A Computational Model for Simulation of Electroosmotic Flow in Microsystems

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ABSTRACT

A numerical model has been developed to simulate three-dimensional and transient electroosmotic flow occurring in various microdevices for handling fluid flow and transport. The model can simulate one fluid flow, with or without a free surface, and two-fluid flow, with or without a sharp interface, using a VOF method. The model is validated by comparing numerical predictions against available analytical solution. Capabilities of the model to simulate processes such as sample focusing, micropumping, and micromixing. are demonstrated through examples.

Keywords: Electroosmotic Flow, Micropump, Micromixer, and Sample Injection

1 INTRODUCTION

Electroosmotic flow or electroosmosis is created by applying an external electrical field on electrical double layers (EDL) formed due to the interaction of an electrolyte solution with a dielectric surface. It appears in a variety of micro fabricated fluidic devices such as valves and pumps for fluid handling and analysis. This kind of flow plays an important role in various micro systems (MEMS and BioMEMS) for fluid handling and analysis. For example, it is utilized in various biomedical lab-on-a-chip devices to transport liquid (buffer or sample) for different purposes, such as sample injection, chemical reactions, and species separation. Due to its importance, electroosmotic flow in microchannels has received considerable attention recently and been investigated both numerically and experimentally [1]-[11].

Patankar and Hu [1] carried out a three-dimensional and steady numerical solution of electroosmotic flow using a finite volume method. The Debye-Huckel approximation was used to linearize the expression for charge density. Electroosmotic flow in a cross-shaped intersection was considered as an example of sample injection. Mitchell et al.[2] made simulations of electroosmotic flow in a straight channel, a cross-shaped intersection, and a T-shaped intersection using a meshless computational method. Combined electroosmotic/pressure driven flows in a straight channel, a cross-shaped intersection, a T-shaped junction, and a Y-split junction were studied by Dutta et al.[3]-[4] using a mixed structured/unstructured spectral element method. Dutta and Beskok[5] also performed an analytical solution of combined electroosmotic/pressure driven flows in a two-dimensional straight channel. Finite Debye layer effects were analyzed. To investigate the effect of channel cross section geometries and nonuniform ζ-potential along the channel walls, the two-dimensional and steady finite difference solutions of electroosmotic flow in straight channels was performed by Ren and Li[6] and Arulanandam and Li[7]. The effect of nonuniform ζ-potential on electroosmosis was also investigated by Potcek et al.[9]. In their simulation, the EDL is approximated by using a slip velocity equal to electroosmotic velocity. Electroosmosic flow in a two-dimensional microcapillary with one liquid solution displacing another solution was studied by Ren et al.[8]. Ermakov et al.[10]-[11] investigated mass transport and fluid flow driven by electroosmosis in two-dimensional channels. Two injection techniques (pinched and gated valves) were simulated. The effects of the electric field distribution in channels for sample transport during different phases of injection were analyzed to get proper injection parameters for an optimal sample analysis.

Most of the work described above on simulation of electroosmotic flow focussed on two-dimensional and steady cases. One exception is the work performed by Patankar and Hu[1] for three-dimensional and steady electroosmotic flow. However, transient simulations can provide more insight into the characteristics of electroosmotic flow important to the biochip operation as reported by Fan and Harrison[12]. They observed that the duration of electroosmotic injection for biochip operation affects the separation efficiency, implying the importance of the transient process. In addition to the importance of transient characteristics of electroosmotic flows, three-dimensional effects are also important and indispensable for the simulation of real micro devices since the channel cross sections in microfluidic devices made by microfabricating technology is close to a rectangular shape and the ζ-potential in a channel wall is not uniform due to the ionic concentration of the electrolyte solution, surface properties of the channel walls or adhesion of particles (DNA and protein) in solution. Therefore, in the present paper, we provide a numerical approach for the simulation of three-dimensional and transient electroosmotic flow. In the following section, the governing equations and their numerical solution are discussed, followed by a section containing model validation and a few examples to illustrate the application of the developed model. Finally, a brief conclusion is drawn.

2 GOVERNING EQUATIONS AND NUMERICAL METHOD

As mentioned earlier, electroosmotic flow is created by applying an external electrical field on the EDL formed on solid-liquid interfaces. The governing equations for this kind of flow with the assumption of an equilibrium Boltzmann distribution of ion concentration for single-charged ions are

$$\nabla \cdot \mathbf{V} = 0 \tag{1}$$

$$\rho \left[\frac{\partial \mathbf{V}}{\partial t} + \mathbf{V}(\nabla \cdot \mathbf{V}) \right] = -\nabla P + \mu \nabla^2 \mathbf{V} + \rho_E \mathbf{E} \tag{2}$$

$$\nabla^2 \phi = 0 \tag{3}$$

$$\nabla^2 \psi = -\frac{\rho_E}{\epsilon} \tag{4}$$

$$\rho_E = 2FC_0 sinh \left(\frac{F\psi}{RT} \right) \tag{5}$$

where $\mathbf{V}$ is the velocity vector, ρ the density, P the pressure, μ the viscosity, ρ_E the charge density, $\mathbf{E}$ $(= -\nabla\phi)$ the electrical field intensity, F is the Faraday's constant, R the gas constant, T the temperature, C_0 the ionic concentration in the bulk solution, ϵ the permittivity, ψ the potential due to EDL, and ϕ the applied potential.

The boundary conditions for Eqns.(1) and (2) are obvious and will not be repeated here. The insulation boundary condition for ϕ is imposed on all solid walls while specified boundary conditions for ψ on all dielectric solid walls are corresponding ζ-potentials.

The above equations in their two-dimensional and steady forms have been solved numerically in [4]-[7], while the three-dimensional and steady numerical solution was carried out in [1], with the Debye-Huckle approximation applied on the right side of Eqn.(4). This is only valid for a small ζ-potential. In the present paper, Eqns.(1) through (5) in their three-dimensional and transient form are numerically solved along with the following Volume-of-Fluid (VOF) equation[13] for the volume of fluid function (F).

$$\frac{\partial F}{\partial t} + \mathbf{V} \cdot \nabla F = \nabla \cdot (\mathcal{D} \nabla F) \tag{6}$$

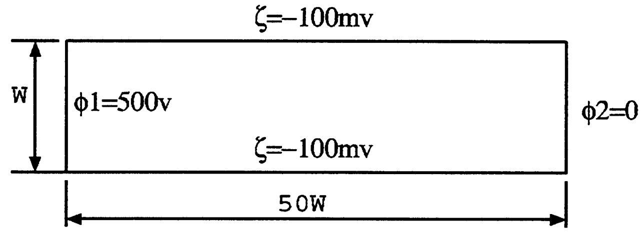

Figure 1: An Illustration of Straight Channel Used for Model Validation

The VOF method is used to track liquid free surface and liquid-liquid interface (for example, sample injection). Alternatively, sample flow and diffusion can also be simulated by a scalar transport equation represented by

$$\frac{\partial C_s}{\partial t} + \mathbf{V} \cdot \nabla C_s = \nabla \cdot (\mathcal{D} \nabla C_s) \tag{7}$$

where C_s is the concentration of sample while $\mathcal{D}$ is the diffusion coefficient. ***FLOW-3D***®—a commercial CFD code—is used to implement this model where a fractional-area-volume-obstacle-representation (FAVOR™) method is used to handle flows in complicated geometries in a fixed-grid of cells. Detailed information can be found in [14]. The capabilities for solution of Eqns.(1)-(2), (6) and (7) are already available in the code and have been widely validated. The Eqns.(3)-(5) are discretized in a fixed-grid of cells and the resulting equations are solved using a GMRES-like iterative method[15]. The ζ-potentials are imposed on obstacles as shown in the illustrated examples later on to facilitate the solution of Eqn.(4).

3 MODEL VALIDATION AND APPLICATIONS

To validate the developed model, the electroosmotic flow through a simple two-dimensional channel was simulated. The numerical predictions were compared with the corresponding analytical solution given by Dutta and Beskok [5]. The channel geometry is shown in Fig.1. Constant ζ-potentials on the top and bottom walls, and external potentials of 500v at left side (inlet) and zero at right sight (outlet) were imposed. It was also assumed that the related parameters of aqueous solution are $\epsilon = 6.95 \times 10^{-10} C^2/Jm$, $\mu = 10^{-3} Ns/m^2$, $\rho = 10^3 kg/m^3$ and $C_0 = 3.723 \times 10^{-6} mole/m^3$. These parameters were also adopted in all simulations of the following examples. Figures 2 and 3 show the potential (ψ) and velocity profiles derived from numerical and analytical solutions. An excellent match between model predictions and analytical solutions was reached.

To illustrate practical applications of the developed model, three examples were presented. In the first exam-

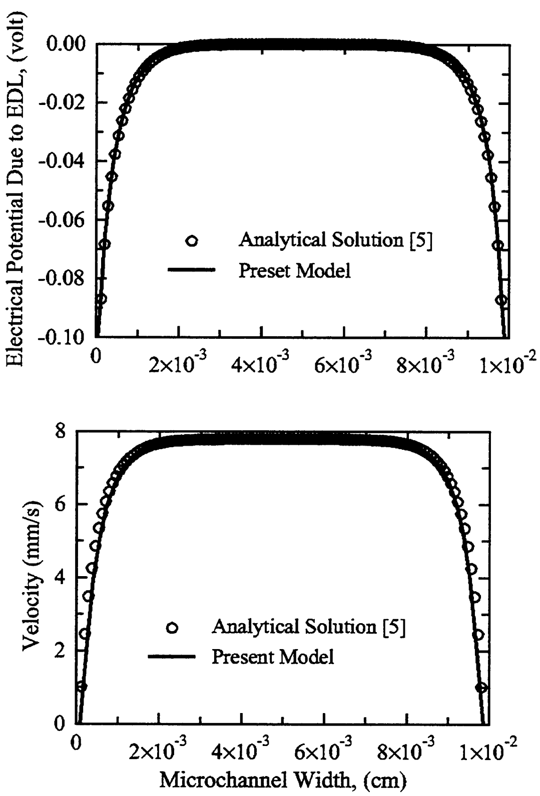

Figure 2: Comparison of Model Predictions and Analytical Solution[5]; Top: potential; Bottom: velocity

ple, a sample focusing process is simulated. The channel size is given in Fig.3. A constant ζ-potential equal to $-150mv$ on all channel walls was imposed. The sample was introduced from the left port while buffer liquid came from the top and bottom ports. The sample focusing was controlled by imposed external potentials at top and bottom ports. The left part of Fig.4 shows the potential (ψ) distribution due to EDL while the steady focused sample shape is shown on the right part of the same figure. In the second example, fluid flow driven by electroosmosis (micropumping) was simulated. Figure 5 shows channel geometry and boundary conditions.

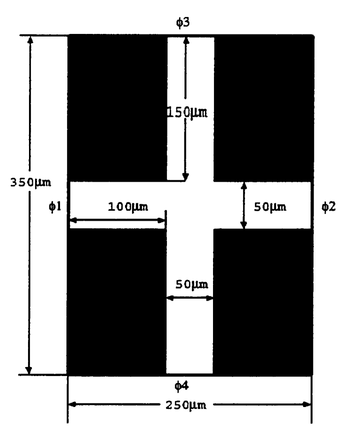

Figure 3: Channel Geometry and Dimensions

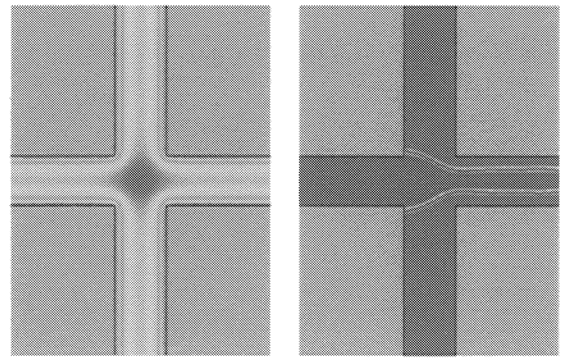

Figure 4: Potential Distribution and Focused Sample Shape

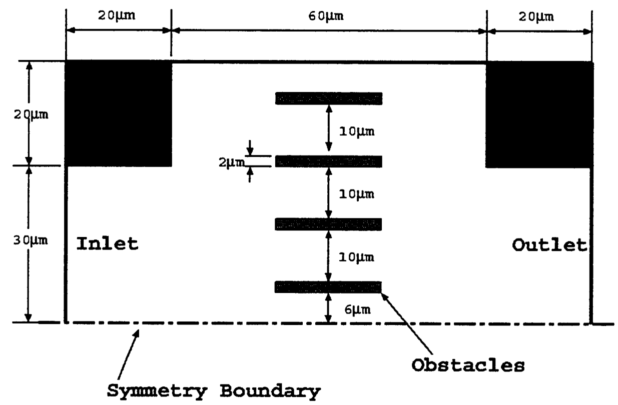

Figure 5: Channel Geometry and Boundary Conditions

The ζ-potential equal to $-150mv$ is imposed on the obstacles indicated in the figure. The external potential was imposed at the inlet while the outlet was grounded. The potential distribution due to EDL and fluid field are shown in Fig.6. The last example simulated the electroosmotic flow through a three-dimensional channel with its wall covered by some charged bands where EDL is formed as shown in Fig.7. External potentials were imposed at the inlet and the outlet of the channel. A helical flow field inside the channel was created as illustrated by streamlines plotted in Fig.8. It is interesting to notice that the fluid field formed due to nonuniform ζ-potential at channel walls can be used for fluid mixing in microdevices. To see the mixing process (fluid stretching and folding), a block of marker particles was initially placed near the channel inlet (the top of Fig.9). Particle distribution at 4 and 8ms, colored by its direction (perpendicular to the paper), is shown on a two-dimensional slice (the bottom of Fig.9). Fluid stretching and folding were clearly observed.

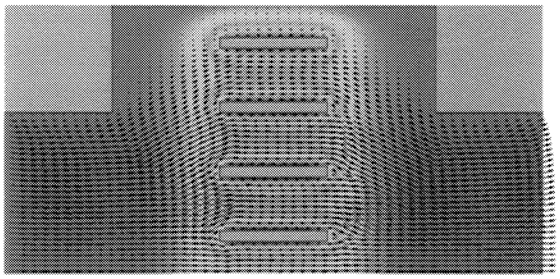

Figure 6: Potential and Flow Distribution

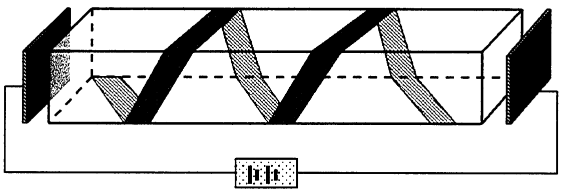

Figure 7: A Three-dimensional Channel with Charged Bands

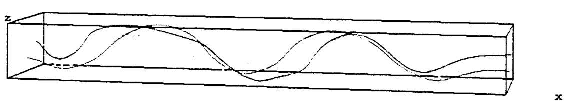

Figure 8: A Few Chosen Stream Lines

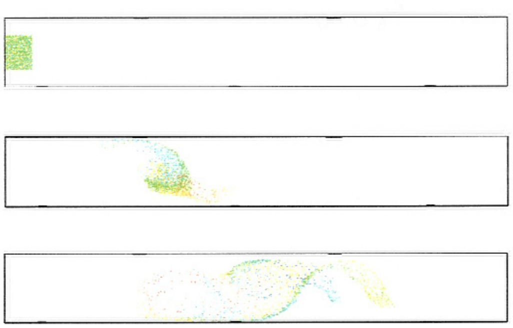

Figure 9: Marker Particle Distribution at Time=4ms and 8ms

4 CONCLUSION

The present paper describes a numerical model for the simulation of three-dimensional and transient electroosmotic flow in microsystems. That has been implemented in the commercial software ***FLOW-3D*®**. The modified code was used to simulate electroosmotic flows in a few representative geometries encountered in microsystems. It was shown that the model is robust and accurate in simulating electroosmotic flows. Nonuniform ζ-potentials in channel walls can be taken advantage of for fluid mixing. The potential applications of the model for the design and operation of microdevices such as micropumps, microvalves, and micromixers, was also demonstrated through examples. The model will be a useful tool for designing and optimizing the operation of microsystems involving electroosmotic flows.

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