Velocity and Concentration Properties of Porous Medium in a Microfluidic Device

Rachel Freeman
Department of Chemical Engineering
University of Washington

ChemE 499 Undergraduate Research
December 14, 2006

Introduction

The purpose of this project is to model the fluid flow and diffusive transport in a microfluidic device that used by Dr. Chee Ng and Professor Suzie Pun in the Department of Bioengineering and the University of Washington. This apparatus is designed to deliver nanoparticles through a semi-permeable membrane to embedded cells. The fluid travels past solid supports before it reaches the embedded cells, which plays an important role in the flow characteristics. The purpose of modeling the flow through this device was to determine the path the nanoparticles will follow and determine how the particles diffuse throughout this device. A schematic of the device is shown below in figure 1.

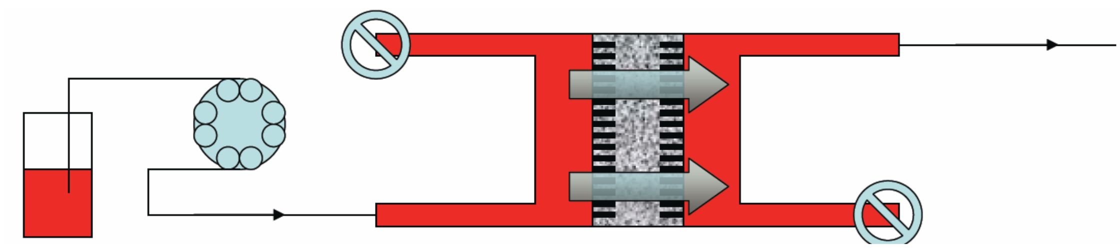

Figure 1. Picture of the microfluidic device

In this figure, the black rectangles represent the supports the fluid must travel around and the gray area represents the section where the cells are located.

Materials and Methods

The flow properties were modeled in COMSOL Multiphysics with diffusive correlations and Darcy's Law. In COMSOL, Darcy's Law follows the form

$$\nabla \bullet \left(-\frac{\rho\kappa}{\eta}\nabla p\right) = F \qquad (1)$$

The variables for Darcy's Law and values in this case are as follows:

$\rho = density = 1000 kg/m^3$

$\kappa = permeability = 2.2x10^{-18} m^2$

$\eta = viscosity = 1x10^{-3} Pa \cdot s$

$p = pressure = 500 Pa$

The variable F is a source term which is set as F=0 for this simulation. Darcy's Law solves for a velocity of the fluid in terms of m/s.

The diffusive properties are calculated in COMSOL through the follow equation

$$\frac{\partial c}{\partial t} + \nabla(-D\nabla c) = u\nabla c \tag{2}$$

$D = diffusivity = 2.2x10^{-11} m^2/s$

$u = velocity[=]m/s$

$c = concentration[=]mol/m^3$

The initial boundary condition for this scenario was a constant concentration at the inlet streams, which was normalized to 1 mol/m^3. The velocity calculated by Darcy's Law was used by the model. The diffusivity was assumed as the Stokes-Einstein Diffusivity for a 10-nm particle.

Three geometries were analyzed in order to compare relative velocity profiles and concentration distributions. The shapes and dimensions of these three designs are summarized below by figure 2. The first case studied was the current design used in the microfluidic device. There are 5 sets of posts spaced evenly throughout the device. The exact dimensions can be found in the figure. The second model uses smaller post sizes, but the number of posts is increased to seven pairs. The goal of this model is to decrease changes in velocity that occur in the middle section of the apparatus. Finally, the third model uses rounded posts. They are of the same relative size and shape as model 1. The goal with this design is to cut down on irregularities created by the posts through expansion and contraction flow. This also reflects the shape the device takes after long usage.

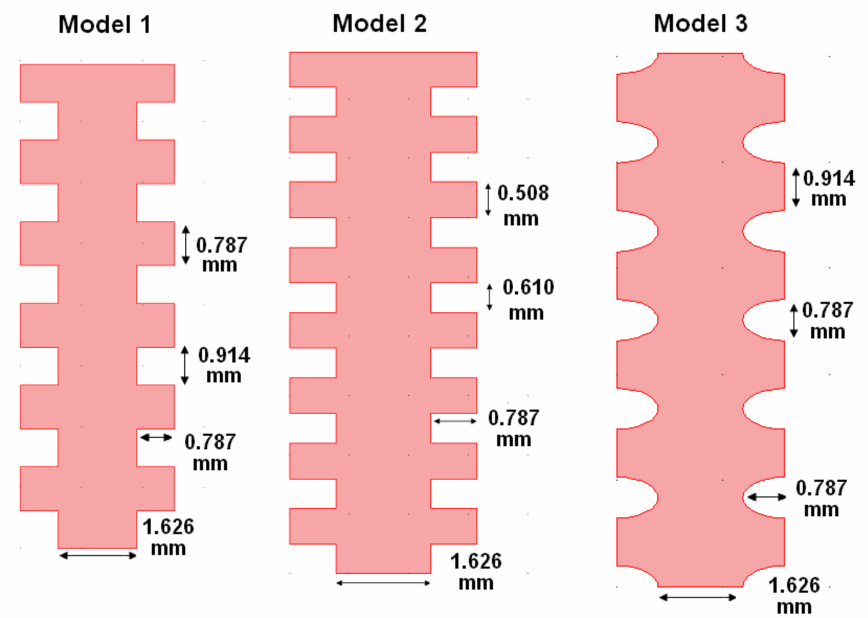

Figure 2. Shapes and Dimensions of three proposed designs

Boundary Conditions

There were three types of boundary conditions used in this set-up. Figure 3 below summarizes these conditions. The first applied to the region where fluid entered the device. These boundary conditions, color-coded blue in figure 3, were set to a pressure of 500 Pa and initial concentration of 1 mol/m^3. The outlet region, color-coded green, was set to a pressure of 0 Pa and convective flux. All other boundaries were set to the insulation/symmetry boundary condition for both Darcy's Law and Convection/Diffusion.

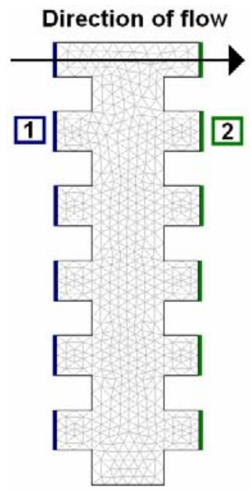

Figure 3. Mesh Refinement and boundary conditions for Model 1

Mesh Refinement

Figure 3, presented above, also displays the mesh refinement for one model. The refinement for each model is summarized in Table 1.

Table 1. Mesh Refinement

	Model 1	Model 2	Model 3
Number of Elements	1032	1264	2552
Degrees of Freedom	4386	5466	5333

Results

Two Dimensional Modeling

The velocities profiles were determined using two-dimensional models. The device, however, does have a depth of 1.56 mm. In order to justify a two dimensional model of this system, the velocity profile a section of the original device was plotted in three dimensions, as shown below in Figure 4. The important aspect of this model is the uniformity in the z-direction. This means a two-dimensional cross section of this device can accurately represent the whole device.

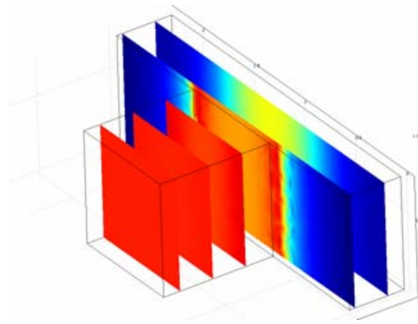

Figure 4. Sectional model of device in three dimensions

Velocity Profiles

The velocity profiles were determined in COMSOL by Darcy's Law. The following figures graph the x-directional velocity along the y-direction of the device. This gives a quantitative representation to the uniformity of velocity in the device. The velocity scale changes in each graph, which must be looked out for.

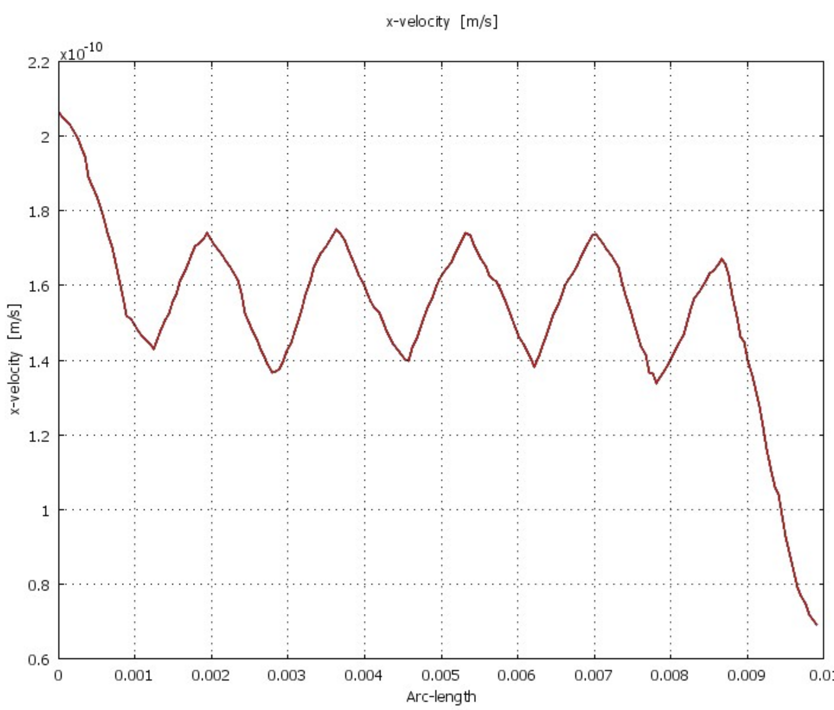

Figure 5. Velocity profile of Model 1

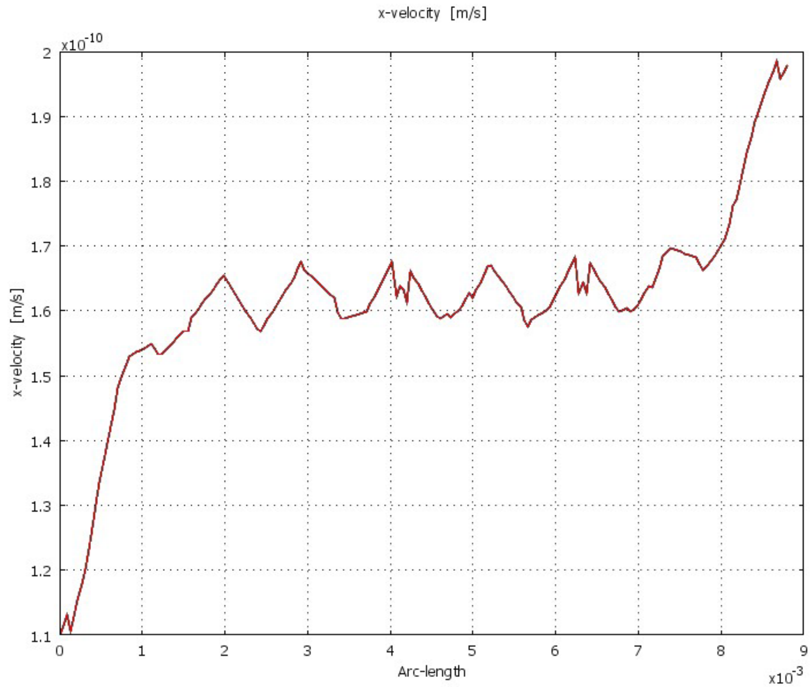

Figure 6. Velocity profile of Model 2

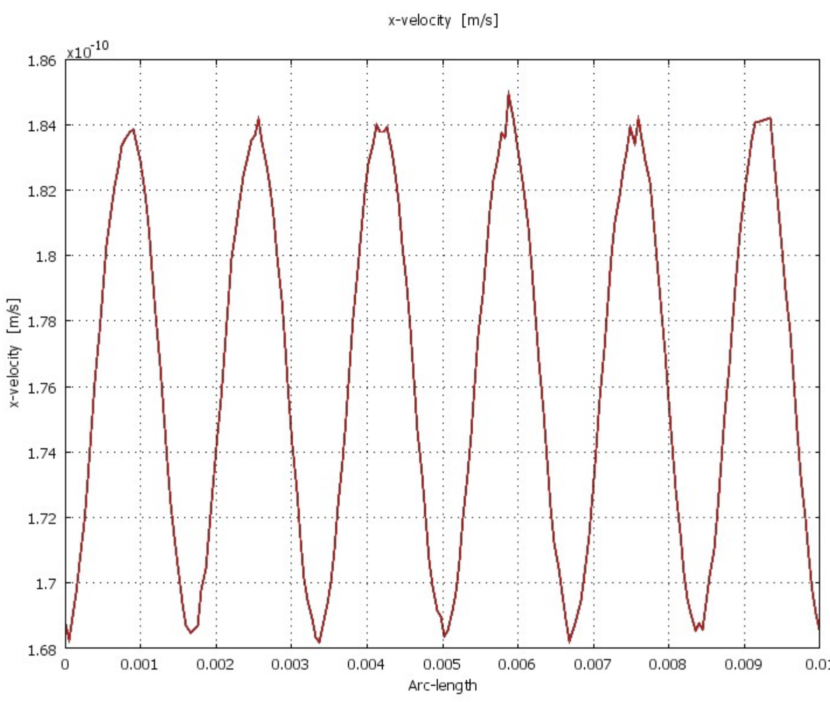

Figure 7. Velocity profile of Model 3

In the case of Models 1, 2 and 3, the velocity varies between ranges of approximately 1.4–1.8 $x10^{-10}$ m/s, 1.5–1.7 $x10^{-10}$ m/s, and 1.7–1.85 $x10^{-10}$ m/s, respectively.

Concentration Profiles

The concentration of the three models after 30000s, as well as the concentration range, is shown in figure 8. The range of concentration at this time is between 0.98 and 1.00. The initial concentration in all three cases was 0.

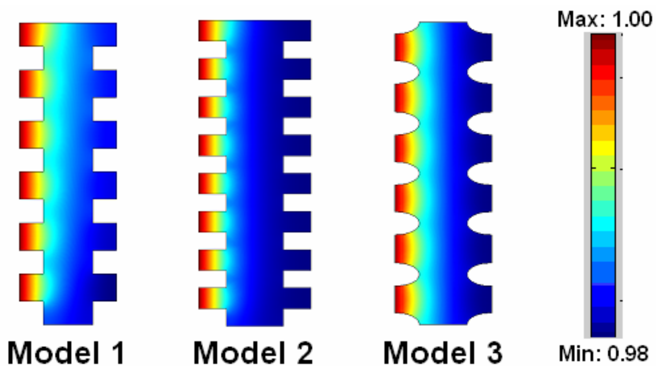

Figure 8. Concentration gradient time t=300000s

There is a relatively small variation in concentration at 30000s, which means each device has a nearly constant concentration at this point in time. The concentration can also be quantified graphically by showing the concentration distribution over time. This analysis is done for Model 1 in Figure 9. The concentration is plotted along the x-axis, which is the direction of flow. The lines represent the concentration at different times, which is displayed in the legend.

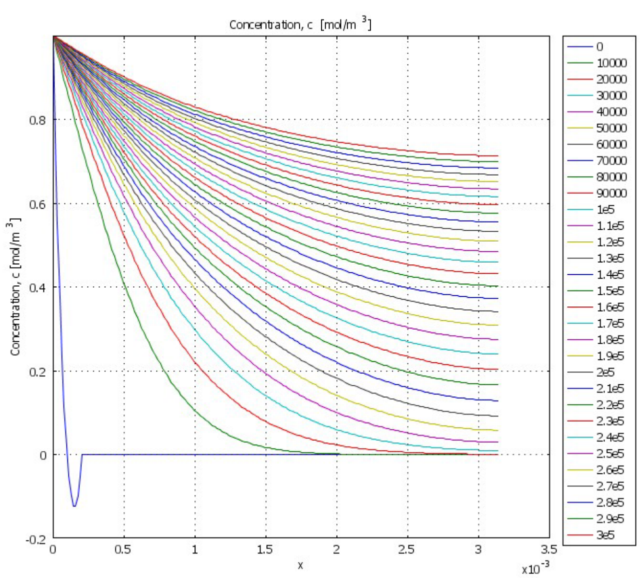

Figure 9. Transient Concentration of Model 1

Conclusions and Recommendations

The results of this project revealed very few surprises. The shape and size of the supports affect how the velocity varies within the device. Smaller or rounded supports, as represented by Models 2 and 3 respectively, reduce the variation in velocity. These supports have little effect on the concentration profile in the apparatus. With enough time, the concentration throughout the device will be nearly uniform.

There are steps that can be taken to further model this device. First, a model of the flow through the entire device should be done, as per the interest of Dr. Ng. This would include the regions before the fluid reaches the support. In addition, more rigorous modeling and refinement can be done on a smaller symmetric region of the device.