Electroosmotic Pumping in Rectangular Microchannels: a Numerical Treatment by the Finite Element Method [*][†]

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Abstract

In this work, the analysis of electroosmotic pumping mechanisms in microchannels is performed through the solution of Poisson-Boltzmann and Navier Stokes equations by the Finite Element Method. This approach is combined with a Newton-Raphson iterative scheme, allowing a full treatment of the non-linear Poisson-Boltzmann source term which is normally approximated by linearizations in other methods.

The computer simulation of fluid flow in microchannels has received an increasing attention recently, due mainly to emerging applications of deep technological significance. We could mention for instance the microchips and laser diode arrays cooling, as well as flow injection mechanisms in biological micro-reactors. Since the use of mechanical fluid propulsion in such devices would impose severe practical limitations (like the difficulty to produce components of microscale pumps), surface electric charge effects may be used to induce fluid flows through microchannel devices free from moving parts [2]. It is a well known fact that ion adsorption, ion dissolution or ionization may transfer electric charges to a surface brought into contact with a polar fluid. Through the so called Electric Double Layer (EDL) effect [1], this induced surface charge affects the ion distribution of the fluid, in such a way that these ions may pull the fluid molecules under the action of an external electric field, applied along the length of the fluid microchannel(the fluid flow direction). In a few words, this is the electroosmotic pumping mechanism. The EDL theory relates the surface electrostatic potential ψ and the charges within the fluid at the surface neighborhood by means of the Poisson equation

$$\frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = -\frac{\rho_e}{\varepsilon \varepsilon_0} \tag{1}$$

where ρ_e is the net charge density, ε_0 is the vacuum permittivity and ε is the dimensionless dielectric constant. It is assumed in this case that the microchannel has rectangular cross-section, the fluid flow is directed along the x-axis and $y - z$ is the cross section plane.

According to the theory, the net charge density ρ_e is given by the Boltzmann distribution (for symmetric electrolytes) as

$$\rho_e = -2n_\infty z e \sinh\left(-\frac{ze}{k_b T}\psi\right) \tag{2}$$

where k_b is the Boltzmann's constant, e is the fundamental charge, n_∞ is the ionic number concentration in the bulk solution, z is the ionic valence and T the absolute temperature.

Therefore, the Poisson equation (1) may now be written as

$$\frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{2n_\infty z e}{\varepsilon\varepsilon_0} \sinh\left(-\frac{ze}{k_b T}\psi\right). \tag{3}$$

If one considers a rectangular cross-section microchannel with length L, height $2H$ and width $2W$, the analysis may be limited to $1/4$ of the section due to symmetry reasons, and dimensionless variables may be introduced as follows:

$$y^* = \frac{y}{D_h}, \quad z^* = \frac{z}{D_h}, \quad \psi^* = \frac{ze}{k_b T}\psi \tag{4}$$

where

$$D_h = \left(\frac{4HW}{H+W}\right) \tag{5}$$

is the hydraulic diameter. Therefore, these dimensionless variables allow a new formulation for (3) as

$$\frac{\partial^2 \psi^*}{\partial y^{*2}} + \frac{\partial^2 \psi^*}{\partial z^{*2}} = (\kappa D_h)^2 \sinh(\psi^*) \tag{6}$$

where κ is the Debye-Huckle parameter, the inverse of the characteristic EDL thickness:

$$\kappa = \left(\frac{2n_\infty z^2 e^2}{\varepsilon\varepsilon_0 k_b T}\right)^{1/2}. \tag{7}$$

The boundary conditions for (6) are

$$y^* = 0, \quad \frac{\partial \psi^*}{\partial y^*} = 0, \tag{8}$$

$$z^* = 0, \quad \frac{\partial \psi^*}{\partial z^*} = 0, \tag{9}$$

$$y^* = \frac{H}{D_h}, \quad \psi^* = \zeta^* = \frac{ze}{k_b T}\zeta, \tag{10}$$

$$z^* = \frac{W}{D_h}, \quad \psi^* = \zeta^* = \frac{ze}{k_b T}\zeta, \tag{11}$$

where ζ is the zeta potential, that is, the electric potential at the shear plane (the Stern plane approximately). Since the solution of (6) is known in the entire domain, (2) gives us the charge density. The pumping effect will be modeled after the knowledge of the fluid velocity distribution. This distribution is given by the Navier-Stokes equation for laminar conditions in a fluid with constant density ρ and viscosity μ, under the action of a force $\vec{F}$ due to the external electric field,

$$\rho\frac{\partial u}{\partial t} + \rho u \cdot \nabla u + \nabla p - \mu\nabla^2 u = \vec{F}, \tag{12}$$

which may be greatly simplified under further assumptions. First one supposes the absence of the pressure gradient. For steady state flows the time derivative is zero, and supposing a fully developed and two dimensional flow one also has $u = u(y, z)$. Therefore, under these assumptions (12) will be given by

$$\mu\left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) = F_x. \tag{13}$$

Since the field strength and electric force are related by $F_x = \rho_e E_x$, and the charge density is given by (2), one has

$$\mu\left(\frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}\right) = -2n_\infty ze\sinh\left(-\frac{ze}{k_bT}\psi\right)E_x. \tag{14}$$

By taking again dimensionless variables

$$u^* = \frac{u}{U}, \qquad E_x^* = \frac{E_x L}{\zeta}, \tag{15}$$

where U is a reference velocity and L the distance between the electrodes, (14) may be written as

$$\left(\frac{\partial^2 u^*}{\partial y^{*2}} + \frac{\partial^2 u^*}{\partial z^{*2}}\right) = -ME_x^*\sinh\left(\psi^*\right) \tag{16}$$

with

$$M = \frac{2n_\infty ze\zeta D_h^2}{\mu U L} \tag{17}$$

and the boundary conditions

$$y^* = 0, \qquad \frac{\partial u^*}{\partial y^*} = 0, \tag{18}$$

$$z^* = 0, \qquad \frac{\partial u^*}{\partial z^*} = 0, \tag{19}$$

$$y^* = \frac{H}{D_h}, \qquad u^* = 0, \tag{20}$$

$$z^* = \frac{W}{D_h}, \qquad u^* = 0. \tag{21}$$

It is clearly remarkable that both the modified Poisson-Boltzmann and Navier-Stokes dimensionless equations ((6) and (16) respectively) have the same structure and are partial differential equations of the Poisson type:

$$\frac{\partial^2 \psi^*}{\partial y^{*2}} + \frac{\partial^2 \psi^*}{\partial z^{*2}} = (\kappa D_h)^2 \sinh(\psi^*), \qquad \left(\frac{\partial^2 u^*}{\partial y^{*2}} + \frac{\partial^2 u^*}{\partial z^{*2}}\right) = M E_x^* \sinh(\psi^*). \qquad (22)$$

In order to solve system (22), the non-linear equation for the electric potential ψ^* will be treated first by the Finite Element Method [3], combined with a Newton-Raphson iterative scheme. In the Finite Element Method, we expand ψ^* as $\psi^* = \sum_k \psi_k^* N_k$, where the N_k's stand for the shape functions in each finite element, and ψ_k^*'s are the unknowns at each nodal point. By taking the Galerkin Method, the residual related to a weight function N_i is given by

$$R_i = \sum_j \psi_j^* \int_\Omega \nabla N_i \cdot \nabla N_j \, d\Omega \;\; + \;\; (\kappa D_h)^2 \int_\Omega N_i \sinh\left(\sum_j \psi_j^* N_j\right) \, d\Omega,$$

and therefore the Jacobian J will be

$$J = \frac{\partial R_i}{\partial \psi_j^*} = \int_\Omega \nabla N_i \cdot \nabla N_j \, d\Omega \;\; + \;\; (\kappa D_h)^2 \int_\Omega N_i \cosh\left(\sum_k \psi_k^* N_k\right) N_j \, d\Omega.$$

According to the Newton-Raphson algorithm, an initial guess solution ψ_0^* is given, and for $m = 0, 1, 2, 3, ...$ one searches a sequence converging to the solution ψ^*, by solving the iterative equations

$$J\left(\psi^{*(m)}\right)\left(\psi^{*(m+1)} - \psi^{*(m)}\right) = -R\left(\psi^{*(m)}\right), \qquad (23)$$

where

$$\left(R\left(\psi^{*(m)}\right)\right)_i = \sum_j \psi_j^{*(m)} \int_\Omega \nabla N_i \cdot \nabla N_j \, d\Omega$$

$$+ \;\; (\kappa D_h)^2 \int_\Omega N_i \sinh\left(\sum_j \psi_j^{*(m)} N_j\right) \, d\Omega, \qquad (24)$$

$$\left[J\left(\psi^{*(m)}\right)\right]_{ij} = \int_\Omega \nabla N_i \cdot \nabla N_j \, d\Omega$$

$$+ \;\; (\kappa D_h)^2 \int_\Omega N_i \cosh\left(\sum_k \psi_k^{*(m)} N_k\right) N_j \, d\Omega. \qquad (25)$$

Once the convergence is reached, the solution ψ^* is replaced in the equation for the velocity field u^*. By taking again an expansion of the form $u^* = \sum_k u_k^* N_k$, the finite

element solution of $\left(\frac{\partial^2 u^*}{\partial y^{*2}} + \frac{\partial^2 u^*}{\partial z^{*2}}\right) = ME_x^* \sinh(\psi^*)$ is given in matrix notation as

$$[S]\{U\} = \{F\},\tag{26}$$

$$S_{ij} = \int_\Omega \nabla N_i \cdot \nabla N_j \, d\Omega,\tag{27}$$

$$F_i = ME_x^* \int_\Omega N_i \sinh(\psi^*) \, d\Omega.\tag{28}$$

Equations (23) to (28) were programmed and solved for some physical situations and parameters, and the results will be discussed in the following paragraphs. Electric potential and velocity field distributions were calculated in one-fourth of a rectangular cross section microchannel. In order to perform the finite element calculations, the domain was discretized into a mesh of second order triangular elements, using an automatic mesh generator based on the Delaunay algorithm [4]. Thus, each element contains six nodes, and the respective shape function, in homogeneous coordinates (u,v), can be written as

$$
\begin{aligned}
N_1 &= -(1-u-v)(1-2(1-u-v)),\\
N_2 &= 4u(1-u-v),\\
N_3 &= -u(1-2u),\\
N_4 &= 4uv,\\
N_5 &= -v(1-2v),\\
N_6 &= 4v(1-u-v).
\end{aligned}\tag{29}
$$

The mesh has a local refinement close to the microchannel walls containing, for the case corresponding to the following figures, 21,438 elements. In the problem under study, sharp variations of both electric potential and velocity occur close to the boundaries, introducing severe numerical errors if a linear approximation is used. Thus, quadratic finite elements must be used in order to obtain a numerically accurate solution.
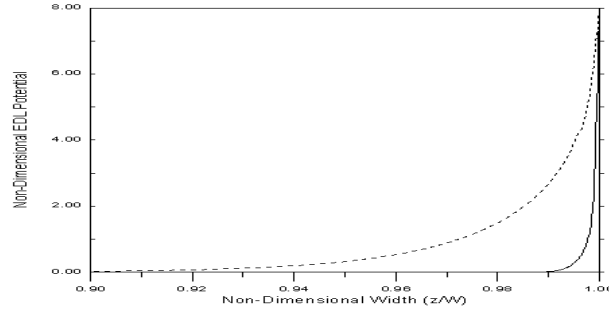
(a) Non-dimensional electric potential along the width of the channel at $y/H{=}0$ for two different hydraulic diameters ($D_h{=}24\ \mu m$ and $D_h{=}250\ \mu m$)

In the figures above and below, the dashed lines correspond to a hydraulic diameter of $D_h{=}24\ \mu m$, and the continuous lines to $D_h{=}250\ \mu m$. We used $H/W{=}2/3$ for the channel aspect ratio, $L{=}1\ cm$ for the inter-electrodes spacing, $U{=}1\ mm/s$ for the

reference velocity, $\zeta = 0.2\ V$ ($\zeta^* = 8$) and $1\ kV/cm$ for the applied electric field ($E_x^* = 5000$). The viscosity was taken as $\mu = 0.9 \times 10^{-3} kg\ m^{-1} s^{-1}$, the relative permittivity is $\epsilon = 80$ and the concentration, $10^{-6}\ M$.
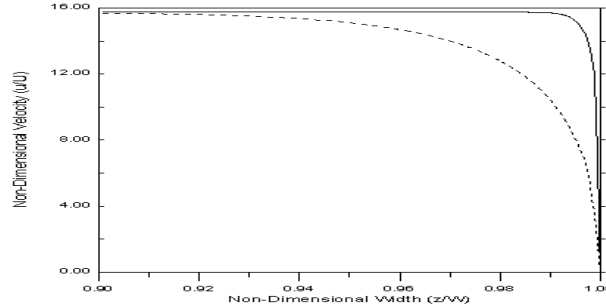
(b) Non-dimensional velocity profile along the width of the channel for the same values of the hydraulic diameter.

These results are quantitatively comparable to those obtained by other methods for the same problem [2]. In particular, the sharp decay of the fields close to the channel walls is perfectly reproduced. Since no approximation was made for the source term in Poisson-Boltzmann equation, this method can be employed for physical situations in which linearizations would be unacceptable. The advantage in our case is the combination of the Finite Element Method flexibility features (the capability for treating complicated domains, for instance) and the robustness of a Newton-Raphson approach for the non-linearity treatment.

References

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