Finite Element Modules for Enhancing Undergraduate Transport Courses: Application to Fuel Cell Fundamentals

Originally published in 2007 American Society for Engineering Education Conference Proceedings

Example 3: Heat Transfer in a Composite Slab with Reaction

Note: This example problem has been used in an elective course "Fuel Cell Fundamentals" which is taken by chemical, mechanical, electrical, and biomedical engineering students as well as students in materials science. The students range in experience from sophomore to seniors level. Thus this problem is meant to illustrate the ease by which the software can be applied to practical problems.

Problem Statement: Consider heat transfer within a fuel cell bipolar plate. A schematic of the geometry is shown below.
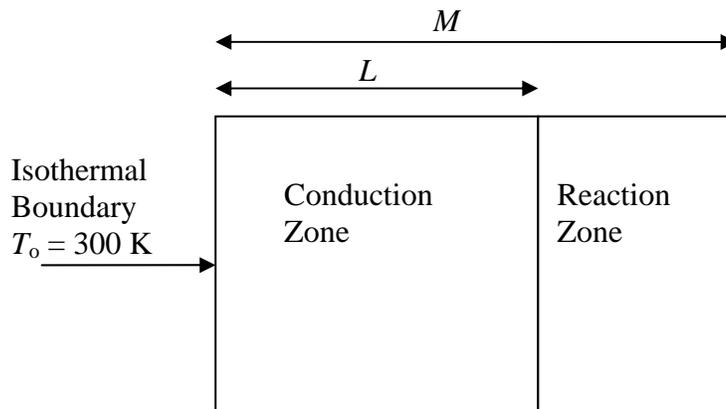
All other external boundaries are insulated and have no heat flux into or out of them. There is continuity of flux and temperature at the conduction zone and reaction zone interface.

The distance from the isothermal boundary to the interface between the conduction and reaction zone is L and the distance from the isothermal boundary to the far edge of the reaction zone is M.

The insulated boundaries on the top and bottom essentially make this a one-dimensional heat conduction problem. In the conduction zone, the governing equation is:

$$k \frac{\partial^2 T}{\partial x^2} = 0$$

and in the reaction zone the governing equation is:

$$k \frac{\partial^2 T}{\partial x^2} = -Q$$

where Q is a uniform heat source per unit volume of 100,000,000 W/m^3 within the reaction zone. The value of k is the thermal conductivity and is equal to 20 W/m-K for the bipolar plate. Your task is to find the maximum temperature for the following parameter choices (all distances are in meters)

- $L = 0.010$, $M = 0.011$
- $L = 0.005$, $M = 0.006$
- $L = 0.001$, $M = 0.002$

and compare with the analytical solution given by:

$$T_{max} = T_o + \frac{Q}{2k}\left(M^2 - L^2\right)$$

Part 1: Create the domain.
1. Start the software.
2. Once FEMLAB / Comsol Multiphysics launches, click on the plus sign at the following locations: "Chemical Engineering Module," "Energy Balance," "Conduction," and then select "Steady State Analysis."
3. Click OK

Part 2: Draw the heat transfer geometry
1. Hold down the shift key and click on the rectangle in the upper left corner of the screen. A window will appear. Insert the following values: For Size use Width = 0.010, Height = 0.1. For Position use x = 0, y = 0.
2. Click OK
3. Repeat step 1, but insert the following values: For Size use Width = 0.001, Height = 0.1. For Position use x = 0.010, y = 0.
4. Click OK
5. Click the "Zoom Extends" button on the main toolbar. It looks like a red cross with a magnifying glass.

Part 3: Apply physical properties
1. From the top menu, select "Physics," then "Subdomain Settings"
2. Select subdomain 1, and enter the thermal conductivity (make sure the isotropic radio button is selected) as 20 (you do not have to enter the heat capacity or thermal conductivity as this is a steady-state problem).
3. Select subdomain 2, and enter the same value for thermal conductivity as in subdomain 1. For heat source, enter a value of 1e8.
4. Click OK

Part 4: Apply boundary conditions
1. From the top menu, select "Physics," then "Boundary Settings"

2. Click on boundary number 1, select "Temperature" from the pull-down menu, and enter 300.
3. Hold down the shift key, and select boundaries 2, 3, 5, 6, and 7. Make sure it says "Thermal Insulation" on the pull-down menu.
4. Click OK

Part 5: Create the mesh
1. Click on the hollow triangle to initialize the mesh.
2. Click on the filled triangle to refine the mesh, once.

Part 6: Solve
1. Click on "Solve" from the pull-down menu, and select Solver Parameters."
2. Select "Stationary Linear"
3. Click OK
4. Click on "Solve" from the pull-down menu, and select "Solve Problem." You should see the geometry with a color spectrum indicating a temperature profile. If you don't see anything, click on "Zoom Extends."
5. Click on the "Zoom Window" button (looks like a magnifying glass with a red square) to zoom in on the right boundary. Click within the geometry to determine the temperature at the right edge.
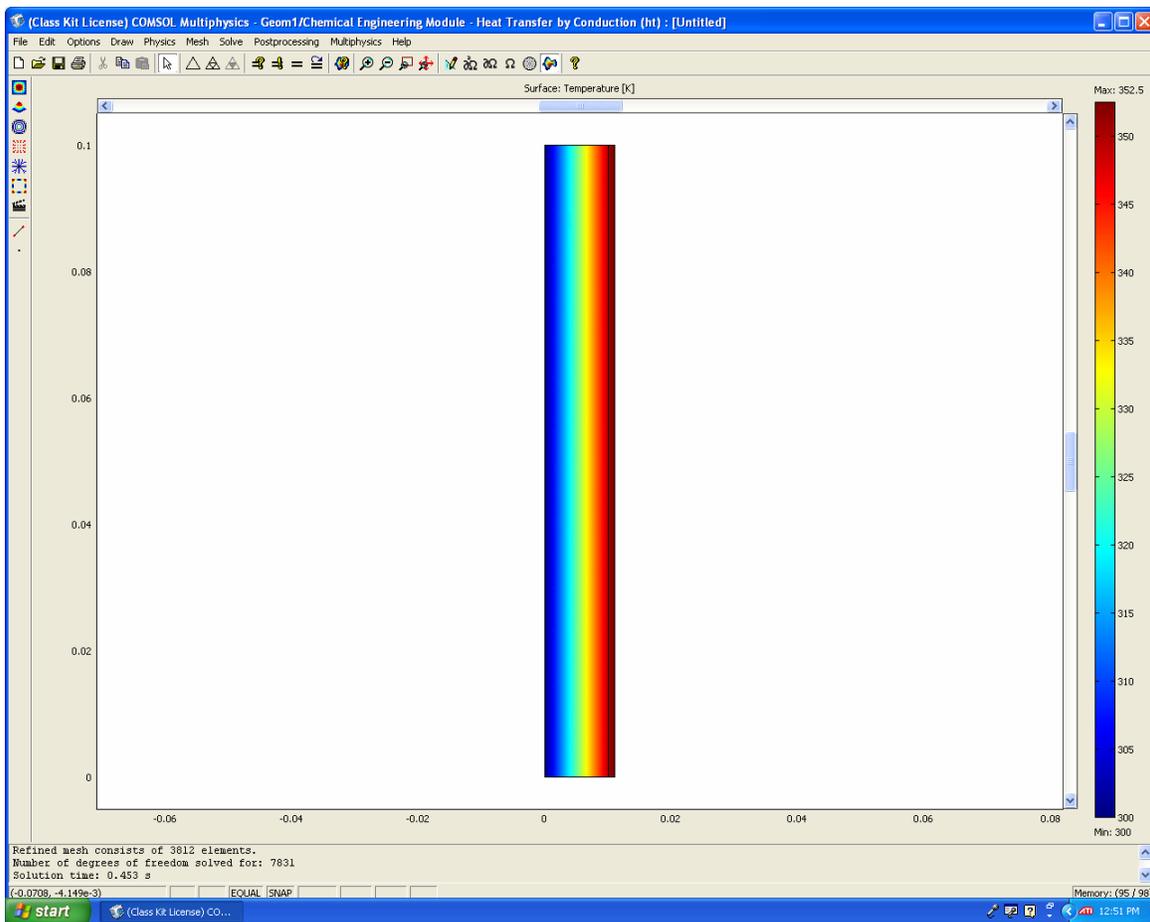
Figure 3.1. Temperature surface plot.

Part 7: Generate plots

1. Select "Postprocessing" from the pull-down menu, then "Cross-Section Plot Parameters," then select "Line/Extrusion."
2. For the cross-section line data, enter x0 = 0.010-L, x1 = M, y0 = 0.05, y1 = 0.05. (Note: for the first subproblem with L = 0.010 and M = 0.011 you would enter x0 = 0 and x1 = 0.011).
3. Verify a straight line between 0 and L and a parabolic, curved line between L and M.
4. Compare your numbers with the analytical solution.

Repeat for the other 2 geometry selections. This can be done by selecting from the pull-down menu, "Draw," then "Geom 1 (2D)". Double click on the large rectangle and re-enter the coordinates as width = L and x = 0.010-L. Remesh your geometry and re-run the simulation as outlined above. Note you must enter numbers for width and x and not the formula given above.

Part 8: Check answers

- L = 0.010, M = 0.011 T_{max} = 352.5 °C
- L = 0.005, M = 0.006 T_{max} = 327.5 °C
- L = 0.001, M = 0.002 T_{max} = 307.5 °C

Example 4: Mass Transfer and Hydrogen Permeation

Note: This problem has been used in a required junior level chemical engineering course "Transport / Unit Operations 2." Two unsteady-state mass transfer problems are illustrated below.

Problem Statement: Consider mass transfer within a slab. A schematic of the geometry is shown below.
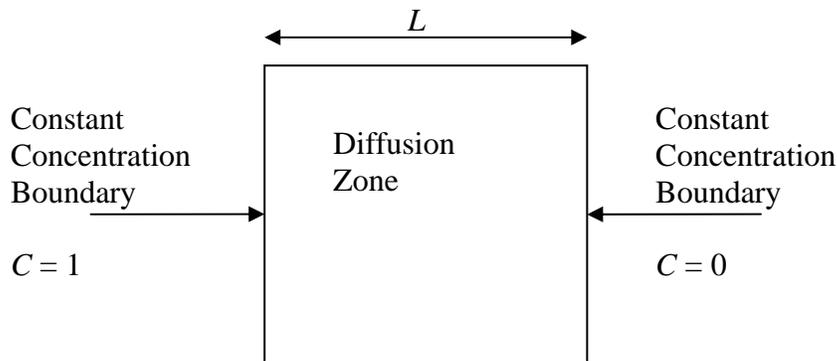
All other external boundaries are insulated and have no mass flux into or out of them. Initially, $C = 0$ everywhere.

The distance between boundaries is $L = 0.10$ m.

The insulated boundaries on the top and bottom essentially make this a one-dimensional mass diffusion problem. In the diffusion zone, the governing equation is:

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

The value of D is the mass diffusivity and is equal to 2.0 x 10^{-5} m^2/s. Your task is to develop a time-dependent FEMLAB / Comsol Multiphysics model and compare the results of the simulation with the analytical solution. Such work is often done to verify computer code.

With $C_o = 1$ the analytical solution given by:

$$\frac{C}{C_0} = \left(1 - \frac{x}{L}\right) + \sum_{m=1}^{\infty} \frac{-2}{m\pi} \exp\left(\frac{-m^2\pi^2 Dt}{L^2}\right) \sin\left(\frac{m\pi x}{L}\right)$$

Part 1: Create the domain
1. Start the software
2. Once FEMLAB / Comsol Multiphysics launches, click on the plus sign at the following locations: "Chemical Engineering Module," "Mass Balance," "Diffusion," and then select "Transient Analysis."
3. Click OK

Part 2: Draw the mass transfer geometry
1. Hold down the shift key and click on the rectangle in the upper left corner of the screen. A window will appear. Insert the following values: For Size use Width = 0.10, Height = 1. For Position use x = 0, y = 0.
2. Click OK
3. Click the "Zoom Extends" button on the main toolbar. It looks like a red cross with a magnifying glass.

Part 3: Apply physical properties
1. From the top menu, select "Physics," then "Subdomain Settings"
2. Select subdomain 1, and enter the diffusivity (make sure the isotropic radio button is selected) as 2e-5.
3. Select the "init" tab and verify the initial condition is 0.
4. Click OK

Part 4: Apply boundary conditions
1. From the top menu, select "Physics," then "Boundary Settings"
2. Click on boundary number 1, select "Concentration" from the pull-down menu, and enter 1.
3. Click on boundary number 2, and verify the boundary condition is "Insulation/Symmetry."
4. Click on boundary number 3, and verify the boundary condition is "Insulation/Symmetry."
5. Click on boundary number 4, select "Concentration" from the pull-down menu, and enter 0.
6. Click OK

Part 5: Create the mesh
1. Click on the hollow triangle to initialize the mesh.
2. Click on the filled triangle to refine the mesh. There should be 1120 elements.

Part 6: Solve
1. Click on "Solve" from the pull-down menu, and select Solver Parameters."
2. Select "Time Dependent"
3. Under "Time Stepping" change it to read 0:10:100 (Note these times are in seconds since D_{AB} is in m^2/s.)
4. Click OK
5. Click on "Solve" from the pull-down menu, and select "Solve Problem." You should see the geometry with a color spectrum indicating a concentration profile.

If you don't see anything, click on "Zoom Extends." This plot is called a "surface plot."
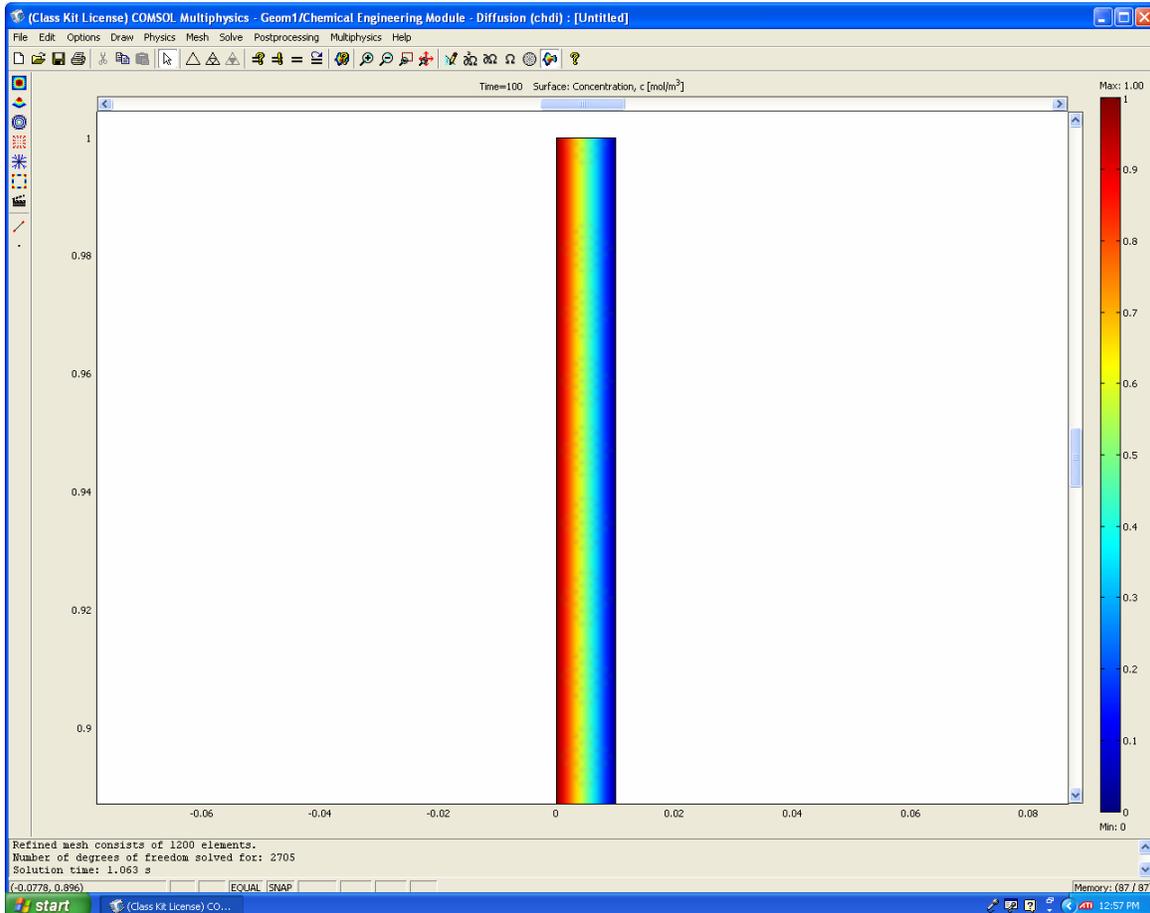
Figure 4.1. Concentration surface plot.

Part 7: Make a color plot
1. Hit the print screen button
2. Start the program called "Microsoft Paint."
3. Click on "edit," then "paste." You should see the picture of your screen.
4. Go to page setup, select landscape, and fit to 1x1 pages, and print on the color printer.

Part 8: Generate concentration profile
1. Select "Postprocessing" from the pull-down menu, and pick "Cross-Section Plot Parameters."
2. Select, under the "General" tab, for "Solutions to Use," the solution at t = 100 only.
3. Then "Cross-Section Plot Parameters," then select "Line/Extrusion."
4. For the cross-section line data, enter x0 = 0.0, x1 = 0.1, y0 = 0.5, y1 = 0.5.
5. On the plot, click on the letters "ASCII" and enter a file name to save the data. Make sure you put it in a folder that you can find later.

6. Within MATLAB or EXCEL, plot this data at increments of $\Delta x = 0.01$ m (thus at $x = 0.00, 0.01, 0.02$, etc. up to 0.10). Plot the data as some sort of symbol (either an x, star, square, etc.)
7. Calculate the Fourier number for this problem, Dt/L^2. If this number is greater than 0.1 you can probably use just one term in the analytical series solution.
8. In the same graph that you created in step 6, plot the analytical solution as a line. Note to have a smooth plot, you should use a smaller Δx.

Part 9: Practice

Consider the cross-section of the bipolar plate, shown below:
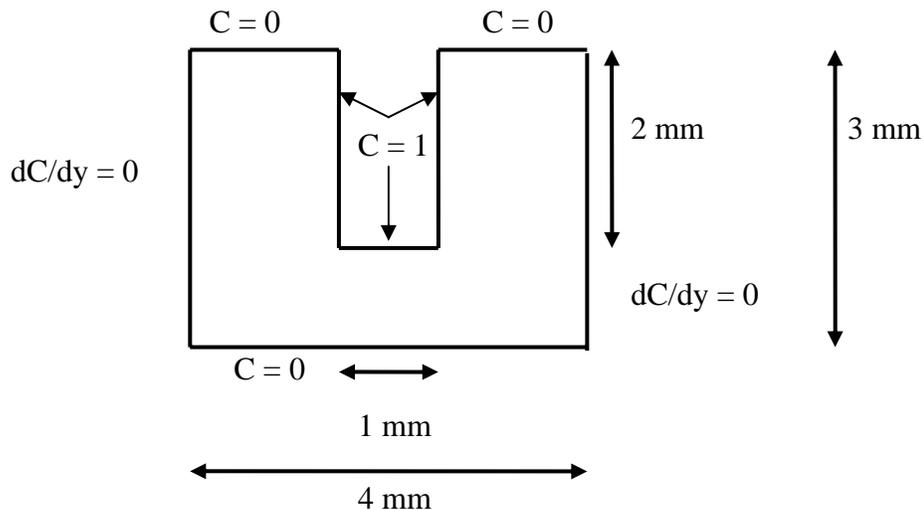
At the top and bottom of the plate, the concentration is always zero. At the left and right of the plate, there is "symmetry" from the region surrounding one channel to the next, so the slope in the concentration is zero. Within the channel itself, the concentration at the plate / channel interface is one. The initial concentration is zero. Note you can use the "difference button" to help you make this geometry.

Note that the diffusion coefficient is $D_{AB} = 10^{-5}$ mm^2/s. (What is this in m^2/s?)

Use FEMLAB / Comsol Multiphysics to determine a "surface plot" of the concentration after 10000 s.