

TECHNICAL BRIEF: NUMERICAL MODELING AND ANALYSIS OF ELECTROOSMOTIC FLOW IN A DNA CHIP

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Abstract- Lab-on-chip devices have many novel applications for the transport of the liquid samples and buffer solutions for varieties of purposes in biochemical applications. One of the efficient methods is through electrokinetic effects, where an electric field will be applied to charged ions such as DNA, a negatively charged ion which is propelled in a microchannel for further processing. These ions, mixed with the buffer, act as carriers of the entire solution through the selective arrangements via the probe region for its detection transporting from inlet to the outlet. COMSOL, commercially available multiphysics software, with its specific MEMS and Chemical Engineering modules was used to run simulation for the fluid flow and chemical analytes analysis throughout the channel of various shapes.

Keywords- µTAS, Bio-MEMS, Electro-osmosis, COMSOL Multiphysics, Electrokinetic flow, Ionic fluid, COMSOL.

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Introduction

Microfluidics or more recently nanofluidic devices are rapidly heightened micro device embedded tools that have enormous applications such as DNA analysis, drug delivery and proteomic analysis [1]. Generally, electro-osmotic, gas-pressure, positive displacement, micro-peristaltic, thermal, micro-hydrodynamic (MHD), and several other pumping modes have been utilized in order to manipulate micro scale fluid propulsion [2]. Computational modeling, simulation and analysis for electrokinetic fluid flow with species transport and chemical reaction involves the multiphysics modeling of the micro-/nano systems [3,4]. One such study includes studying variation of particle velocity along the axis of the nanopore under the application of electric fields [4]. Based on a main model used from COMSOL library, various models of microchannels were studied.

Geometrical Modeling

A micro-conduit having dimensions for its height, width and length was selected to study electrokinetic fluid flow by two dimensional analysis as shown below in [Fig-1].

Mathematical Modeling

Based on the main model used from COMSOL library as shown in [Fig-1], charged solution is formed to the wall surfaces during the electrokinetic fluid motion. This layer is referred to as a diffuse layer. The layer is dependent on the material used; and the type of charged groups formed i.e. negatively or positively charged groups on the wall's surfaces. The potential difference imposed between its different parts produces a flow in the vertical or horizontal direction, depending on the direction of imposed field. The control model geometry shown in [Fig-2] was modified to see the flow variation. The electric potential differences at the open boundaries between inlets and outlets were applied where fluid was allowed to enter or enter the channel port. The flow is expected to be laminar with of very low Reynolds number (Re<10). In order to justify the electro-osmotic flow the Stokes flow equations could be used. From a published work, the stokes flow equations were derived from the Navier-Stokes equations assuming that the inertial term is zero [3]. Unlike the Navier-Stokes equations, the Stokes equations form a nearly linear system of equations.

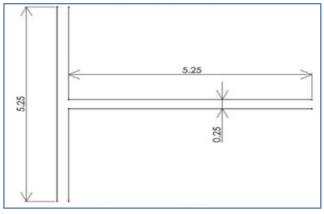


Fig. 1- Control Model microfluidic chip A- COMSOL Model Library (All dimensions are in mm)[3,5]

In general, the fluid motion in the microchannel is modeled by the

Journal of Biomedical and Bioengineering ISSN: 0976-8084 & E-ISSN: 0976-8092, Volume 3, Issue 1, 2012 Navier Stokes equation and continuity equation; assuming the fluid is incompressible.

$$\nabla . u = 0 \tag{1}$$

$$\rho \left[\frac{\partial u}{\partial t} + (u \cdot \nabla) u \right] = -\nabla p + \mu \nabla^2 u + \rho_e E$$
⁽²⁾

Where p_e is the charge density (C/m³), ρ denotes the fluid's density (kg/m³), E is the electric field intensity (V) and μ is the dynamic viscosity (m²/s) and u is the velocity (mm/s), p is the pressure (Pa). The slip velocity at the edge of the electric double layer is given by Similarly, ionic concentration of bulk solution in the microchannel is given by:

$$u = \frac{\varepsilon_0 \varepsilon_r \varsigma_0}{\eta} \nabla V \tag{3}$$

$$\frac{\partial c}{\partial t} + \nabla (-D_i \nabla c_i - z_i u_{mi} F c_i \nabla V) = 0$$
(4)

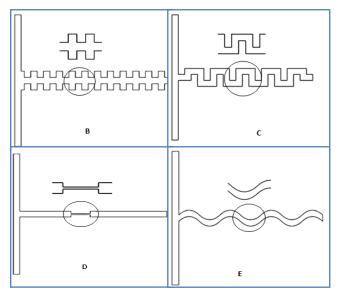


Fig. 2- Modified microfluidic chip models B, C, D and E

Where, η denotes the dynamic viscosity (Pa·s), u is the velocity (mm/s), ε_0 denotes the permittivity of free space (F/m), ε_r is the relative permittivity of water (dimensionless), ζ_0 refers to the zeta potential at the channel wall (V), and V denotes the electric potential (V), c_i is the concentration of i species (mol/m³), D_i represents the diffusivity of the species (m²/s), z_i equals the charge number of i species (which equals 1 for this model), u_{mi} is the mobility of i species (s·mol/kg), and F is Universal Faraday's constant (C/mol).

Results and Discussion

The T-shaped microfluidic chip model of 0.25 mm width with saline solution supplied through an inlet was modeled.

Modeling and simulation was performed using COMSOL. Physics setup including fluid flow and ionic mass transport was applied [3]. The model was then modified with varying shapes as shown in [Fig -2]. Initially, the two inlets were applied electric potentials of 119 V and 79V across the outlet port in order to measure the maximum electroosmotically driven fluid velocity in the channel. Similarly for mass transport same model was created based on published work

and simulation was done in order to determine the concentration distribution in the outlet section of the chip [6].

Different potential differences were applied between the two inlet ports that were supplied with analyte solution and the buffer. Similarly, various potential differences were applied at the outlet. Thus designed computer simulation produced the results for the effect of voltage difference on the velocity of analyte solution. Effect of this change in voltage difference on the concentration distribution of the ionic analyte solution is also presented below.

The velocity at the outlet section of microchannel decreases with decreasing potential differences. Initially the voltage difference between inlet and outlet was chosen as 119 V as this particular potential difference produced an optimal values of fluid driving motion. Lower velocities were obtained applying the lower voltage differences keeping other parameters constant. Since other parameters are constant, only parameter that effects the formulation of high velocity was potential difference between inlet and the outlet. The maximum velocity was seen in the highlighted part of the model D whereas the velocity obtained for model E was least [Fig-3] [Fig-4].

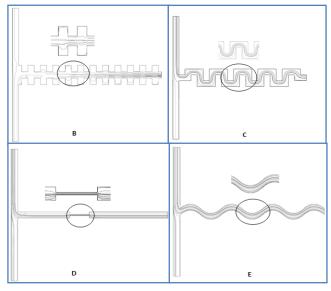


Fig. 3- Modified geometries of microfluidic chip models showing velocity streamlines field (models B, C, D and E)*

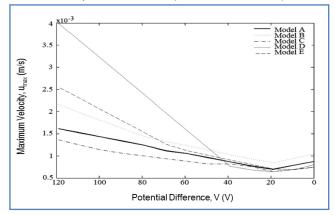


Fig. 4- Modified geometries of microfluidic chip models showing maximum velocities at any point in the outlet section Vs. potential differences across sample inlet and the outlet (models B, C, D and E compared with model A)

Journal of Biomedical and Bioengineering ISSN: 0976-8084 & E-ISSN: 0976-8092, Volume 3, Issue 1, 2012 For each model, the velocities were found to be decreasing till the voltage difference was applied 20V, and then started to slightly rise as it lowered to 20V. [Fig-4] illustrates the velocity profiles of fluid in different models plotted against applied potential differences. Similarly, effect of potential difference in concentration distribution and transient analysis in concentration distribution in microfluidic chip can also be analyzed. This will be discussed in our future publications. Recent work on microfluidics on mixing and electrokinetic flow has shown a promising development in the near future [7,8] including some subsequent publications [9-13].

Conclusions and Recommendations

The geometrical modifications in the analysis chamber of the Tshaped micro channel and its effect on the fluid velocity has been reported. Electrical and transient parametric analysis to maximize the species concentration will be further explored and reported in our future publications. Ionic fluid velocity showed promising results in order to design an effective microfluidic chip that may be used for mixing, pumping and detection purposes in bio-analytical applications.

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