A NUMERICAL MODEL FOR SIMULATION OF COMBINED ELECTROOSMOTIC AND PRESSURE DRIVEN FLOW IN MICRODEVICES

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ABSTRACT

With the development of microfabrication technologies, microdevices are becoming more and more important to engineers examining microscale systems, especially those for chemical or biological analysis. Simulation of fluid flows through various microdevices will facilitate engineers to derive better design for controlling and handling fluid flows through microdevices. Present paper presents a numerical model to simulate combined electroosmotic and pressure driven flow. The model is validated by comparing numerical results against the corresponding analytical solution and very good match between data and model is obtained. To illustrate the application of developed model, fluid flow in a three-dimensional microchannel is simulated.

1 INTRODUCTION

Microfluidic devices that perform various chip-based chemical, biological, and medical analysis have received significant attention recently due to their advantages in shortening analysis times, reducing sample volumes, and cutting operation and manufacturing costs. These devices are usually called “lab-on-a-chip" devices and they attempt to incorporate many necessary components and functionalites observed in a typical laboratory on the surface of a substrate. The major components of these devices consist of micropumps, microvalves, and micromixers etc. which are used to handle and control fluid flow on a chip.

Hydrodynamic pressure is customarily used as a driving force in such devices, but for very small channels, pressure-driven flow exhibits a parabolic velocity profile and average velocity is proportional to the second power of transverse channel dimension. As a result, the required pressure drop could be too large and may become impractical in very small devices. As an alternative, electrokinetic body forces can be utilized to drive fluid flow. This is known as electroosmotic flow or electroosmosis. These forces are created by applying an external electric field on an electric double layer (EDL), which is formed by the interaction between electrolyte solution and dielectric surface, and function efficiently near a surface. Considered a microchannel flow due to electroosmosis, a plug-like velocity profile is obtained. As a consequence, the average velocity of electroosmotic flow is roughly independent of the device size. Due to this fact, electroosmatic flow has drawn a great attention from engineers and scientists examining microsystems, and is more and more frequently used in handling and controlling fluid flow in various microdevices [1-9]. In present paper, a model for combined pressure and electroosmotic driven flow is presented and validated against available analytical solutions. To demonstrate the application of presented model, a sample simulation is provided. In Section 2, the governing equations and numerical solution algorithm are discussed while model validation along with a sample simulation and conclusion are given in Sections 3 and 4 respectively.

2 GOVERNING EQUATIONS AND NUMERICAL METHODS

As mentioned earlier, electroosmotic flow is created by applying an external electrical field on the EDL formed on the solid-liquid interface. Considering this fact and with the assumption of an equilibrium Boltzmann distribution of ion concentration, the governing equations for combined electroosmotic and pressure driven flow are:

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

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

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

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

$$\rho_E = -2F \sum_i c_{i0} z_i exp\left(-\frac{z_i F \psi}{RT} \right) \tag{5}$$

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_{i0} the ionic concentration in the bulk solution, ε the permittivity, ψ the potential due to EDL, z_i valance, and ϕ the applied potential.

The boundary conditions for Eqns.(1) and (2) are obvious and will not be repeated here. The insulation or specified value 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 [2-5], while the three-dimensional and steady numerical solution was carried out in [6], 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 [7] for the volume of fluid function (F)

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

to simulate fluid flow with a free surface or the replacing of one fluid by another fluid in microchannels due to electroosmotic flow (for example, sample injection). Alternatively, sample flow and diffusion can also be simulated by a scalar transport equation represented by

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

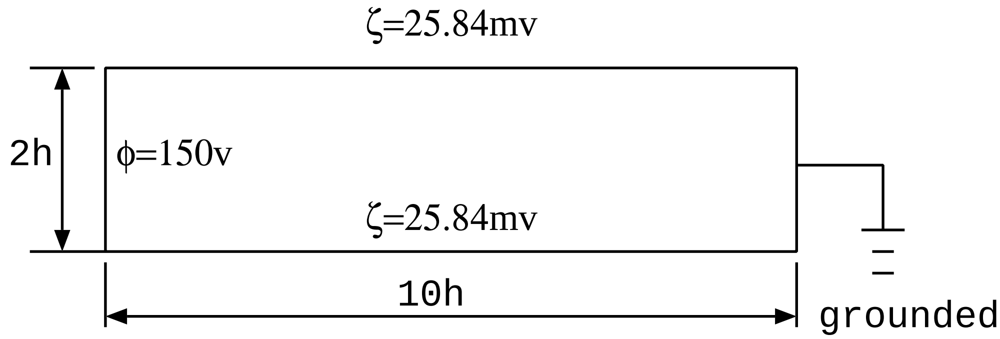

Fig. 1 An Illustration of Straight Channel Used for Model Validation

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 the aforementioned model where a fraction-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 [8]. The capabilities of solution of Eqns.(1)-(2), (6) and (7) are already available in the code and has 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 method [9]. The ζ-potentials are imposed through obstacles as shown in the illustrated examples later on to facilitate the solution of Eqn.(4).

3 MODEL VALIDATION AND SAMPLE SIMULATION

3.1 Model validation

To validate the developed model, the combined electroosmotic and pressure driven flow through a simple two-dimensional channel is simulated. The channel geometry is shown in Fig.1. Constant ζ-potential on the top and bottom walls, and external potential of 150v at left side (inlet) and zero at right sight (outlet) are imposed. It is also assumed that related parameter of aqueous solution are $\varepsilon = 6.95\times10^{-10}C^2/Jm$, $\mu = 10^{-3}Ns/m^2$, $\rho = 10^3 kg/m^3$ and $c_0 = 3.723\times10^{-6} mole/m^3$. These parameters are also adopted in the sample simulation presented below. The analytical solution for this problem was performed by Dutta et al.[2-3] and predicted velocity profile across the channel is:

$$\frac{u(\eta)}{u_p} = -\frac{1}{2}\frac{dP^*}{d\xi}(1-\eta^2) + [1-\psi(\eta)/\zeta] \tag{8}$$

where u_p, P^* and ψ^* are defined by

$$u_p = \frac{\zeta\varepsilon E}{\mu} \tag{9}$$

$$P^* = \frac{P}{\mu\left(\frac{u_p}{h}\right)} \tag{10}$$

while ξ and η are nondimensional coordinates defined by:

$$\xi = \frac{x}{h}\,;\ \eta = \frac{y}{h} \tag{11}$$

x and y are coordinates in horizontal and vertical directions respectively with origin located at center of channel inlet. The numerical predictions are compared with the corresponding analytical solution given

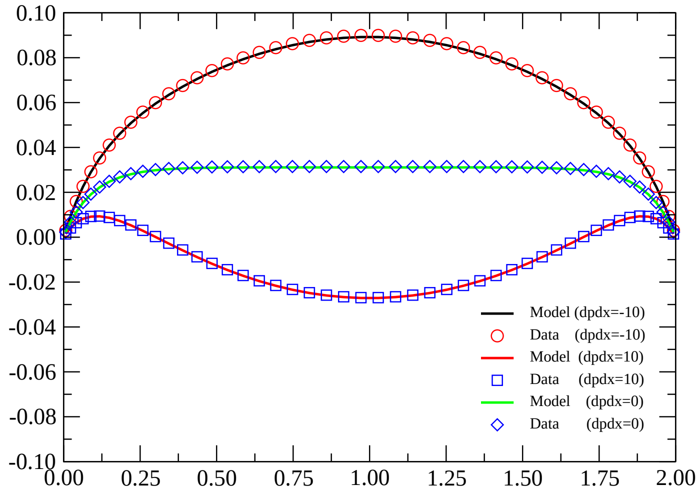

Fig. 2 Comparison of Analytical and Numerical Solutions

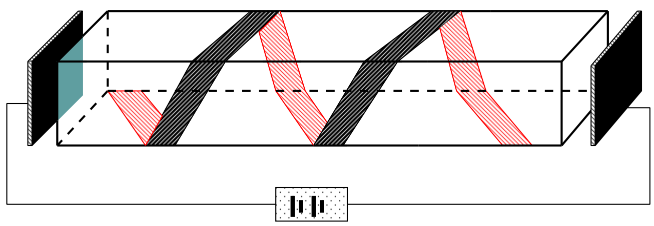

Fig. 3 A Three-dimensional Channel Covered by Some Charged Bands

in Eqn.(8) with different pressure gradients. The numerical solution fit with analytical predictions very well.

3.2 Sample simulation

To illustrate the application of the developed model, the combined electroosmotic and pressure driven flow through a three-dimensional channel with its wall covered by some charged bands where EDL is formed as shown in Fig.3. The pure electroosmotic flow for this geometry was presented in [1] where a helical flow through channel was observed and fluid folding and stretching were obtained. The motivation of creating helical flow in this device is to increase fluid mixing and residence time when it passes through the channel. Since velocity in MEMS devices is very small and related transport process need longer time, without this helical flow, a very long channel could be required. In present work, a pressure gradient (10Pa across channel length) was added against the electroosmotic flow. If considered the path of a fluid particle coming from channel inlet, its path length will be longer and thereby fluid particle residence time will be increased. Figs.4 through 7 show pressure and ζ-potential distributions along with velocity vectors at different cross sections along channel length. Fig.8 shows pressure and velocity distribution in a vertical slice cut through the middle of the channel width. From these figures, you will see helical flow structure is still maintained by adding a pressure gradient against electroosmotic flow.

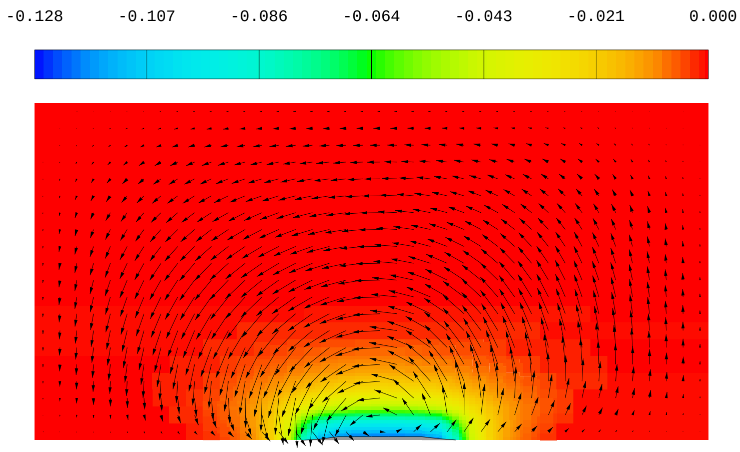

Fig. 4 Velocity and ζ-potential Distribution on a Cross Section at 33.75 *μm* from channel inlet

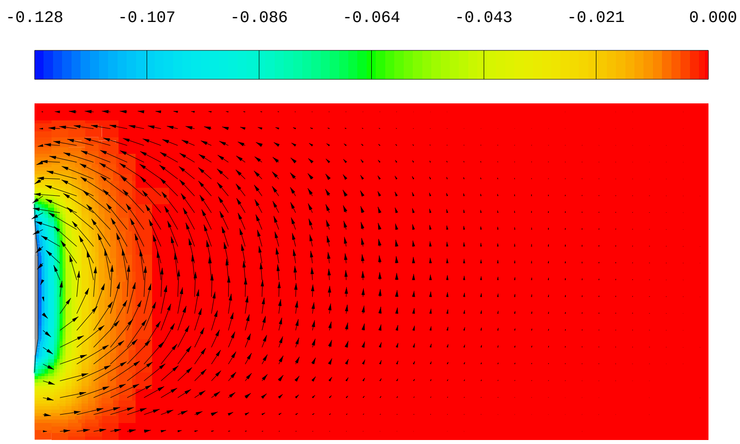

Fig. 5 Velocity and ζ-potential Distribution on a Cross Section at 78.75 *μm* from channel inlet

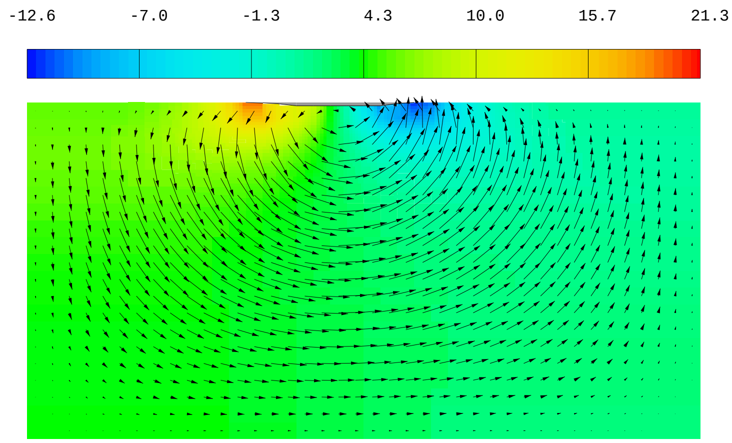

Fig. 6 Velocity and Pressure Distribution on a Cross Section at 118.8 *μm* from channel inlet

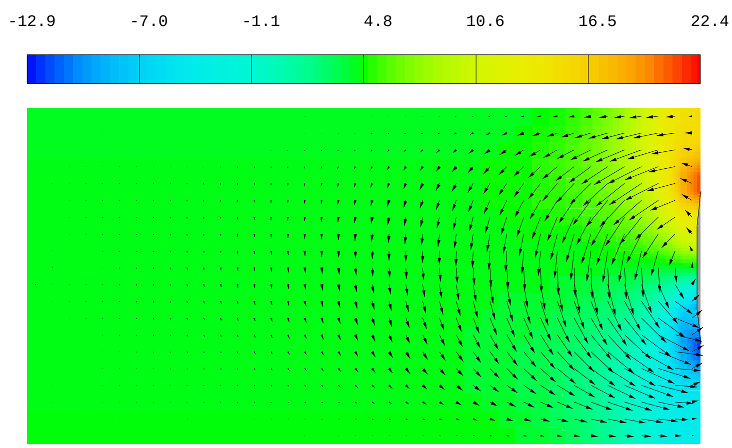

Fig. 7 Velocity and Pressure Distribution on a Cross Section at 163.7 *μm* from channel inlet

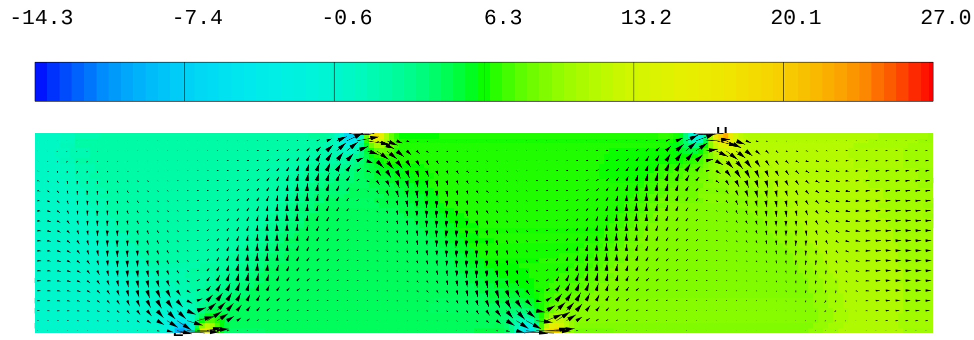

Fig. 8 Velocity and Pressure Distribution on a Vertical Slice Cut through Middle of the Channel

4 CONCLUSION

In present paper, a numerical model for the simulation of three-dimensional, transient, and combined electroosmotic and pressure driven flow in microsystems was developed and implemented in ***FLOW-3D®***. The model is validated by comparing numerical results and corresponding analytical solutions. Application of developed model is illustrated by simulating a complex three-dimensional channel flow. The developed model will be a useful tool for design and optimal operation of various microsystems for controlling and handling fluid flow through them.

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