using current solution	
ager and select Initial	O Current solution	
	O Initial value expression evaluated using stored solution	
llowing result after	O Stored solution	
	o Domain Plot Parameters	X
blotted and request a	Pc	
strusion tab and select	General Line/Extrusion Point	
	Line/Extrusion plot	
did not use the	Plot type	
and not use the	Line plot O Extrusion plot	
	y-axis data	
	Predefine Line Settings	
	Expressio	
	Subdoma Line childry Califating	- 1
	Line style. Solid line	
	OK Cancel	
	Line Settings Surface Settings	
	OK Cancel Appl	<u>y</u>
Cutlip and Shacham 7.13a		
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	400	
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	: : : 1500	
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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.

Line Setting	şs	
Line color:	Cycle	Color
Line style:	Solid line	×
Line marker:	None	✓
🗹 Legend		
		OK Cancel

Cross-Section Plot	Parameters	X
General Point		
_y-axis data		
Predefined quantiti	ies: Concentration, c 💌 💌	
Expression:	с	
Coordinates		
x: O	0.001 0.002 0.003 0.004	
Line Settings]	
	OK Cancel Apply	,



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

$$N_{A} = k_{c} (C_{A0} - C_{Ai}) = k_{c} (C_{A0} - KC_{A}|_{x=0})$$

33. To modify this for the COMSOL boundary conditions

$$N_{A} = k_{c} \left(C_{A0} - K C_{A} \right|_{x=0} \right) = K k_{c} \left(\frac{C_{A0}}{K} - C_{A} \right|_{x=0} \right)$$

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.