AC Electroosmotic Flow in Electrolytes Generated by Two Coplanar Microelectrodes

K. Adamiak

Dept. of Electrical and Computer Engineering
Univ. of Western Ontario, London, Ontario, Canada N6A 5B9, kadamiak@eng.uwo.ca

ABSTRACT

A numerical model for the AC electroosmotic flow in aqueous solutions is presented. It is assumed that the electrodes are ideally polarizable, the fluid is well-conducting, and the Debye double layer is much smaller than dimensions of the electrodes. The electric potential is calculated by solving the Laplace equation with the boundary conditions resulting from approximate analysis of the ionic concentration in the double layer. The net electric charge in this area interacts with the electric field, leading to generation of a force causing the fluid motion. The effect of voltage frequency on the electric field distribution and flow characteristics is presented.

Keywords: AC electroosmosis, microfluidics, electric field, fluid flow

1 INTRODUCTION

In many microfluidic applications there is a need for pumping of small volumes of fluid. Several techniques have been proposed, most importantly electromechanical, electrothermal and electroosmotic. The fluid motion in microsystems can also be produced using the so-called AC electroosmotic effect [1,2]. The pumping effect requires an asymmetric geometry: usually periodic array electrodes with different widths, although other configurations are also possible [3].

Ramos et al. [4] used a circuit model to analyze electric potential distribution and charge density generated in the layer of conductive fluid by two microelectrodes. The flux tubes were used and the double layer was represented by a distributed capacitor. A similar circuit model was also used to analyze an AC electroosmotic pump [1,2]. In [5] this model was criticized as over-simplified. A much more complete theoretical model of electrode polarization was presented in [6]. However, this model is too complicated for the flow simulation. The numerical model of Gonzales et al. [7] implemented a linear one-dimensional analysis of the double layer and the obtained results compared well with the experimental data. However, the boundary conditions derived in that paper are practically identical with the capacitor approximation [4].

This paper attempts to provide a missing link between a fundamental approach presented in [6] and the practical capacitor model of Ramos et al. [4]. It is shown that for applications with dimensions much larger than the Debye thickness, both methods lead to practically identical results.

2 MATHEMATICAL MODEL

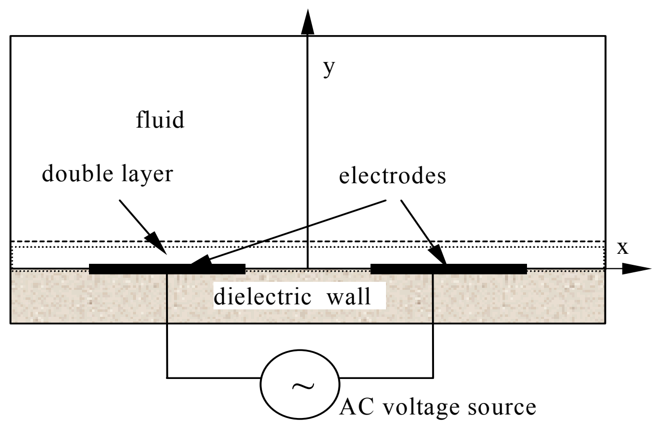

Figure 1: Schematic configuration of the problem

AC electroosmotic pumping of fluids is studied in the model consisting of two thin coplanar electrodes, deposited on a dielectric substrate and placed in an aqueous solution (Fig. 1) [7, 8]. An AC voltage is supplied to the electrodes and a cloud of space charge forms in a very thin layer close to the conducting surfaces. It is assumed that the electrodes are ideally polarizable (there is no charge injection from the electrodes) and the fluid is well-conducting with an unlimited number of positive and negative ions; however, only one negative and one positive ionic species are considered to have identical properties, except for their polarity. When an AC voltage is applied the ions form a so-called dynamic double layer, with ions traveling towards and away from the electrodes. In the bulk of fluid densities of positive and negative ions are practically identical, so the fluid is neutral. Only in the thin Debye layer is there an excess of one-polarity ions [6]. The problem is formulated separately for both areas. As the length of the system is much longer than its width, it is invariant in the z-direction and a 2D model in x-y plane will be considered.

2.1 Scalar electric potential

An approximate model for this problem is based on the Debye-Hückel theory of the double layer and involves the electric potential and the electrochemical potentials for both charged species. Because thickness of this layer is very small (typically 10-50 nm) only one component, normal to the electrode surface, can be assumed, so 1D model is sufficient [6]. Applied voltage is small and the model is linear with respect of the electric potential Ψ.

The balance of electrical, drag, and thermodynamic forces yields the following equation for the densities of the positive, n_+, and negative, n_-, ionic species [6,9]

$$k_B T \frac{d \ln n_+}{dx} + e\frac{d\Psi}{dx} + v_+ \lambda_+ = 0 \quad (1)$$

$$k_B T \frac{d \ln n_-}{dx} - e\frac{d\Psi}{dx} + v_- \lambda_- = 0 \quad (2)$$

where k_B is the Boltzmann's constant, T – the absolute temperature, e – the electronic charge, v_+ *and* v_- – the ions velocity and λ_+ and λ_- – the drag coefficients, for positive and negative ions, respectively.

Defining the average ion velocity as a gradient of the velocity potential the ionic densities can be calculated [6]:

$$n_+ = n_0^+ \exp(-e\frac{\Psi - \Phi_+}{k_B T}) \quad (3)$$

$$n_- = n_0^- \exp(e\frac{\Psi - \Phi_-}{k_B T}) \quad (4)$$

where Φ_+ and Φ_- are the velocity potentials for positive and negative ions, respectively.

The scalar electric potential is governed by the Poisson equation $-\varepsilon\nabla^2\Psi = \rho$, where ρ is the net space charge density, $\rho = e(n_+ - n_-)$. In a symmetrical electrolyte the mobilities of the positive and negative ions are approximately equal, so it can be assumed that

$n_0^+ = n_0^- = n_0$, $\lambda_+ = \lambda_- = \lambda_0$ and $\Phi_+ = \Phi_- = \Phi$

and that the densities of both species can be expressed using the linearized formulae

$$n_+ = n_0(1 - e\frac{\Psi - \Phi_+}{k_B T}) \quad (5)$$

$$n_- = n_0(1 + e\frac{\Psi - \Phi_+}{k_B T}) \quad (6)$$

All these idealizations lead to the following Poisson equation for the electric potential Ψ

$$\frac{d^2\Psi}{dx^2} - \frac{2e^2 n_0}{\varepsilon k_B T}(\Psi - \Phi) = 0 \quad (7)$$

The mass conservation equation for the ionic species also has to be satisfied, what after the model linearization [7], neglecting the convection current and conversion to the complex phasor notation, leads to a second equation for the flow potential [6]

$$\frac{d^2\Phi}{dx^2} + \frac{i\omega\lambda_0}{k_B T}(\Psi - \Phi) = 0 \quad (8)$$

where $i = \sqrt{-1}$ and ω – the radian frequency of the supply voltage.

Eqs. (7) and (8) form a set of two differential equations of the second order for the scalar electric and flow potentials. In order to simplify the solution, they can be written in a non-dimensional form. Normalizing Ψ with respect to k_BT/e, distance x with the Debye length $\lambda_D = \sqrt{(\varepsilon k_B T)/(2n_0 e^2)}$ and frequency with $\omega_s = k_B T/(2\lambda_0\lambda_D)$, Eqs. (7) and (8) are expressed as:

$$\frac{d^2\psi^*}{dx^{*2}} - \psi^* + \varphi^* = 0 \quad (9)$$

$$\frac{d^2\varphi^*}{dx^{*2}} + i\omega^*(\psi^* - \varphi^*) = 0 \quad (10)$$

One function can be easily eliminated and in this case the equation of the fourth order is obtained

$$\frac{d^4\psi^*}{dx^{*4}} - (1 + i\omega^*)\frac{d^2\psi^*}{dx^{*2}} = 0 \quad (11)$$

General solutions for ϕ^* and ψ^* derived from this equation have the form

$$\psi^*(x^*) = C_3\exp(-ax^*) - (C_2 + C_1 x^*)/a^2 \quad (12)$$

$$\varphi^*(x) = C_3(1-a^2)\exp(-ax^*) - (C_2 + C_1 x^*)/a^2 \quad (13)$$

where a^2=1+iω, C_1, C_2 and C_3 are constants to be calculated from the boundary conditions: at x^*=0 $\psi(0)=V_0/2$ and the normal component of the current density vanishes since the electrode is ideally polarizable [7]. At $x=\lambda_d$ (x^*=1.0) the scalar potential and its normal derivative in the double layer should be equal to the corresponding values in the bulk of the liquid, which is electrically neutral [7]. After performing all the necessary calculations and changing the space normalization from the Debye length to the electrode length L, and electric potential normalization from k_BT/e to V_0, the following boundary condition for the electric potential in the bulk of electrolyte, which is governed by the Laplace equation, can be derived:

$$\frac{\partial\tilde{\Phi}}{\partial n} + \alpha\tilde{\Phi} = \alpha \quad (12)$$

where $\alpha = \dfrac{-2i\omega}{\sqrt{1 + 2i\omega\lambda_D/L}(1 + \sqrt{1 + 2i\omega\lambda_D/L})}$

In most practical cases $\lambda_D \ll L$ and the coefficient α simplifies to the value first suggested in [7], $\alpha = -i\omega$.

2.2 Flow velocity

The fluid flow velocity distribution has been calculated by solving the Navier-Stokes equation. As the expected flow velocity is usually very small, the Reynolds number for these cases is in the order of 10^{-3}. There is also no body force, because the fluid is electrically neutral. Under such conditions the Naver-Stokes equation can be written as:

$$\eta\nabla^2\boldsymbol{v} = \nabla p \quad (13)$$

where η is the dynamic fluid velocity. The mass conservation equation should also be satisfied

$$\nabla \cdot \boldsymbol{v} = 0 \qquad (14)$$

Only in the diffuse layer there is an interaction of the electric charge and the electric field, produced by electrodes, what results in the Coulomb force. The flow is produced with an electro-osmotic slip velocity as provided by the Helmholtz-Smoluchowski formula [4]

$$v_s = \frac{\lambda_D}{2\eta} \mathrm{Re}(\rho_s \frac{\partial \psi^*}{\partial y}) \qquad (15)$$

where ψ* is a conjugate of ψ and

$$\rho_s = \frac{2e^2 n_0 \lambda_D^2}{kT(1-a)} \frac{\partial \psi}{\partial x} \qquad (16)$$

In the non-dimensional form this leads to

$$\tilde{v}_s = \mathrm{Re}\{\frac{1}{1-a} \frac{\partial \tilde{\psi}}{\partial \tilde{x}} \frac{\partial \tilde{\psi}^*}{\partial \tilde{y}}\} \qquad (17)$$

where $\tilde{v}_s = v_s / v_0$ and $v_0 = e^2 n_0 \lambda_D^3 V_0 / (4\eta k_B T L^2)$.

2.3 Numerical algorithm

The equations for the electric potential and fluid flow were solved using the FEMLAB 3.2 commercial software. Due to symmetry only half of the domain shown in Fig.1 was discretized into about 20000 triangular elements with quadratic interpolation of the solution. For the electric potential distribution the Laplace equation has to be solved with the boundary conditions of the third kind given by Eq. (12). As these conditions involve complex numbers, the potential will also be complex, meaning that potentials at different points don't have to be in the same phase. Calculated normal and tangential derivatives of the potential on the surface of the electrode were substituted to the Navier-Stokes solver for the calculation of the flow velocity. Both components of the velocity vector and pressure distribution were calculated at a different point of the channel and at different frequencies of the supplied voltage.

3 RESULTS

3.1 Electric Potential

Distributions of the real and imaginary parts of the electric potential are shown in Fig. 3. The real value of potential ψ is mainly affected by the voltage supplied to the electrodes with some corrections, which are most significant near the electrode edges. In the middle of the electrode real(ψ) is very close to the electrode potential, as grad(ψ) is relatively small. Closer to the electrode edges the gradient of ψ increases, as does the difference between V_o and ψ. This pattern is, of course, affected by the frequency. For higher values of ω the voltage drop on the capacitive double layer can be very small, parameter α in Eq.(12)

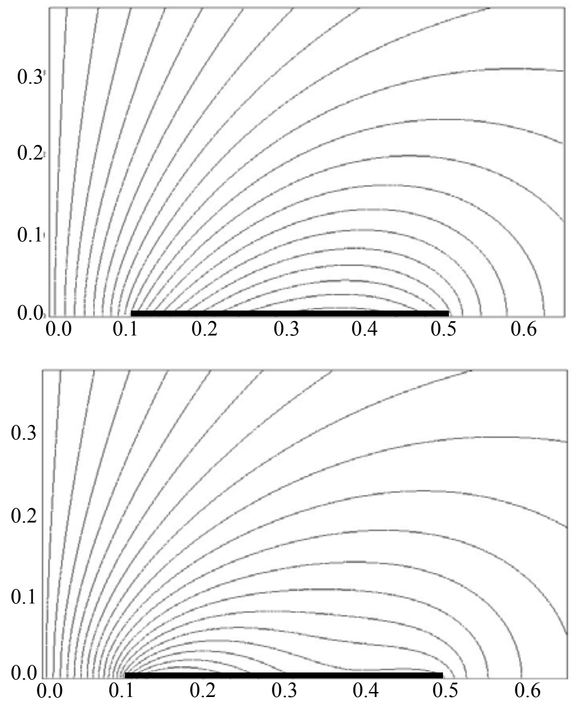

Figure 2: Distribution of the real and imaginary values of the electric potential (ω^*=10).

increases and the entire potential drop occurs practically across the electrolyte volume. At lower frequencies, the voltage drop can be substantial and can cause a substantial difference between ψ and V_o.

The imaginary part of the potential ψ is generated by the normal derivative of real(ψ). Therefore imag*(ψ)* has the maximum values near the electrode edges and it increases for smaller coefficient α, i.e. for smaller frequencies.

3.2 Fluid flow velocity

An interaction between the electric field created by electrodes and the electric charge produces an electrical (Coulomb) force. It exists only in the area where the charges exist, meaning in a very thin double layer. The thickness of this layer has been neglected, because it is much smaller than channel dimensions, so the force acts only on the fluid surface. Only a horizontal component of the force causes fluid motion and it is proportional to the tangential electric field, which reaches the largest values at points close to the electrode edges. Therefore, the fluid is strongly attracted to the inner electrode edge and it moves from the inter-electrode gap, creating the velocity pattern shown in Fig. 3. The force acting on the outer edge is much weaker, so even if the second vortex exists, it is practically invisible.

Because of the surface nature of the electric force, the flow velocity dramatically changes in the direction perpendicular to the electrodes (Fig. 4). The maximum

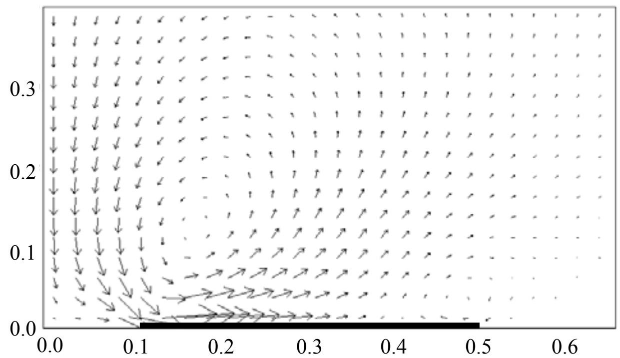

Figure 3: Velocity distribution near the electrode for the relative frequency ω^{*}=5.

velocity occurs at the fluid surface at a point near the inner electrode edge. Moving away from the electrodes the velocity decreases and eventually changes direction, which is necessary to satisfy the flow continuity.

The frequency of AC voltage significantly affects the flow pattern [3] (Fig.5). At frequencies smaller than the charge relaxation frequency in the fluid, the surface velocity is small and distributed rather uniformly along the electrode surface. As the frequency increases, the velocity increases as well, and becomes less uniform. For high ω, the velocity forms a very sharp peak near the electrode edge with much smaller values at all other points. The maximum value of this velocity eventually decreases, if ω is sufficiently large.

4 CONCLUSIONS

A new numerical model for the AC electroosmotic has been presented. Starting with equations for the concentration of ions in the electrolyte, the model has been simplified by assuming just two ionic species (positive and negative) with identical mobilities. Linearization of this model allowed us to formulate the boundary conditions for the electric potential in the electrolyte. For channels with dimensions much larger than thickness of the Debye layer,

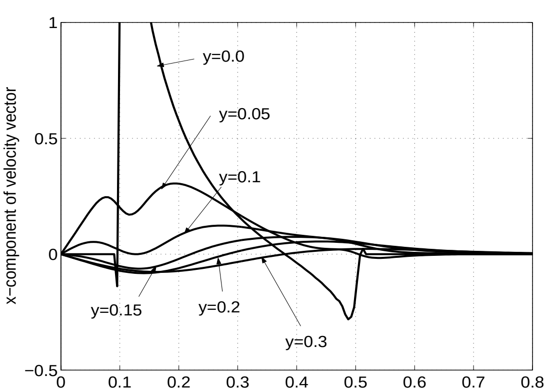

Figure 4: Horizontal fluid velocity at different altitudes above the electrode for the relative frequency ω^{*}=10.

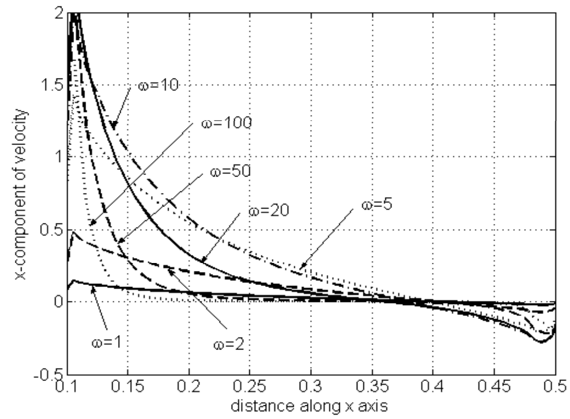

Figure 5: Fluid velocity on the fluid-dielectric interface (y=0.0) for different frequencies.

these boundary conditions are practically identical with those suggested in [7].

The presented algorithm was used to simulate the flow in a layer of fluid generated by two symmetrical electrodes deposited on a dielectric layer and supplied with an AC voltage. The electric potential and fluid flow velocity were calculated using the Finite Element Method.

The largest fluid velocity was calculated close to the inner edge of the electrode. This velocity decreases in the vertical direction and eventually changes its direction. A much weaker vortex is created near the outer edge. The flow pattern is strongly affected by the voltage frequency. There is an optimum frequency causing the maximum flow velocity.

ACKNOWLEDGMENTS

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC).

REFERENCES

[1] A.B.D. Brown, C.G. Smith and R.R. Rennie, Phys. Rev. E, 63, 016305, 2002.

[2] A. Ramos, A. Gonzales, A. Castellanos, N.G. Green and H. Morgan, Phys. Rev. E, 67, 056302, 2003.

[3] A. Ajdari, Phys. Rev. E, 61, R45-R48, 2000.

[4] A. Ramos, H. Morgan and N.G. Green, J. Colloid Inter. Sci. 217, 420-422, 1999.

[5] M. Scott, K.V.I.S. Karel and R. Paul, J. Colloid Inter. Sci. 238, 449-451, 2001.

[6] M. Scott, R. Paul and K.V.I.S. Kaler, J. Colloid Inter. Sci. 230, 377-387, 2000.

[7] A. Gonzales, A. Ramos, N.G. Green, A. Castellanos and H. Morgan, Phys. Rev. E, 61, 4019-4028, 2000.

[8] N.G. Green, A. Ramos, A. Gonzales, H. Morgan and A. Castellanos, Phys. Rev. E, 66, 026305, 2002.

[9] E.H.B. DeLacey and L.R. White, J. Chem. Soc., Faraday Trans. 2, 78, 457-479, 1982.