Effect of Pore Geometry on the Diffusion Reaction Rate in a Fuel Cell

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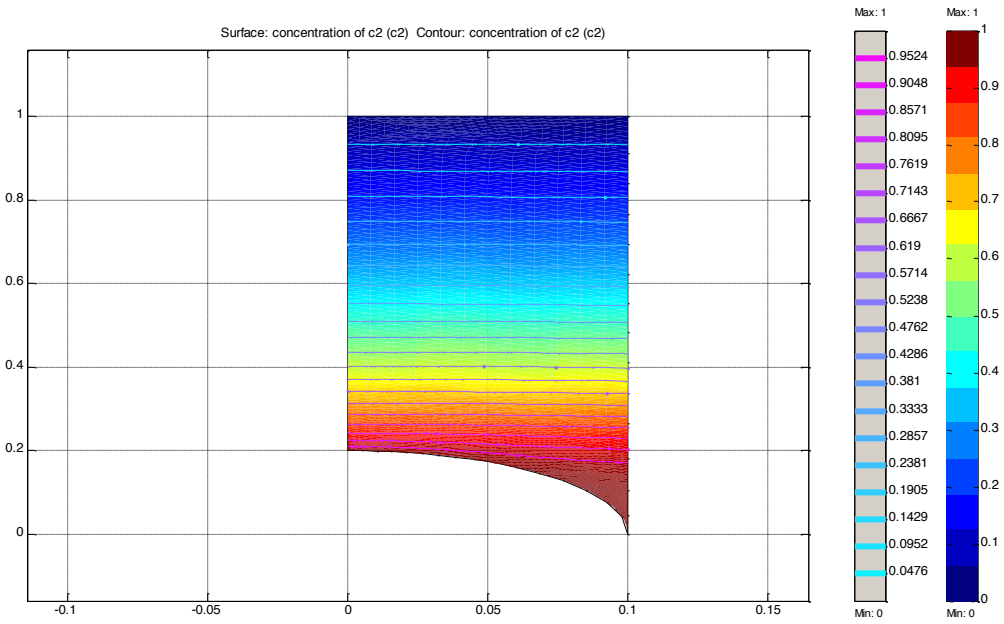
Date: March 14, 2003



I. Introduction

The purpose of this research was to determine the impact of the pore geometry on the reaction rate for a fuel cell. This research is an addition to the research previously completed by Dr. Finlayson in his report "Reaction Diffusion Problem for Neah Power." The main feature of this problem is a reaction diffusion of oxygen into an electrolyte, and then a reaction along a surface that is doped with a catalyst. The key parameters are the properties of the oxygen and electrolyte, the pore geometry, and the reaction kinetics.

The actual system is comprised on many pores through which the reaction occurs, but in order to gain some perspective into the effect of the geometry just one pore is considered. The pore geometries considered are shown in Figures 1-3. These geometries were chosen for many reasons. The Cylinder was taken to be the base case. The Cone represents a non-ideal manufacturing process that resulted in incomplete etching of the cylindrical pore. The solenoid represents additional processing prior to pore etching that would increase the available surface area. Previous research presented at fuel cell conferences has shown that inducing wavy boundaries on pores is something that is feasible from a manufacturing stance. The main trade off to the situations with increased surface areas is the increased resistance to diffusion.

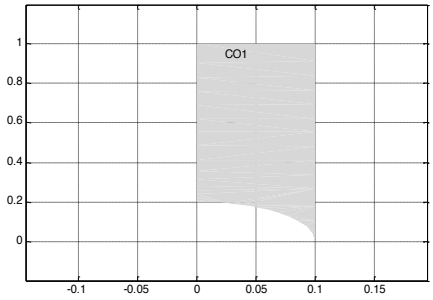


Figure 1: Cylindrical Geometry

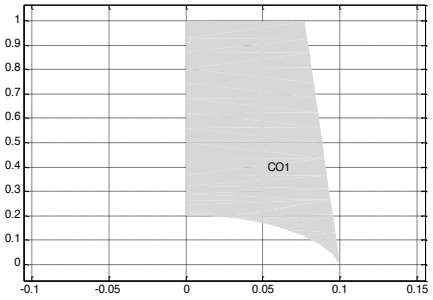


Figure 2: Conical Geometry

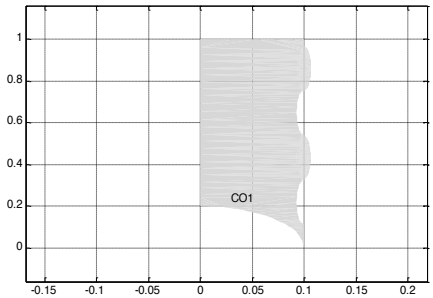


Figure 3: Solenoid Geometry

In order to quantify the impact of the different geometries, the overall reaction rate will be compared based on an effectiveness factor found by integrating the concentration of

the oxygen and electrolyte along the reacting boundary. The effectiveness factor is a measure of how much oxygen is reacted, taking diffusion resistance into account.

The boundary conditions for this system are shown in their non-dimensional form below. The derivation of these equations can be found in Dr. Finlayson's report.

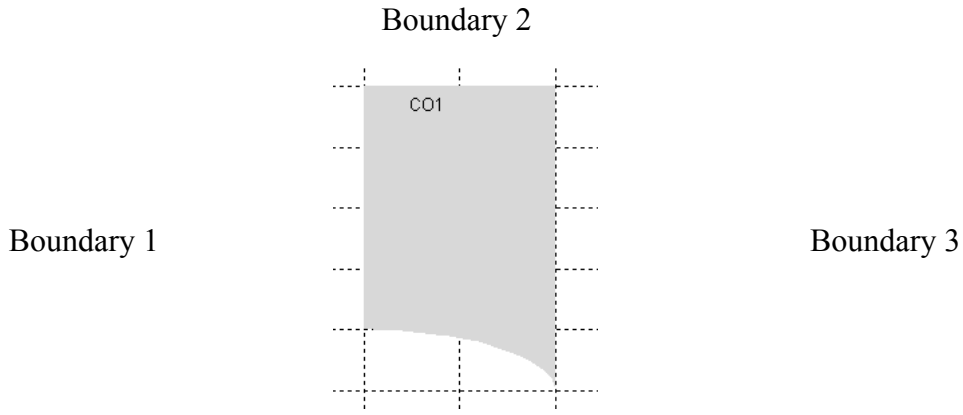


Figure 4: Schematic of model showing the Boundary numbering

Boundary 1:

$$\frac{\partial c_i^*}{\partial n} = 0, i = 1,2$$

Boundary 3:

$$\frac{\partial c^*_1}{\partial n} = -\frac{Da}{DR} * c_1^* * c_2^*$$

$$\frac{\partial c^*_2}{\partial n} = -\frac{Da}{4} * 1000 * c_1^* * c_2^*$$

Boundary 2:

$$c_1^* = 1$$

$$c_2^* = 0$$

Boundary 4:

$$\frac{\partial c^*_1}{\partial n} = 0$$

$$c^*_2 = 0$$

Table 1: Non-Dimensionalized Boundary Conditions

The range of Damkohler numbers that will be considered are 0.0005-10. There are two different diffusivity ratios that will also be considered 43 and 0.8. The diffusivity ratios were given by Tom Madden and Susan Snyder of Neah Power, and the range of Damkohler numbers were chosen to be able to compare my results for the cylinder to Dr. Finlayson's results.

Method

1. Open Matlab, and type the command Femlab
2. When the Model Navigator opens use the following specifications
    a. Chemical Engineering Module

b. Axisymmetry
c. Mass Balance
d. Diffusion
e. Stationary Linear

3. Once the model is specified, enter the draw mode
4. Draw a rectangle with an aspect ratio of 10:1 (length to width), and an ellipse with one quarter of the total ellipse covering the bottom of the rectangle. If the draw function has the word SNAP highlighted in the toolbar, the drawing will be restricted to just the gridlines. To turn that feature off, just double click on the word SNAP.
5. Highlight both the rectangle and the ellipse, and then use the toolbar on the left hand side of the model subtract the ellipse from the rectangle. The three union buttons will add or subtract the highlighted geometries.

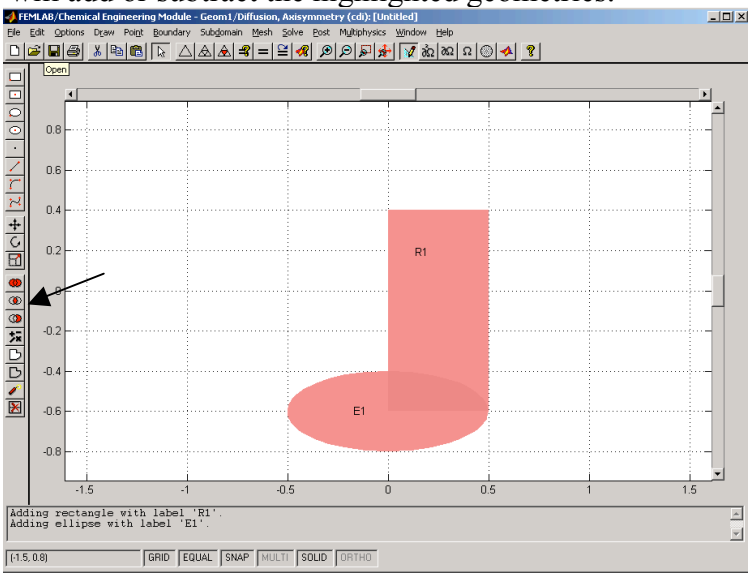


Figure 5: Toolbar example for creating composite figures

6. To make the different geometries, just change the shape of the rectangle for the cone, or add a series of ellipses for the solenoid.
7. Under the Options, define the variable for the Damkohler number and Diffusivity ratio. Use those variable names when setting the boundary conditions to make solving each system easier.
8. Then you must add another variable. Under MultiPhysics, Add/Edit Modes, add another variable that has the same specifications as the model.
9. Under Multiphysics, highlight either the oxygen or the electrolyte variable name. Then go to boundary settings, and insert the boundary conditions. Repeat this for both variables. When entering the boundary conditions, you must put a period between the two concentrations (c.*c2).
10. Under Solve, change the Solver Parameters to stationary non-linear.
11. Initialize the mesh by clicking on the triangle button on the top tool bar.
12. Finally, solve the equation by clicking on either the equal button or the equal button with an arrow. The equal button with the arrow solves the problem using the previous solution as the initial value.

13. Once a solution is returned, go under Post, Plot parameters to plot concentration lines and surfaces.
14. Then you can integrate the boundary. Under Plot, Boundary Integration, integrate boundary 3 with respect to c.*2.

Additionally, you can create a movie to show the effect of the range of Damkohler numbers on the oxygen concentration. To do this

1. Under Options, create a new expression that is Da*t, where Da is the Damkohler number and t is time.
2. Update the boundary conditions by replacing the Damkohler number with the new expression
3. Under Solve, Solver parameters, change that to time dependent.
4. Under the Timestepping tab, change the values for the initial time, final time and step size to accommodate the entire range
5. Under Options, update the initial Damkohler number as the lowest value within the range
6. Hit solve on the model
7. Once the solution has compiled, under the Post section, go to Plot Parameters, Animate. At this point you can set the number of frames per second, and you can save the movie as a mpeg.

Results

Ability to Recreate Previous Results

Da	η (Diff Ratio = 43) Previous	η (Diff Ratio = 43) My Results	η (Diff Ratio = 0.8) Previous	η (Diff Ratio = 0.8) My Results
	0.531	0.533	0.529	0.529
	0.491	0.492	0.488	0.488
	0.399	0.399	0.392	0.392
	0.355	0.335	0.325	0.326
	0.293	0.292	0.280	0.280
	0.244	0.243	0.225	0.245
	0.192	0.191	0.162	0.152
	0.159	0.157	0.120	0.120
	0.129	0.126	0.0833	0.083
	0.102	0.100	0.0535	0.535
	0.0714	0.077	0.0269	0.0277
	0.526	0.0507	0.0151	0.155
	0.0375	0.036	0.00811	0.008681
	0.224	0.218	0.00345	0.00347

Table 2: Compares my results with the previously reported results for the effectiveness of the Cylindrical pore at various Damkohler numbers.

Table 2 shows that the results that I was able to obtain were within a reasonable range of the previously reported values. Slight deviations were likely the result of the shape of the oxygen bubble within the cell. The small deviation shows that the approximate size and shape of the oxygen bubble was within reason for modeling the actual reaction. Table 2 also shows that the effectiveness of the system decreases with increasing Damkohler numbers. This trend was also shown in the concentration profiles at various Damkohler numbers.

Effectiveness

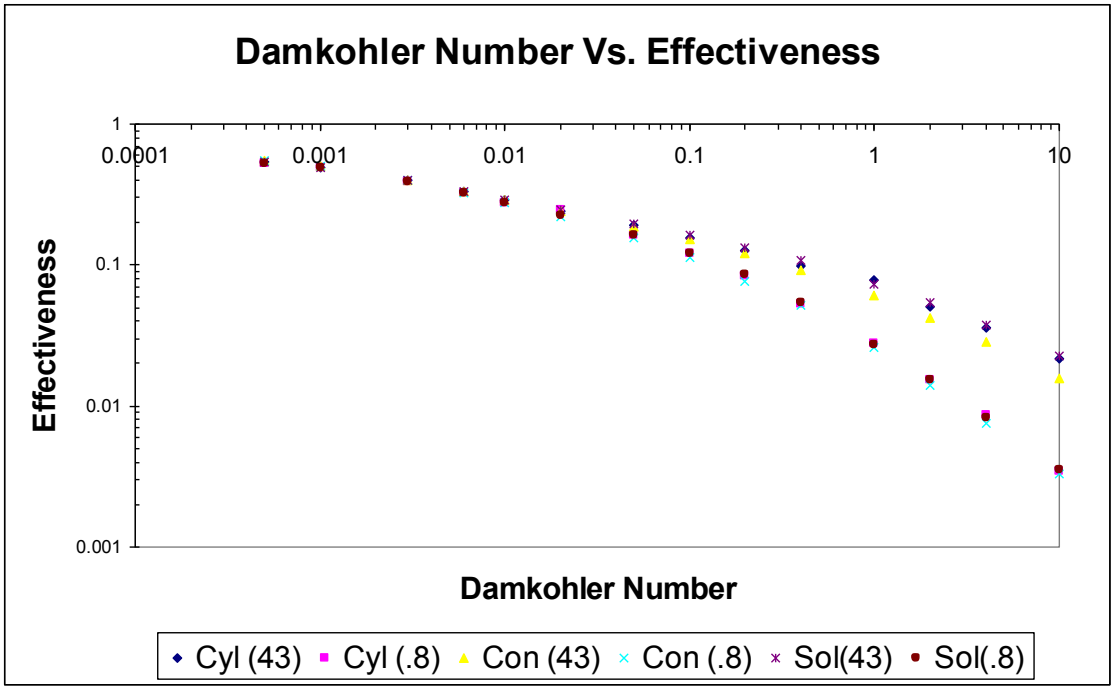


Figure 6: Plot of the Damkohler number versus the Effectiveness on a log-log scale. The legend at the bottom describes the geometry and diffusivity ratio that is represented within the graph.

Figure 6 is a graphical representation of the effect of the pore geometry both as a function of the diffusivity ratio and the Damkohler number. Although the calculated effectiveness for the three different geometries at the same Damkohler number and diffusivity ratio are not significantly different, the overall reaction rate of the system will change. This is due to the fact that the effectiveness is multiplied by the internal surface area of the system. The internal surface area in order from smallest to largest is: Cylinder, Cone, Solenoid. Therefore the reaction rate for the solenoid is better than the cylinder, but is not quantified in this report. Figure 6 also shows the effect of the diffusivity ratio on the effectiveness. The two diffusivity ratios begin at around the same effectiveness, but as the Damkohler number increases, the effectiveness of the smaller diffusivity ratio does not drop off as much as the larger one.

Effect of Damkohler Number on Concentration Profile

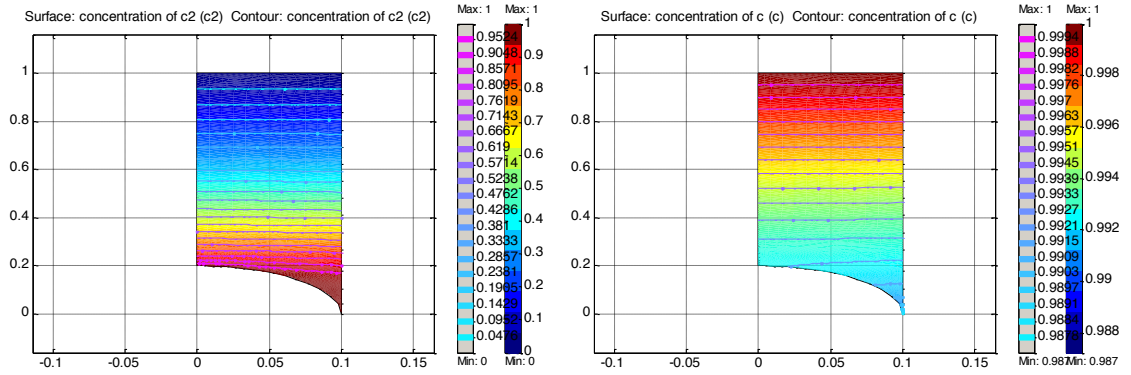


Figure 7 and 8: Concentration Profiles for Oxygen (c2) and the Electrolyte (c) for a Diffusivity Ratio = 0.8, Damkohler Number = 0.001

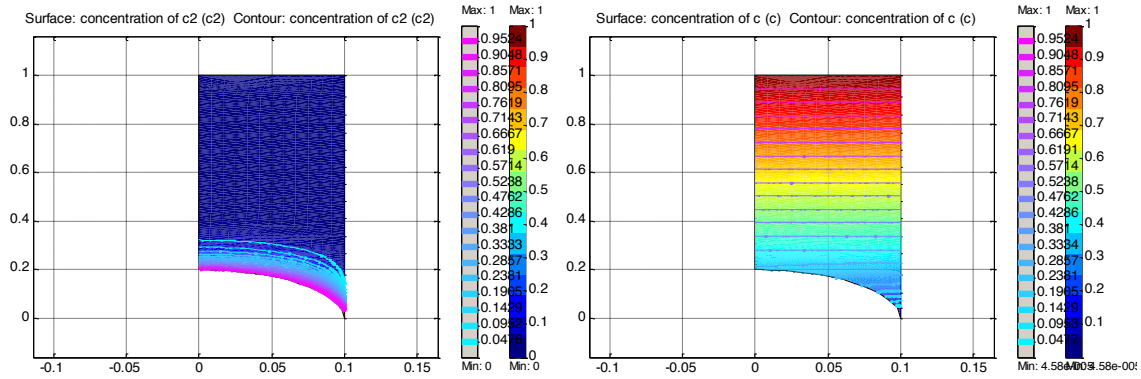


Figure 9 and 10: Concentration Profiles for Oxygen (c2) and the Electrolyte (c) for a Diffusivity Ratio = 0.8, Damkohler Number = 10

The set of Figures 7-10 show the effect of the Damkohler number on the concentration profiles. The most dramatic effect is on the diffusion of the oxygen to the reacting surface. As the Damkohler number increases, the bulk of the reaction takes place close to the pinch point of the oxygen bubble. The scale on the electrolyte concentration is somewhat misleading because in both cases the ratnge of the electrolyte is from 1-.988. The scale for Figure 10 was copied wrong from the figure for an unknown reason. The concentration lines in both cases for the oxygen profile show that the reaction on boundary 3 reduces the concentration as expected.

Effect of Diffusivity Ratio

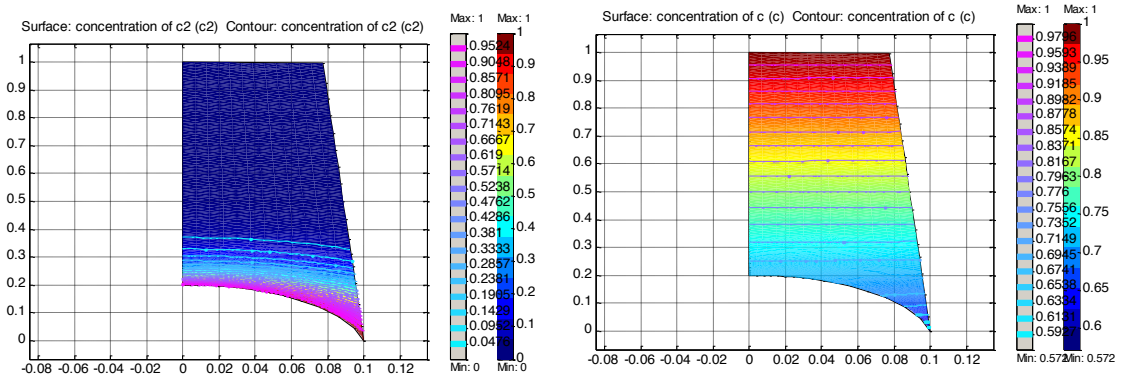


Figure 11 and 12: Concentration Profiles for Oxygen (c2) and the Electrolyte (c) for a Diffusivity Ratio = 0.8, Damkohler Number = 0.1

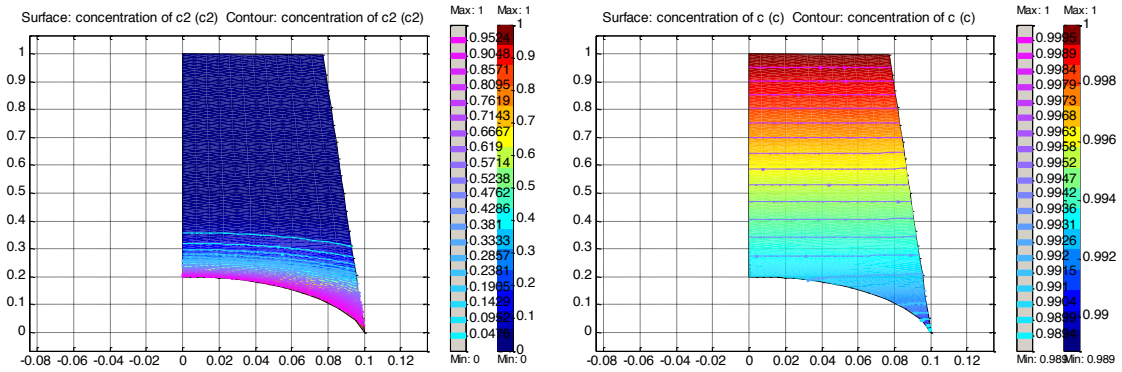


Figure 13 and 14: Concentration Profiles for Oxygen (c2) and the Electrolyte (c) for a Diffusivity Ratio = 43, Damkohler Number = 0.1

The set of figures 11-14 show the effect of the Damkohler number on the effectiveness. Based on Figure 6, I would expect to see a small degree of difference in the oxygen profile, which is shown in Figure 11 and 13. As the Damkohler number increases, I would expect to see a larger degree of separation.

Additional figures for concentration profiles at various Damkohler numbers and Diffusivity ratios can be obtained from the femlab files that are attached to this report. In the interest of time, and file size the results were limited to just a few figures. The file for the solenoid was contaminated when I tried to solve it as a time dependent model, and since the ellipse placement has an effect on results, additional figures were not used.

Conclusions

Overall my research successfully recreated results previously found for the cylindrical pore geometry. This would imply that the method I used to create my models would give proper results. I have shown the general trend for the effect of the Damkohler number and diffusivity ratio on each system.

Finally, the true purpose of this research was to be able to make some recommendations about the most effective pore geometry. Although some conclusions can be drawn from Figure 6, I would hesitate to make a recommendation to begin to focus more time and energy on trying to create a process to induce a wavy border on the pore. The reason for my hesitation is that there is not a dramatic enough increase in the effectiveness of the overall reaction rate. Also, the impact of the simplifications on the model could introduce a large degree of uncertainty in the calculated reaction rate. In my mind, the better conclusion is that the current manufacturing processes are acceptable since there is not a drastic increase in the reaction rate for the different pore geometries.