

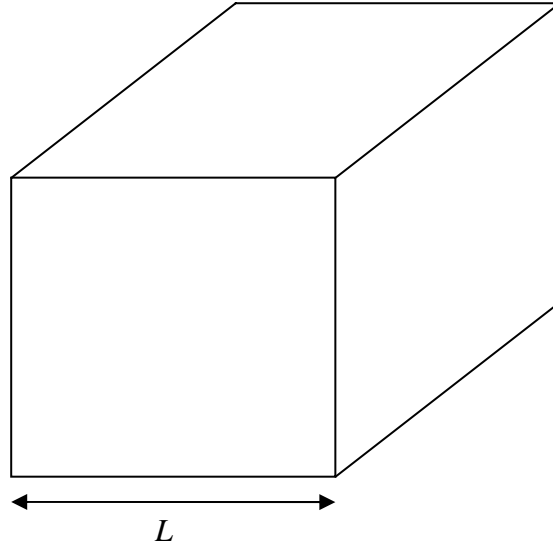
## Finite Element Modules for Enhancing Undergraduate Transport Courses: Application to Fuel Cell Fundamentals

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### Example 5: Transport Effects on Kinetics

**Note:** This problem can be used in a required junior level chemical engineering course “Transport / Unit Operations 2.” Three steady-state mass transfer problems with reaction are illustrated below.

**Problem Statement:** Consider the problem of species diffusion and first order reaction within a catalyst “cube” of length  $L$ . A schematic of the geometry is shown below.



All external boundaries have constant concentration  $C = C_o$ .

Within the cube, the governing equation is:

$$D \left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) = kC$$

where  $D$  is the species diffusivity and  $k$  is the reaction rate coefficient. In dimensionless terms, choosing  $C^* = C/C_o$ ,  $x^* = x/L$ ,  $y^* = y/L$ , and  $z^* = z/L$ , and defining the Thiele modulus as  $\phi^2 = kL^2/D$  we have:

$$\left( \frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2} \right) = \phi^2 C$$

Your task is to find the effectiveness factor for the following parameter choices for  $\phi^2$ : 0.1, 1.0, and 10.0.

### **Part 1: Create the domain**

1. Start FEMLAB / Comsol Multiphysics.
2. Once FEMLAB launches, select 3D from the “Space Dimension” pull-down menu.
3. Click on the plus sign at the following locations: “Chemical Engineering Module,” “Mass Balance,” “Diffusion,” and then select “Steady State Analysis.”
1. Click OK

### **Part 2: Draw the mass transfer geometry**

1. Hold down the shift key and click on the block in the upper left corner of the screen. A window will appear. Insert the following values: Style: Solid, Base: Corner, Axis Base Point:  $x = 0, y = 0, z = 0$ , Length:  $x = 1, y = 1, z = 1$ .
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 1.0 and the reaction rate as  $-0.1 \cdot c$ .
3. Click OK

### **Part 4: Apply boundary conditions**

1. From the top menu, select “Physics,” then “Boundary Settings”
2. Select all boundaries 1-6, select “Concentration” from the pull-down menu, and enter 1.
3. Click OK

### **Part 5: Create the mesh**

1. Click on the hollow triangle to initialize the mesh. There should be about 18,000 elements!

### **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.” Have some fun rotating the geometry around. Make sure it is a “slice plot.”

5. Write down the minimum concentration.

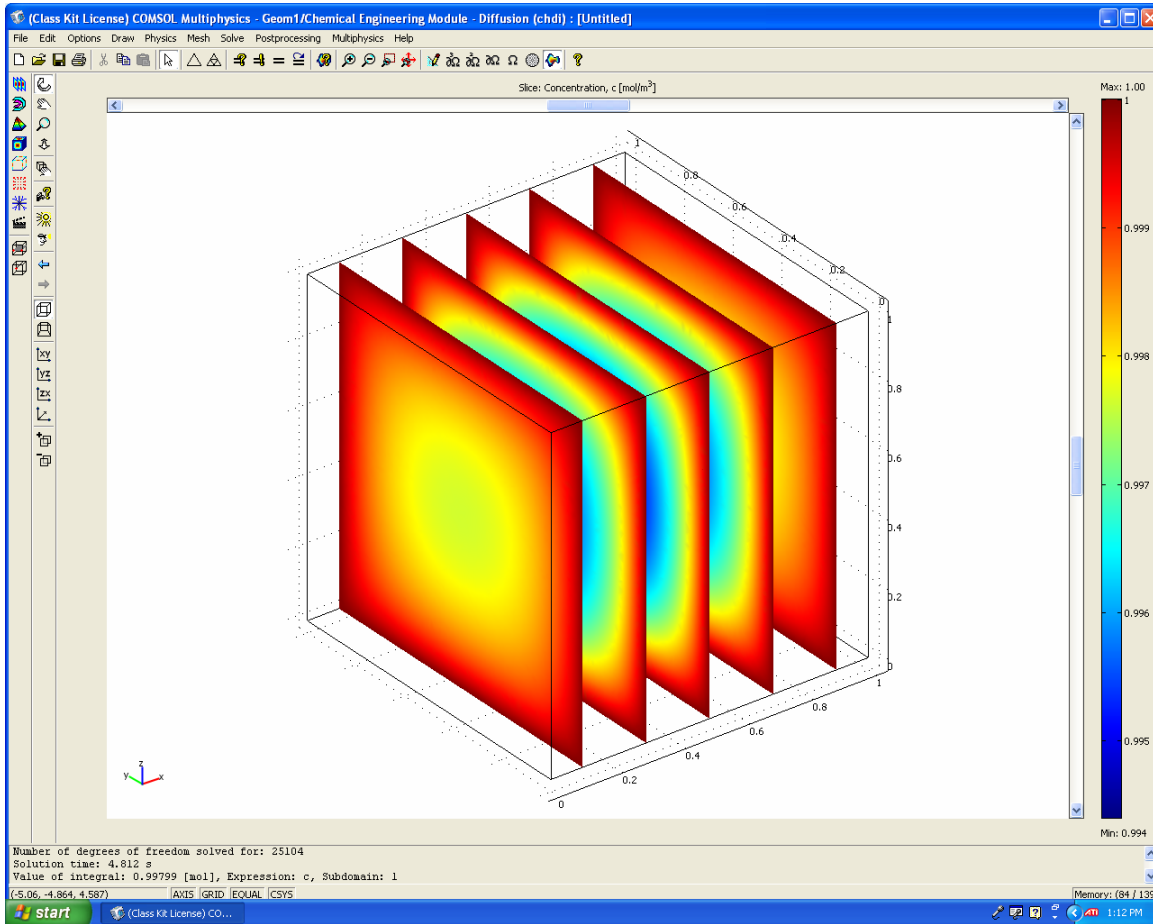


Figure 5.1. Concentration surface plot.

**Part 7: Generate plots**

The effectiveness factor is defined according to the integral  $\eta = \frac{k \iiint C dx dy dz}{k_c L^3}$

In terms of our dimensionless variables, this is given as:

$$\eta = \iiint C^* dx^* dy^* dz^*$$

1. This is easily accomplished within FEMLAB. Select “Postprocessing” from the pull-down menu, then “Subdomain Integration” then select OK.
2. Write down your result for the effectiveness factor.

Repeat for the other 2 parameter selections, when  $\phi^2 = 1.0$  and  $10.0$ .

Note that in class we used the half width of the catalyst “slab” to render the system dimensionless. Here, we use the entire length of the cube. Thus, the results cannot really be compared with each other without making some adjustments.

**Part 8: Check answers**

- $\phi^2 = 0.1$ ,  $C_{min} = 0.994$ ,  $\eta = 0.997$ .
- $\phi^2 = 1.0$ ,  $C_{min} = 0.946$ ,  $\eta = 0.980$ .
- $\phi^2 = 10.0$ ,  $C_{min} = 0.601$ ,  $\eta = 0.845$ .

**Part 9: Practice**

For what value of  $\phi^2$  does  $\eta = 0.5$ ? (Hint:  $\phi^2$  is a multiple of 10.) What is the minimum concentration under these conditions? Also try to get  $\eta$  for a “cone catalyst pellet”, with radius = 1, height = 1, and semiangle = 45, with  $\phi^2 = 10$ .