Numerical Simulation of Micromixing by Surface Charge Heterogeneity using CoventorWare

MCEN5248 MEMS II - Independent Project Progress Report

Paul JooYoung Lee

1. Project definition revisited

Electroosmosis is one of the mechanisms that is used for fluid transportation in microfluidics. Electroosmotic flow (EOF) occurs when the channel wall is surface charged due to the presence of a buffer solution and because of the surface charge a diffuse layer of charged ions called double layer is created along the cross-section of the fluid. If a voltage potential is applied across the channel, the double layer translates, dragging the fluid along by viscosity effects. This in turn creates a unique bulk flow with almost-columnar fluid velocity profile. Using appropriate geometry and voltage boundary conditions, one can have a fine control over the fluid flow pattern in the microchannels.

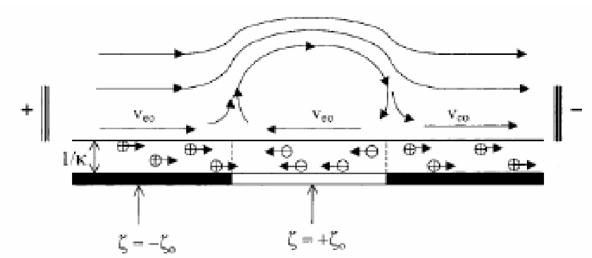


Figure 1. The schematic of micromixing by surface charge heterogeneity electroosmosis.

Another important application of EOF is for microscale fluid mixing. In the microfluidics, flow is of laminar nature and mixing is one of the challenges for microfluidic MEMS devices. There are several published works which corporate the use of channel geometries with different voltage potential boundary conditions. This project aims to come up with another but simpler micromixing channel design, which uses heterogeneously charged surface coatings to induce turbulence around the channel wall (Figure 1). The design will utilize a simple bar geometry with both positive charged and negative charged polymer coatings.

2. Schedule and milestones

In order to come up with a new design, a validation model had to be first built against a published result. After an extensive literature search, a journal article by Fu [1] was found viable and it contains results of both simulation and experiment of micromixing in T shaped microchannel using homogeneous surface charge.

After validation, properties of polymer coatings for making surface charge will be collected for the new design. The polymer coatings from the Davis and Bowman group from Dept. of Chem. Eng., Univ. of Colorado at Boulder will be used as the surface charge coatings. Using the information, several designs of surface charge heterogeneity channels will be simulated for good mixing scheme.

At this point, the author has completed the validation simulation and has collected information for the coatings through a meeting with the members of the Davis group. Mr. Good and Mr. Brothert from Davis group have also provided some journal articles about surface heterogeneity channel designs.

3. Validation simulation settings

The validation model by Fu [1] has a basic T-form mixing channel shown in figure 2. The high voltage potential is applied across the channel, alternating between the two inlets at the ends of the T channel. A constant voltage of 90*V/cm* is applied all times at both inlets and then with alternating extra voltage potential between two positive electrodes.

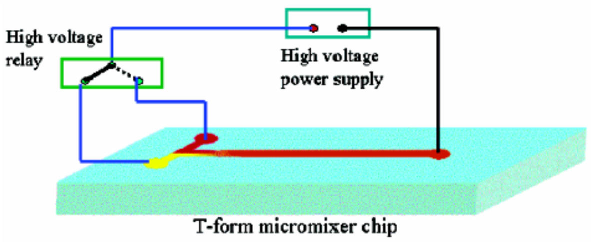


Figure 2. The layout of the T channel micromixer by Fu [1]

There were three validation simulations: (a) steady state simulation with constant voltage at both inlets, (b) switching voltage mixing at 1 Hz and (c) switching voltage mixing at 2 Hz.

The channel model was built using the Fluidics mesh generator of Coventorware™ using the T-geometry with the *Finer* mesh settings. T channel was built with the dimensions shown in figure 3 and the simulation was treated as a 2D problem. NetFlow module was used with the following parameters derived from Fu's work [1].

1. No. of Transported species: Carrier + 1
2. Species concentration applied as species surface boundary condition: $10^{-4}M = 100\mu M$
3. Electroosmotic mobility coefficient (EoM): 53100
4. Species diffusion coefficient: $10^{-10}\ m^2s^{-1} = 100\ \mu m^2s^{-1}$
5. Wall and wall effects boundary condition at Wall face

The EoM was calculated using equation 1 since the parameters given in the Fu's paper was:

1. Dielectric constant, $\varepsilon = 80$
2. Zeta potential, $\zeta = -75mV = 0.075V$
3. Dynamic viscosity, $\mu = 10^{-3}\ N.s/m^2 = 10^{-9}\ kg/\mu ms$

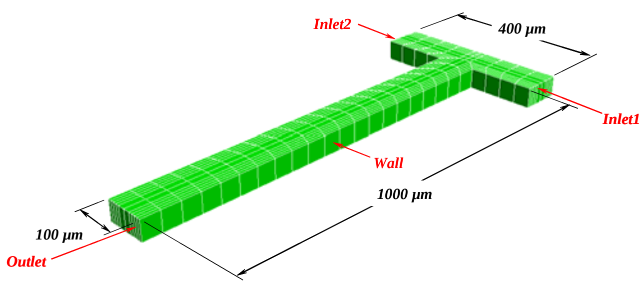


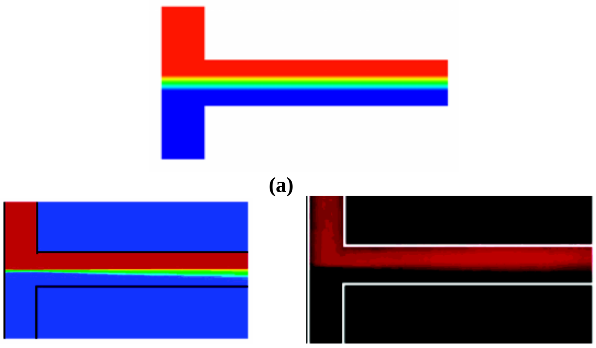
Figure 3. The T-channel model dimensions and the face names. Mesh was made with Fluidics mesh generator, ConventorWare™

$$EoM = \frac{\varepsilon \times \varepsilon_0 \times \zeta}{\mu} \qquad (1)$$

This equation was taken from the NetFlow theory section of the CoventorWare™ tutorial. For the transient analysis, the voltage was applied using an input file option with two text files for inlet1 and inlet2 voltages. For 1 Hz analysis, the driving voltage alternated between 9*V* and 11.25*V* every one second, and for the 2 Hz analysis the switching was made every ½ second. The driving voltage was calculated using the voltage gradient value of 90*V/cm* i.e. 90*V/cm* x 1000*μm* (0.1*cm*) = 9*V* and the higher voltage is obtained by dividing by 0.80 according to the figure 4 of the Fu paper [1]. The guideline to setting transient voltages using an external input file and various other methods is discussed in the CoventorWare analyzer microfluidics reference and tutorials page F2-74. The total simulation time was 5 seconds with 0.2 second output time and 0.01 second time steps.

4. Results and discussions

The results of the CoventorWare™ simulations were identical to the published results. In fact, author's results show better match with the experimental results in the paper than Fu's numerical simulations. Figure 4 shows that three steady state solutions are identical.

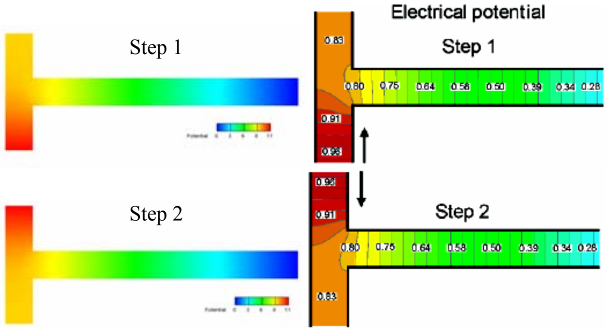


(a)

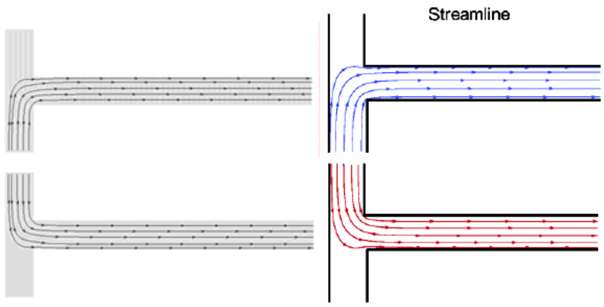
(b) (c)

Figure 4. Steady state solution with a constant driving voltage at both inlets (a) CoventorWare simulation, (b) numerical solution by Fu (c) experimental solution by Fu.

Figure 4 is the voltage potential plots and the streamline plots. The streamline was plotted using the streamtrack plot function under the contour menu of results viewer, CoventorWare™. The plots also show a good match in this case.



(a) (b)



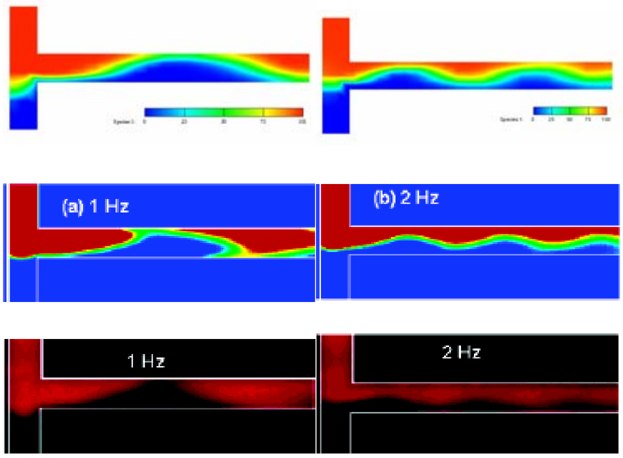
(c) (d)

Figure 5. The voltage potential plot and streamline plot for the transient analysis. The voltage is switched every step between the two inlets. (a) and (c) are the CoventorWare™ results and (b) and (d) are the numerical results from Fu.

Figure 6 is the transient analysis results at 1 Hz and 2 Hz each. The top plots, which are the results from CoventorWare™ simulation by author, conform well to the published experimental results at the bottom. The numerical solution by Fu at 1 Hz is somewhat different from the experimental results and proves the more accurate results by author's simulation.

In conclusion, all three simulation results prove the validity of using CoventorWare™ NetFlow module for simulating a new design. The simulation results exhibit better results than the published numerical solutions.

The next step for the project will be to simulate surface charge heterogeneity and try various designs. According to Davis group members, they can coat the wall surface with any polymer of zeta potential between 50mV and -50mV. They use the photolithographic technique to photopattern the polymers on the surfaces with help from surface adhesion catalyst. This catalyst ensures that they can coat almost every polymer with good adhesions.



(a) (b)

Figure 6. The transient analysis results at 1 Hz (a) and 2 Hz (b) switching frequencies. From the top to bottom: CoventorWare simulation, numerical simulation by Fu and experimental results by Fu.

[1] C.H. Lin, L.M. Fu, Y.S. Chien, *Microfluidic T-Form Mixer Utilizing Switching Electroosmotic Flow*, Anal. Chem.2004, v76, p5265-5272