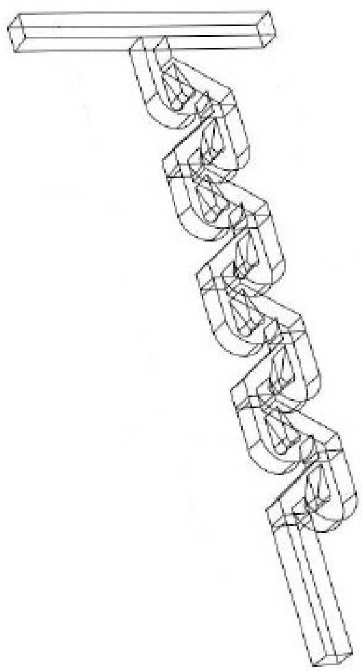
Microfluidic Device Research: Spring Quarter 2009



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Introduction

In order to investigate and report on the operating effectiveness of the microfluidic device design given (shown on the following page in Fig. 1), three unique problems were developed independently. In the order that they are present in the device, a Tesla mixer device composed of ten individual mixer units in parallel are used for the initial mixing of a sample of a particular concentration and a diluent. Following the mixer, a long straight channel induces further mixing due to diffusion. The final important problem to be modeled is a simple T-shaped junction. The important, and complicating, detail is that the velocity in the intersecting channel is time dependent in order to generate a slug of concentrated material.

The operation of these devices will be analyzed at a single inlet velocity for both the sample and diluent feeds. All other properties will be maintained throughout the analysis of each component as well. All fluid properties are being approximated as those of water, implying a density of 1000 kg per m^3, and a viscosity of .001 Pascal seconds. Likewise, for purposes of diffusion calculations, the diffusivity of the sample will be set at 10^{-9} m^2 per second.

All modeling of the Tesla mixer and transient T-shaped junction was performed using Comsol Multiphysics due to their complexity. The diffusive mixing in the straight channel was performed using Matlab. Because of the length of the straight channel, it would be difficult to adequately model the straight channel simply because of the size of the mesh that would be necessary, and therefore the number of calculations and therefore virtual memory that would be required.

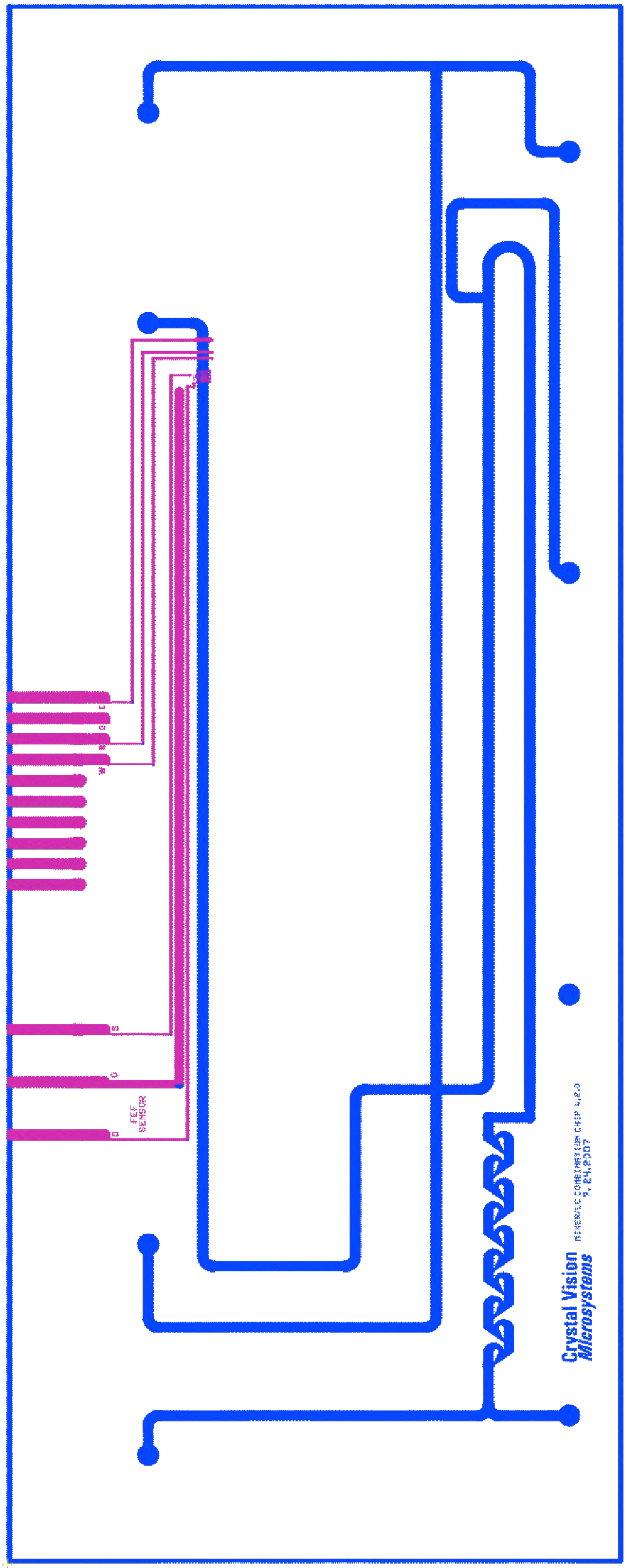

Figure 1. Microfluidic Device, Source: Gilbert, Scott. "Microfluidic LC Chip for On-line Monitoring".

Because of this fact, and the simple nature of the geometry, Matlab code was compiled to perform a finite difference analysis of the diffusion that occurs in the straight channel.

Tesla Mixer

Given how the Tesla mixer takes advantage of the Coanda effect to diverge streams and, possibly, improve mixing characteristics, it is far easier to model its operation using Comsol Multiphysics. One of the first points to note is that the modeling is being performed only in two dimensions. From my own previous work on the Tesla mixer, it appears and has been shown that there is little unique influence from modeling the mixer fully in three dimensions. Because of the additional difficulty in modeling in three dimensions and the minimal benefit, this will not be done.

The mixer channel is 500 _m in width and has ten individual mixer units in series. Also, to simplify the inlet conditions, two individual streams combine prior to the first mixer, one representing the sample with a dimensionless concentration of one, and the diluent, with a concentration of zero. The Navier-Stokes equations are solved using a mesh composed of 17,970 elements comprising 83, 868 degrees of freedom. The Diffusion equations are solved using a mesh of 28,401 elements comprising 58, 228 degrees of freedom.

For the geometry designed, the boundary conditions upon which the Navier-Stokes and Convective-Diffusion equations will be solved must be defined. The fluid flow characteristics require that the two inlets of the mixer have prescribed flows, while the outlet is set to have normal flow and stress. All other surfaces are defined by the “No-Slip” condition. The Convective-Diffusion equations is defined at the inlets by concentrations, the outlet is set as having convective flux. The remaining walls are not permeable, and so are set as insulated surfaces.

In order to provide an example of how the geometry was drawn, and also to show an example of the Navier-Stokes, Fig. 2 is provided. For this instance, the sample feed inlet flow rate is 5 _L per minute, and the diluent is set at 100 _L per minute, providing a 1:20 dilution ratio.

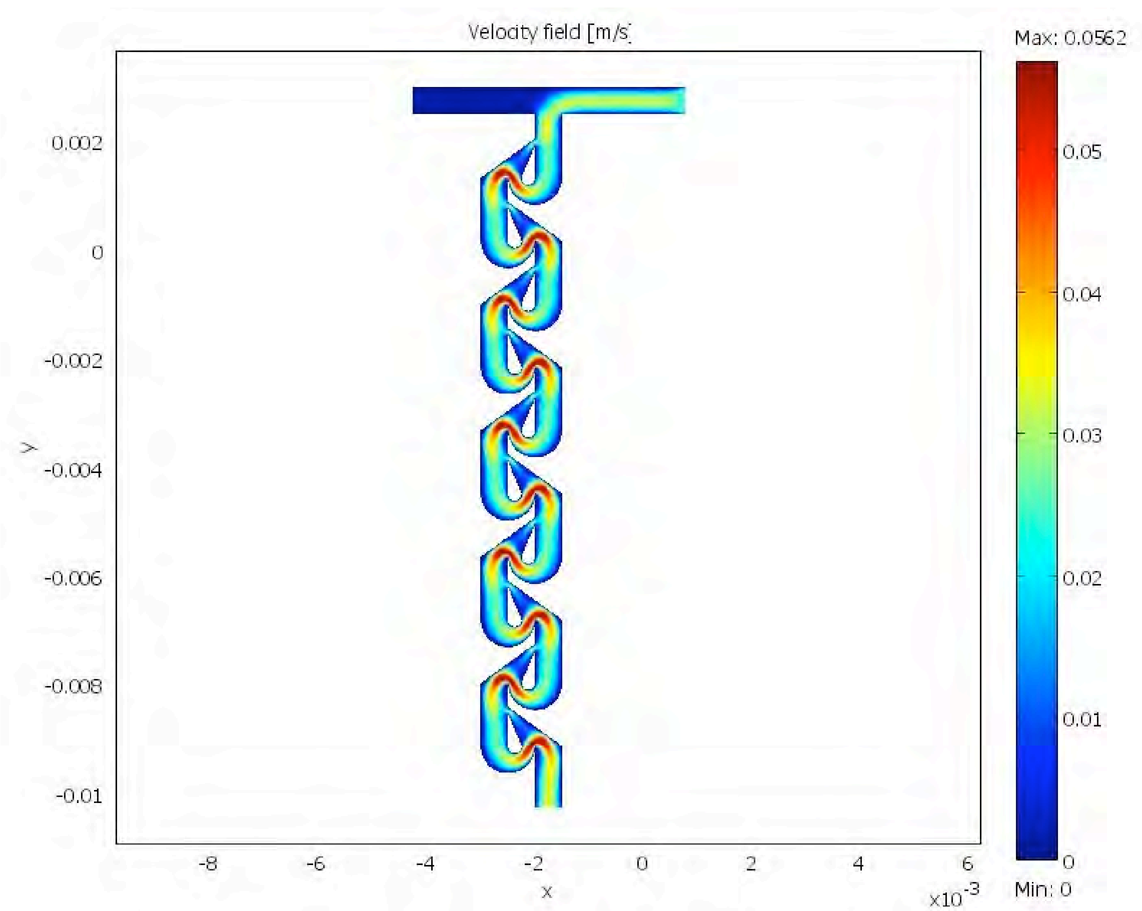

Figure 2. Solution of the Navier-Stokes Equations for the Tesla Mixer

The more important solution of this analysis is the concentration profile of the outlet, which provides the inlet details for describing diffusion in the straight channel. Figure 3 shows this concentration profile. This profile was fitted to a 5th order polynomial in order to obtain data points which are evenly distributed, as needed for the finite-difference analysis performed on the straight channel. To clarify the term, the profile position denoting the x-axis of Fig. 3 represents the position across the width of the mixer outlet, so -.002 to -.0015 is the entire width of the mixer. Additionally, these numbers are negative simply because that was the position of the outlet in the <u>Comsol</u> simulation, there is no other significance.

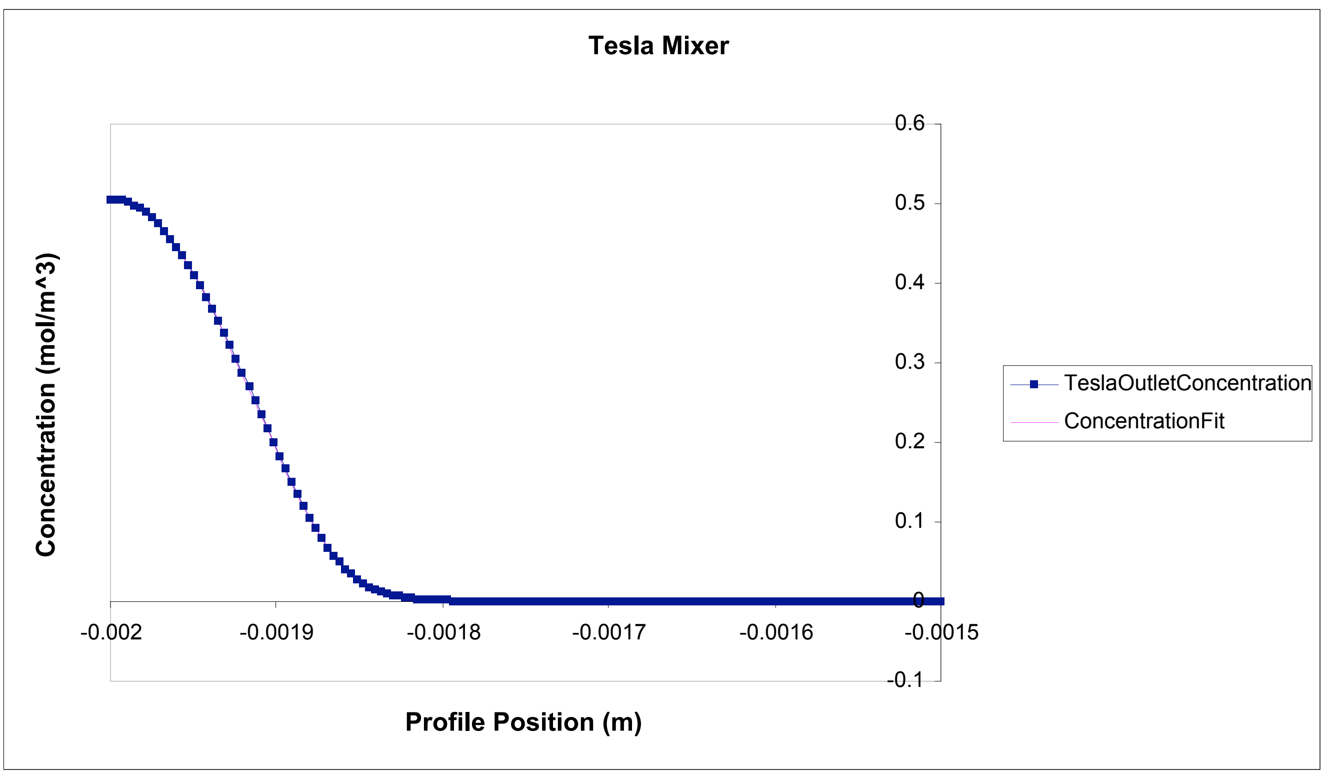

Figure 3. Tesla Mixer Outlet Concentration Profile.

Straight Channel

Because of the length of the straight channel, modeling the fluid flow and diffusive mixing using Comsol would necessitate a large number of mesh elements, and so make obtaining solutions with a fine mesh difficult. Fortunately, the simple geometry makes modeling this portion of the device relatively easy to do without a program such as Comsol. Code for solving the differential equations which compose the Convective-Diffusion equations using the finite difference method was compiled in Matlab to calculate the outlet concentration profile from the channel. The entire code, written by Prof. Finlayson, is shown in the appendix. The channel width is maintained at 500 _m, and the length of the channel is approximated as 90 mm. However, the velocity for this device is held constant at 5 _L per minute as the velocity is reduced to this value after leaving the Tesla mixer and prior to entering the straight channel.

Figure 4 shows the outlet concentration from the straight channel as well as the outlet of the Tesla mixer which is the inlet concentration profile for the straight channel. Because of the length of the straight channel as well as the low velocity compared to the Tesla mixer, far more complete mixing was observed in the straight channel. In fact, as can be seen, a nearly uniform concentration profile is the result of the mixing in the straight channel. For the purposes of the final simulation, this concentration was assumed to be constant across the outlet, as it nearly is, to slightly simplify the inlet conditions of the intersecting channels.

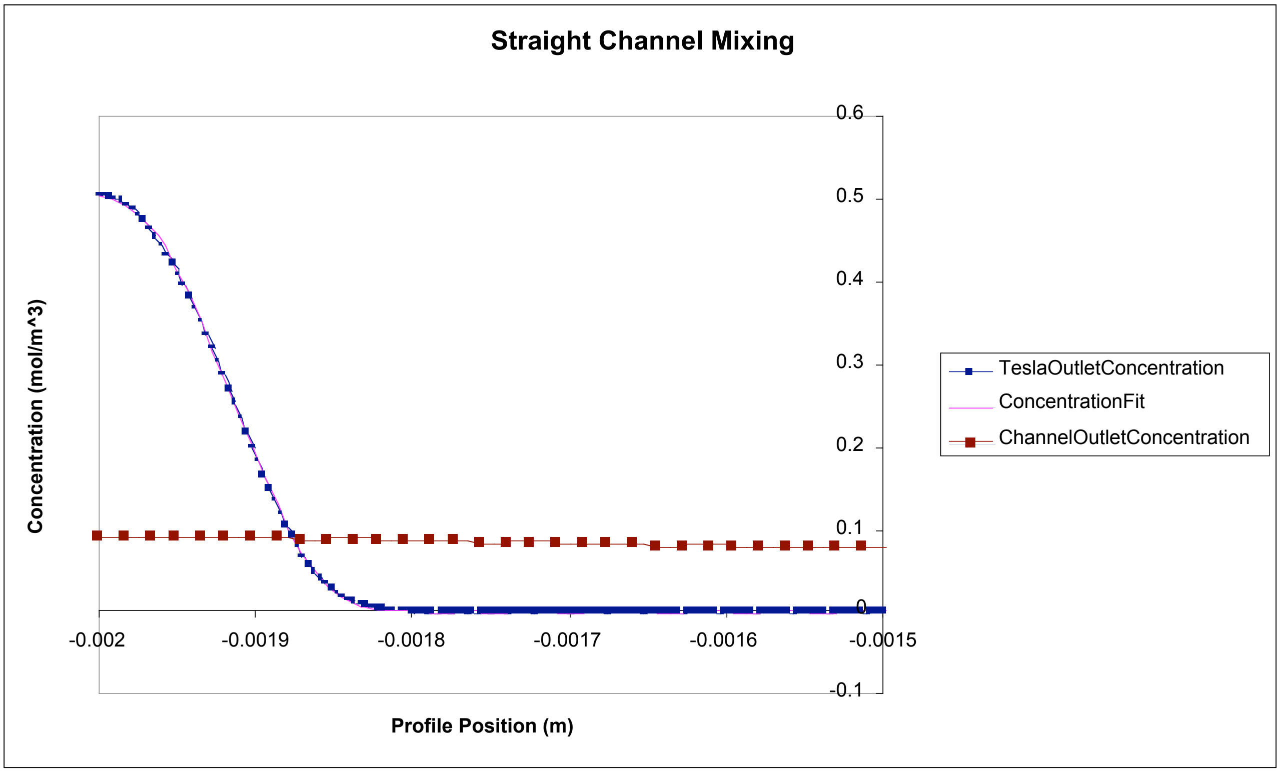

Figure 4. Mixing in the Straight Channel.

Crossed Channels

The final of the three components of the microfluidic device to be simulated was the intersecting channels which generate the concentrated plug of the sample needed. While the geometry, shown in Fig. 5 on the following page, is simple, the transient nature of the simulation makes the simulation far more complex, so performing this kind of analysis with Matlab would be quite difficult, or at the very least far beyond my abilities. The sample enters from the bottom with the intersecting flow coming from the right. The slug of material, if correctly generated, would exit at the top of the geometry. With the concentration provided by the Tesla mixer and straight channel simulations, the only other inlet conditions to specify were the inlet velocities of the sample and of the intersecting channel. Similar boundary conditions to that of the Tesla mixer were used for this simulation as well. Outlets were either described by normal flow and convective flux while walls were defined by the "No-Slip" condition and insulation. Inlets have prescribed velocities and concentrations.

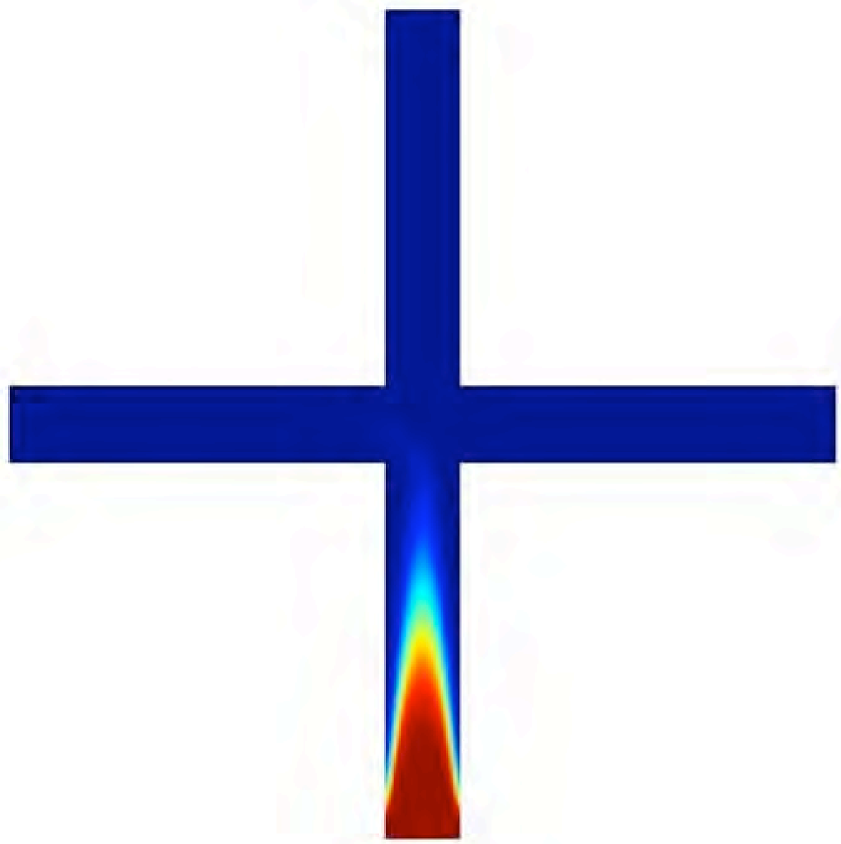

Figure 5. Crossing Channels Geometry.

The sample flow was steady at 5 _L per minute for the duration of the simulation, but in order to generate the plug of material, the intersecting inlet velocity had to be varied with time. The velocity was initially maintained at a constant of 5 _L per minute and was maintained at this value until 5 seconds in order to maintain steady state. It should be noted that it may have been better to allow the flow to remain steady for a greater duration of time in order to be entirely confident that a steady state had been obtained. Doing so would be an entirely superficial addition to the simulation and so there is no complicating factor preventing one from doing. At five seconds, the velocity was dropped exponentially for .125 seconds to 0 _L per minute, which it maintained for .75 seconds. After that period, the velocity increased exponentially back to its initial condition of 5 _L per minute. This change in velocity is represented by Fig. 6 which gives the average outlet velocity for the channel in which the plug was generated. It can be seen that for a period of time from five to six seconds, the velocity decreases to half of its steady value and then returns.

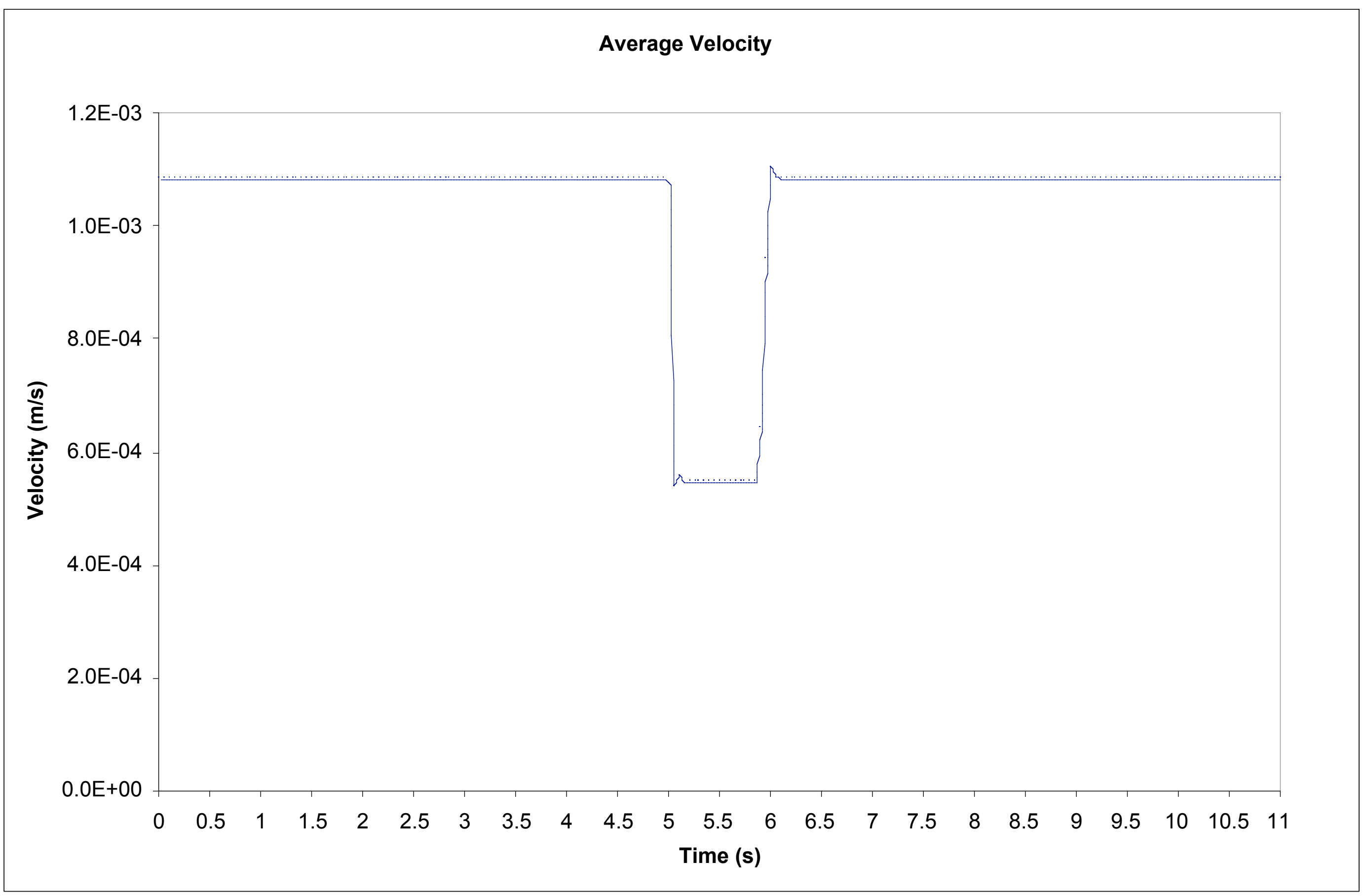

Figure 6. Average Velocity at Plug Outlet of Crossing Channels.

As a result of this decreased velocity the average concentration at the intended plug outlet experiences a spike shown in Fig. 7.

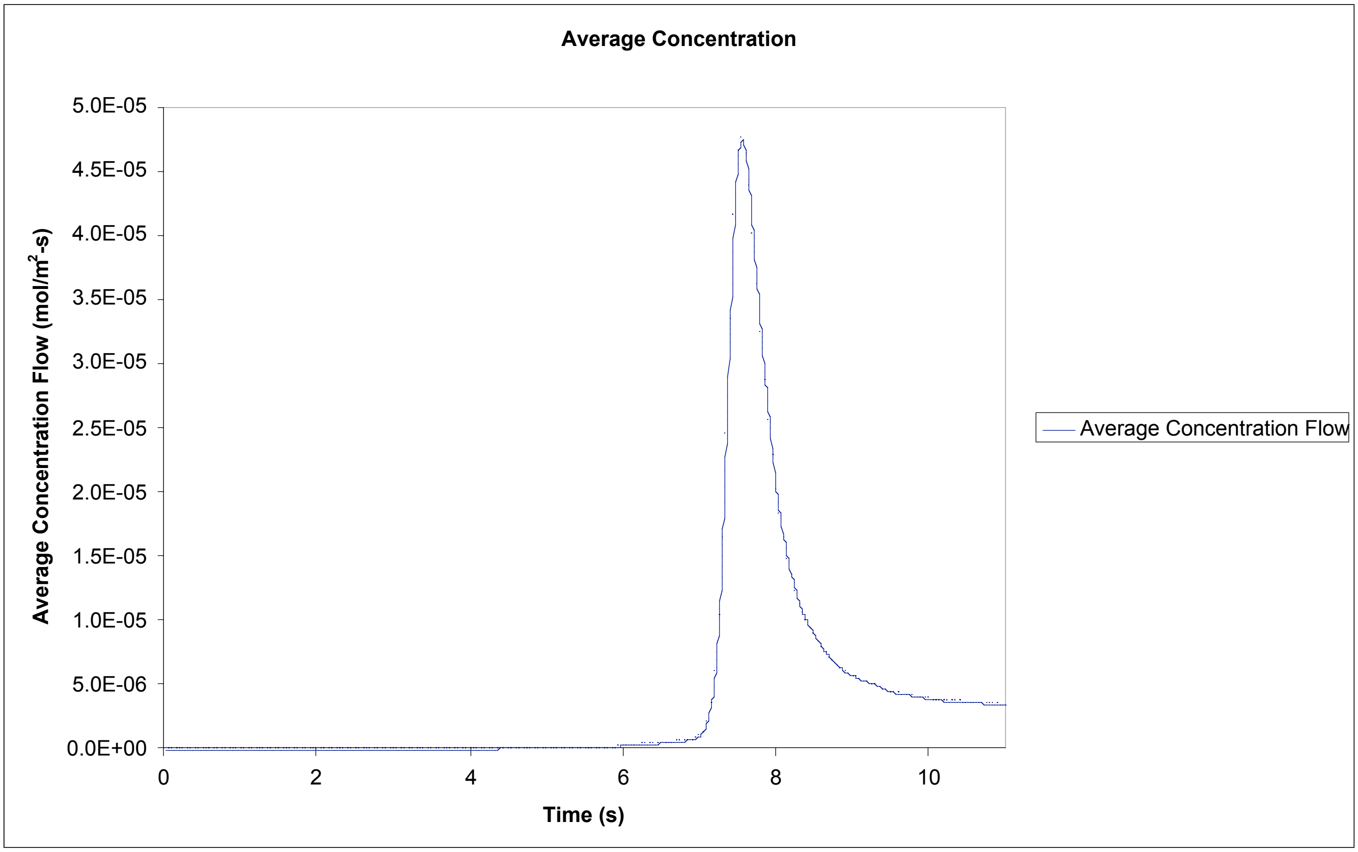

Figure 7. Outlet Concentration of Plug Channel.

It is clear that there is certainly a period in which concentrated material is exiting the channels, and so it appears as though a concentrated plug of the sample is certainly being generated. It can be seen though that the plug is certainly not a discrete plug like would ideally be the case. The duration of the simulation was 11 seconds (Chosen arbitrarily and assumed to be sufficient to observe plug creation), and Fig. 7 certainly shows that while there is an acute peak of heightened outlet concentration, it does not return to its initial condition as rapidly as does the velocity. It would seem that while a plug is certainly being generated, it may have a tail of the sample and is not such a simple shape. The results of the Comsol simulation absolutely confirm this is the case as shown in Fig. 8 which is the Convective-Diffusion solution at 6.75 seconds. The plug is clearly visible, as is the tail of the concentrated sample which results as the plug is cleaved by the increasing velocity of the intersecting channel.

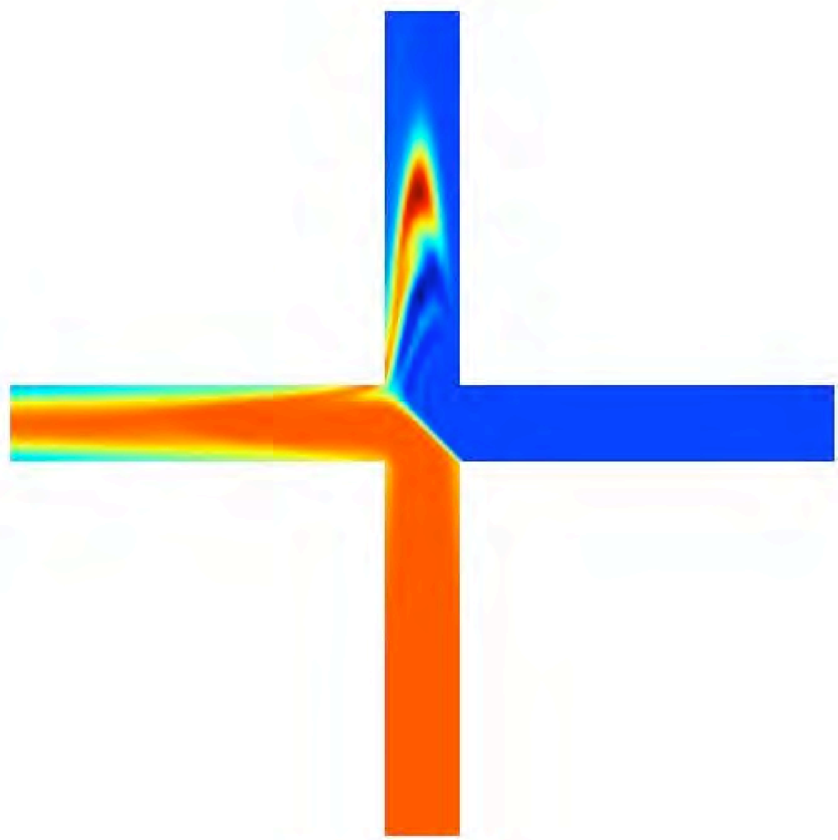

Figure 8. Plug Formation in Crossed Channels.

To describe how the plug forms, the decreased velocity from the right inlet allows the sample from the bottom to begin to move to the top outlet. However, the velocity is decreased for only a short period, so no steady flow is established, but a bubble of the sample forms in the intersection. As the intersecting velocity increases, this bubble is cleaved from the normal flow of the sample, giving the plug seen in Fig. 8. However, because the velocity of the right inlet does not instantaneously increase, the plug is not perfectly formed, giving the tail seen. Also, because the velocity of the intersecting inlet is decreased to 0 _L per minute, this is the largest plug that could possibly be generated with all of the other conditions maintained as constants. However, whether the plug generated is satisfactory is dependent on the device user.

Citations

Finlayson, Bruce A. Introduction to Chemical Engineering Computing. Hoboken: John Wiley & Sons, Inc., 2006.

Gilbert, Scott. “Microfluidic LC Chip for On-line Monitoring”.

Appendix A: Matlab Code

File 1: diffusion.m

```
% diffusion.m
function ydot=diffusion(z,y)
global diffusivity width vavg n delx2

ydot(1)=diffusivity*2*(y(2)-y(1))/(delx2*vavg);
for i=2:n
   ydot(i)=diffusivity*(y(i+1)-2*y(i)+y(i-1))/(delx2*vavg);
end
ydot(n+1)=diffusivity*2*(-y(n+1)+y(n))/(delx2*vavg);
ydot = ydot';
```

File 2: run_diffusion_5uls.m

```
% filename run_diffusion.m
global diffusivity width vavg n delx2
% physical case
diffusivity=1e-9 %m^2/s
width = 0.5e-3 %m
vavg = 0.00111 %m/s
% numerical parameters
n=32
delx=width/n
delx2=delx^2;
% need n+1 points y0
y0 = [0.5064   0.4953 0.4668 0.4192 0.3552 0.2809 0.2038 0.1323 0.0736 0.0327 0.011
               0.0049 0.0046 0      0      0      0      0      0      0      0
               0      0      0      0      0      0      0      0      0      0
               0      0]
zspan=[0:1e-3:.09]; %m
[t y] = ode45(@diffusion,zspan,y0);
plot(t,y)
pause
nplot=size(y)
for ij=1:nplot(1)
   c=y(ij,:);
   sum=(c(1)-0.5)^2;
   for i=2:n
      sum=sum+2*(c(i)-0.5)^2;
   end
   sum=sum+(c(n)-0.5)^2;
   variance(ij)=sum*delx/(2*width)
   length(ij) = t(ij);
end
plot(length,variance)
```