Motion of Uncharged Particles in Electroosmotic Flow through a Wavy Cylindrical Channel

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Abstract: A finite element model is employed to describe the electric potential distribution and electroosmotic flow field inside a wavy cylindrical channel. The model uses coupled Laplace and Poisson-Boltzmann to evaluate the electric potential distribution inside the channel. It also contains continuity and Navier–Stokes equations for the solution of fluid flow. A particle trajectory model was presented to analyze the motion of the particles traveling through the wavy channel. As the ratio of the particle to channel radii changes at different axial position of the wavy channel, wall correction factors for a straight cylindrical channel are used for different particle to channel radii ratio. The effect of waviness on the wall correction factors is neglected. Particles are released at different initial points of the entry plane. The positions of the particles are recorded at the downstream of the channel after travelling few wavelengths distance.

Keywords: Electroosmotic flow, wavy channel particle trajectory, hindered transport.

1. Introduction

The hindered motion of particles suspended in a fluid flowing through a microscopic or nanoscale cylindrical channel has been a topic of central interest in numerous microfluidic and nanofluidic applications e.g. drug delivery, biomedical applications, and micro-pumping mechanism [1-4]. With the advent of microfluidics-MEMS in the last decade, the study of the motion of small particles in narrow channels was revisited and applied to many chemical and biological applications. In such applications, electroosmosis becomes a very effective means of transporting micro liter amount of fluid through narrow capillaries from one reservoir to another. Colloidal particles present in such flow will travel along with the fluid. However, the motion of the particles will be hindered because of the proximity of the channel wall. The motion of the particle can be tracked correctly by using appropriate wall correction factors or lag factors. The particle moving in the center line of a circular cylindrical channel is well studied both analytically [5-7] and numerically [8-10]. However, there exist a group of problems that are yet to be analyzed comprehensively, such as particle moving off the center line of the channel, particle moving in a wavy cylindrical channel, or particle motion in an electroosmotic flow.

In the present paper, an electroosmotic flow model is described. A finite element model (LPB-NS: Laplace-Poisson-Boltzmann Navier-Stokes) has been developed. The model consists of Laplace and Poisson-Boltzmann equations dictating external electric potential, and total electric potential, respectively. These two equations are coupled in manner that Laplace equation governs the external electric potential across the channel where electric charge neutrality holds. On the other hand, the Poisson-Boltzmann equation dictates the potential distribution near the channel wall and allows the solution of Laplace equation to hold elsewhere. This coupled model is superior to the models that use superposition of external electric potential across the channel (obtained from Laplace equation) and electric potential near the channel wall (obtained from Poisson-Boltzmann equation). Navier-Stokes with electrical body force term was then solved to obtain fluid velocity fields in the channel.

A particle trajectory code was written to track individual uncharged particle that is present and travelling along with the fluid. As the motion of the particle is hindered due to the wavy channel wall, appropriate wall correction factors are necessary to estimate particle displacements at each time step. The velocity fields of undisturbed electroosmotic flow of the central part of the channel was exported from the LPB-NS model and used to estimate the particle velocity at different positions as the particle moves in the channel. Few particles are released at the different radial positions, their motions are tracked, and final positions are recorded.

2. Formulation of the Problem

2.1 Governing Equations

An electroosmotic flow in a cylindrical channel can be characterized by channel radii b, channel wall potential ψ_p, and external electric field E_∞. Due to the presence of surface potential of channel wall, an electric double layer (EDL) is formed near the wall. Under the external electric field E_∞ an electroosmotic flow is developed in the channel. To evaluate the electric potential across the channel caused by the external electrical field Laplace equation is used,

$$\nabla^2\phi = 0 \quad (1)$$

where ϕ is the external electrical potential. Poisson-Boltzmann equation is employed to govern the electric potential near the channel wall and in the bulk,

$$\nabla^2\psi = \rho_f = \frac{2n_\infty ze}{\varepsilon} sinh\left[\frac{ze}{kT}(\psi - \phi)\right] \quad (2)$$

where ψ is the electrical potential, ρ_f is the free charge density, n_∞ is the bulk concentration of the ions, z is the ionic valence, e is the elementary charge, ε is the dielectric constant of the medium, k is the Boltzmann constant, and T is the temperature. Surface charge density is defined differently here than that of the most electroosmotic analysis. Instead of assuming bulk potential to be zero, it is considered to be the external electric potential obtained from solution of the Laplace equation. Typically, equilibrium electroosmotic flow model solves Laplace equation for external fields and Poisson-Boltzmann equation for potential near the channel wall and uses a linear superposition to obtain total electric potential of the reservoir-channel system. However, the present coupled model (LPB-NS) model is superior to such liner superposition model, as LPB-NS can operate in the cases of higher external electric fields or higher channel surface potential where linear superposition is no longer valid.

The Navier-Stokes equation with an electric body force term and continuity equation that govern the fluid flow are given as,

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho\boldsymbol{u}\cdot\nabla\boldsymbol{u} = -\nabla p + \mu\nabla^2\boldsymbol{u} - \rho_f\nabla\psi \quad (3)$$

$$\nabla.\boldsymbol{u} = 0 \quad (4)$$

where ρ is the fluid density, $\boldsymbol{u} = (u, v)$ is the fluid velocity vector with u and v being the radial and axial components, respectively, μ is the viscosity of the fluid, and p is the pressure. The solution of the above eqns.(1-4) provides the electroosmotic flow of the computational domain.

2.2 Geometric Description and Boundary Conditions

An axisymmetric model of a cylindrical wavy channel-reservoir system having a mean channel radius b and channel length L is considered in the present analysis. The channel-reservoir configuration is shown in Fig.1. Two large reservoirs, one each at the each channel end, are introduced to minimize the end effects. Sufficiently large sized reservoirs were chosen to reduce any reservoir size affect. Typical dimensions of the capillary considered for present analysis are of length $L/_b = 20$. It is observed that a reservoir of radius $R_r = 5b$ and length $L_r = 5b$ are sufficient to offset any reservoir size effect. The amplitude α and wavelength λ of the wavy channel are generated by using second order Bezier curve [4]. The amplitude of the asperity i.e. a single crest or trough point, can be calculated by

$$\alpha = \frac{w_1P_1}{1 + w_1} \quad (5)$$

In the current analysis, $w_1 = 0.5$ is used while P_1 is controlled to obtain the desired amplitude. Say for instance, to make an undulation amplitude $\alpha = 0.2$ we can easily calculate the control point $P_1 = 0.6$.

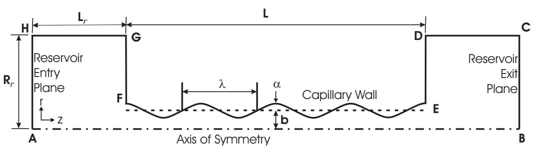

Figure 1: Axisymmetric model of the wavy cylindrical channel. Fluid is driven from one reservoir to another due to electroosmotic flow.

Symmetry boundary conditions are assigned at the axis of symmetry (AB) for potentials and velocity. A constant surface potential boundary condition is assumed for the channel wall (EF). No-slip condition for fluid velocity on the channel wall is assigned.

Capillary wall:

$$\boldsymbol{u} = 0; \quad \psi = \psi_w; \quad \frac{\partial\phi}{\partial n} = 0 \quad (6)$$

At the reservoir entry plane (AH), pressure is assumed to be zero. To apply the external electric field across the channel, a potential difference between the entry (AH) and exit (BC) plane is assumed. Potentials ϕ_{in} and ϕ_{out} are assigned at entry and exit plane, respectively.

Capillary Entry:

$$p = 0; \quad \frac{\partial \psi}{\partial n} = 0; \quad \phi = \phi_{in} \qquad (7)$$

On the reservoir exit plane (BC), a hydrodynamic stress is assumed to be zero and other conditions are,

Capillary exit:

$$\boldsymbol{\sigma_h} = 0; \quad \frac{\partial \psi}{\partial n} = 0; \quad \phi = \phi_{out} \qquad (8)$$

For reservoir walls (FG and DE) adjacent to the channel, zero charge (potential gradient zero) and no slip boundary conditions were chosen. For other walls (CD and GH), zero charge density and slip-symmetry conditions were assigned.

2.3 Non-dimensional Equation

All governing equations are non-dimensionalized. The characteristic length is chosen to be the channel radius b. All symbols with a superscript * represent a non-dimensional parameter. Non-dimensional parameters are chosen as

$$u^* = \left(\mu b/\varepsilon\right)\left(ze/kT\right)^2 u, \Psi = \left(ze/kT\right)\psi,$$

$$p^* = \left(b^2/\varepsilon\right)\left(ze/kT\right)^2 p,$$

For steady state condition, non-dimensional form of the Navier-Stokes equation becomes,

$$Re^* u^* \nabla^* \boldsymbol{u}^* = -\nabla^* p^* + \nabla^{*2} \boldsymbol{u}^*$$
$$(\kappa b)^2 \sinh(\Psi - \Phi) \nabla^* \Psi \qquad (9)$$

$$\nabla^* . \boldsymbol{u}^* = 0 \qquad (10)$$

where $Re^* = \left(\rho\varepsilon/\mu^2\right)\left(kT/ze\right)^2$ is Reynolds number and $\kappa^{-1} = \left(\varepsilon kT/2e^2 z^2 n_\infty\right)^{1/2}$ is the Debye screening length.

Non-dimensional forms of the Poisson-Boltzmann and Laplace equations are obtained as,

$$\nabla^{*2} \Psi = (\kappa b)^2 \sinh(\Psi) \qquad (11)$$

$$\nabla^{*2} \Psi = 0 \qquad (12)$$

2.4 Particle Trajectory Model

The colloidal particles present in the fluid will move along in the direction of the electroosmotic flow. However, the velocity of the particles will not assume the fluid velocity due to the proximity of the channel wall. Hydrodynamic wall correction factors or lag coefficient are necessary to correlate the particle velocity with the fluid velocity.

A particle trajectory model is employed in this study to track a particle moving in the wavy cylindrical channel due to electroosmotic flow. Neglecting rigid body rotation, the particle trajectory equation originates from Newton's second law of motion for a particle suspended in a liquid,

$$\boldsymbol{R} = \boldsymbol{r}(t + \Delta t) - \boldsymbol{r}(t) = \left[\frac{\boldsymbol{F}_{drag}}{6\pi\mu a}\right](\Delta t) \qquad (13)$$

where $\boldsymbol{r}$ is the position vector of the particle's center, t is the time, a is the particle radius, and $\boldsymbol{F}_{drag}$ is the fluid drag. The fluid drag is given as,

$$F_{drag} = 6\pi\mu a u_p = (6\pi\mu a)\boldsymbol{K}.\boldsymbol{u} \qquad (14)$$

where u_p and $\boldsymbol{u}(u, v)$ are particle velocity due to fluid flow and the undisturbed (by the presence of the particle) electroosmotic fluid velocity respectively. The drag coefficient $\boldsymbol{K}$ represents hydrodynamic interactions between the particle and the neighboring channel wall. For the axial motion of the particle moving in the cylindrical channel, drag coefficient is taken from are taken from Cox and Mason [11]. However, to the best of author's knowledge, wall correction factor for the particle moving in the radial direction inside a cylindrical channel does not exist to date. To simplify the problem, we assume that the particle does travel in the close vicinity of the channel wall, and hence, wall correction factor for a particle approaching perpendicular to a flat plate can be applied in the current scenario [12].

3. Solution Methodology

Non-dimensionalized governing equations (9-12) are solved by the finite element package COMSOL Multiphysics 3.4 to obtain the solution. Triangular quadratic Lagrange elements were employed to discretize the computational domain. Fine meshes were used on the channel wall to capture the sharp change of potential in EDL. Relatively coarse meshes were used in reservoir region. Mesh sensitivity analysis was carried out and approximately 20,000-25,000 elements were decided upon to obtain the result.

The three sets of equations, Laplace equation for external electric field, Poisson equation for electric field, and Navier-Stokes equation for fluid were solved sequentially. The flow field of the domain is exported and later used to track the motion of the particle. A MATLAB code was written to track the particle trajectory based on eqn.(13).

4. Results and Discussions

A cylindrical channel of uniform circular cross-section of radius b was considered to validate the model. Analytical solution for an external electric field E_∞, and channel wall potential ψ_w is given by

$$v(r) = \frac{b^2 p_z}{4\mu}\left[1 - \left(\frac{r}{b}\right)^2\right] - \frac{\epsilon \psi_p}{\mu}\left[1 - \frac{I_0(\kappa r)}{I_0(\kappa b)}\right] E_z \qquad (15)$$

where v is the fluid velocity in z-direction, and I_0 is the zeroth-order modified Bessel function of the first kind.

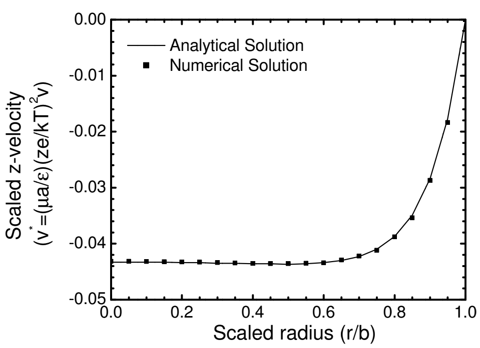

Figure 2: Comparison of electroosmotic flow velocities (v) in the z-direction. Numerical solution is obtained by solving the LPB-NS model and compared against analytical solution. Solution is given for a scaled channel surface potential $\Psi_p = -1.0$, applied external electric potential difference $\Psi_{in} - \Psi_{out} = 1.0$, and $\kappa b = 10$.

The numerical solution was obtained for a scaled channel radius $b = 1$, and length $L = 20$. A scaled channel wall potential $\Psi_p = -1.0$ was considered and a scaled external potential difference $\Psi_{in} - \Psi_{out} = 1.0$ was applied across the channel. The solution was obtained for $\kappa b = 10$. To compare with the analytical solution, the values p_z and E_z were obtained from the numerical solution and put in eqn.(15) to generate the corresponding analytical velocity profile. The obtained numerical solution was compared against the analytical solution and shown in Fig. 2, which shows an excellent agreement with a percentage of error around 1%.

LPB-NS model is applied to a wavy cylindrical channel of mean radius $b = 1$, and channel length $L = 40b$. Waviness was generated with a wave length $\lambda = 4b$ for each undulation on the channel surface. The amplitude is set for $\alpha = 0.2b$ which suggests that channel radii varies from 0.8 (at trough position) to 1.2 (at crest position). Like straight cylindrical channel two reservoirs were added at each end. Same reservoirs size and mesh elements were employed to obtain the solution. Same parametric values are considered as in straight channel: scaled channel wall potential $\Psi_p = -1.0$, a scaled external potential difference $\Psi_{in} - \Psi_{out} = 1.0$, and $\kappa b = 10$.

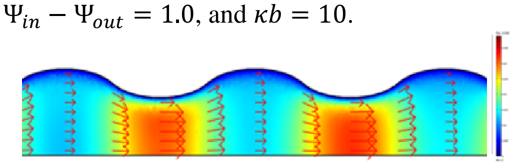

Figure 3: Electroosmotic flow in a wavy cylindrical channel obtained by solving the LPB-NS model. A wavy channel parameters considered are: mean channel radius $b = 1$, channel length $L = 40b$, wave length of each undulation on the channel surface $\lambda = 4b$ and amplitude of $\alpha = 0.2b$. The Solution is obtained for a scaled channel surface potential $\Psi_p = -1.0$, applied external electric potential difference $\Psi_{in} - \Psi_{out} = 1.0$, and $\kappa b = 10$. Velocity vector shows that near the channel wall fluid velocity has a non-zero radial component unlike that of a straight channel.

The middle section of the wavy channel (approximately $0.4L - 0.6L$) was chosen as the test ground for the particle trajectory analysis, as shown in the Fig. 3. The figure shows velocity vector has a non-zero component in the radial direction suggesting particle will move not only in the axial direction but also in the radial direction. The velocities of this region were exported and a MATLAB code was written to use the velocities to estimate particle velocity using wall correction factors reported in [11-12]. Few particles were released from at a certain crest position and at different radial distances ($r = 0.1, 0.3, 0.5, 0.7, 0.8$). The particle motion was tracked and final destination (radial distance) was recorded after travelling a z-distance of $dz = 8$ (two wave length distances).

Table 1: Initial and final radial position of the five released particles

Particle no	Initial radial position	Final radial position
1	0.1	0.0858
2	0.3	0.2618
3	0.5	0.4467
4	0.7	0.6315
5	0.8	0.6358

Trajectory results show that the released particles tend to move toward the center of the cylindrical channel. It should be noted that the particles are released individually and hence no diffusion effect is considered. The particle's tendency to move to center of the channel is only due to the radial component of the velocity vector.

5. Conclusion

In this paper a finite element model consisting of Laplace, Poisson-Boltzmann, and Navier-Stokes equations is presented. The model is used to obtain the electroosmotic flow field in a wavy cylindrical channel. A particle trajectory model was employed to use the velocity distributions and track the motion of the particles with the help of appropriate wall correction factors. The particles are not considered to be released very close to the channel wall as the appropriate wall correction factor for radial direction is not known. Such analysis will be very important to estimate the deposition of the particles on the wavy channel walls.

6. References

1. T. M. Squires, and S. R. Quake, Microfluidics: Fluid physics at the nanoliter scale, *Reviews of Modern Physics*, **77(3)**, 977-1026 (2005).
2. D. J. Beebe, *et al.*, Physics and applications of microfluidics in biology, *Annual Review of Biomedical Engineering*, **4**, 261-286 (2002).
3. D. J. Laser, and J. G. Santiago, A review of micropumps, *Journal of Micromechanics and Microengineering*, 14(6), R35-R64 (2004).
4. N. Quddus, *et al*, An electrostatic-peristaltic colloidal micropump: A finite elemental analysis. *Journal Computational and Theoretical Nanoscience*, **1(4)**, 438-444 (2005).
5. P. Dechadilok, and W. M. Deen, Hindrance factors for diffusion and convection in pores, *Industrial & Engineering Chemistry Research* **45(21)**, 6953-6959 (2006).
6. W. M. Deen, Hindered transport of large molecules in liquid-filled pores. *AICHE Journal* **33(9)**, 1409-1425 (1987).
7. J. Happel, and H. Brenner, *Low Reynolds Number Hydrodynamics*. Noordhoff International Publishing, Leyden, The Netherlands (1973).
8. N. A. Quddus *et al*, Motion of a spherical particle in a cylindrical channel using arbitrary Lagrangian Eulerian method. *Journal of Colloid and Interface Science*, **317(2)**, 620-630 (2008).
9. J. J. L. Higdon, and G. P. Muldowney, Resistance functions for spherical particles, droplets and bubbles in cylindrical-tubes. *Journal of Fluid Mechanics,* **298**, 193-210 (1995).
10. A. Ben Richou, *et al*, Correction factor of the stokes force undergone by a sphere in the axis of a cylinder in uniform and poiseuille flows. *European Physical Journal-Applied Physics,* **24(2)**, 153-165 (2003).
11. R.G. Cox, and S. G. Mason, Suspended particles in fluid flow through tubes, *Annual Review of Fluid Mechanics*, **3**, 291- (1971).
12. R.G. Cox, and H. Brenner. Slow motion of a sphere through a viscous fluid towards a plane surface: small gap widths including inertial effects, *Chemical Engineering Science*, **22(12)**, 1753- (1967).
13. A. Mansouri, *et al*, Transient streaming potential in a finite length microchannel. *Journal of Colloid and Interface Science,* **292(2)**, 567-580 (2005).
14. J. H. Masliyah, and S. Bhattacharjee, *Electrokinetic and Colloid Transport Phenomena*. John Wiley and Sons, New York (2006).
15. N. Quddus, *et al*,. The effects of surface waviness and length on electrokinetic transport in wavy capillary. *Canadian Journal of Chemical Engineering,* **84(1)**, 10-16 (2006).