Simulation of AC-Electroosmotic flows for Concentration of Particles on Biosensors

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ABSTRACT

Artificial concentration of particles in a fluid is a major challenge for micro- and nanobiosensors to enhance sensitivity and to reduce the time of response. We present here a numerical simulation of electroosmotic flows for particles concentration dedicated to biosensors. First a theoretical description of the electric potential in the fluid is presented, and the equation is numerically solved by spectral collocation. The result is used to obtain a slipping flow velocity condition above the electrodes as well as the dielectrophoretic force. Then Navier-Stokes equations are solved with this boundary condition using the same numerical method. Typical vortices are obtained through simulation and their aspects can be modified through electrical and geometrical parameters to enhance the concentration patterns. Either planar or cylindrical symmetries can be simulated through this method. Finally forces acting on particles are evaluated to obtain a better understanding of the particles trajectory.

Keywords: electroosmostic flows, concentration, particles, spectral collocation.

1 INTRODUCTION

Sensors are one major field of research in micro and nanotechnology. Several aspect of a sensor can be developed and optimized to increase the overall sensitivity. The optimisation of the dedicated electronics, of the fluidics and of the materials used for the fabrication of sensors allows achieving detection at roughly femtomolar concentration [1]. Such sensitivity can also be achieved through size reduction [2]. But the leading phenomenon for particles deposition on the active surfaces is the diffusion of the different species in the fluid. As shown in [2], the whole capacity of nano-sensors can not be exploited using this concentration scheme. In fact, diffusion becomes negligible at this scale. Therefore a direct and dedicated transport of particles is necessary to plainly exploit these sensors and reduce the time of response to acceptable values. This can be achieved through electroosmotic flows.

Examples of effective concentration can be found in the literature using this phenomenon [3]. Moreover this way of particles concentration can also be used on microscale sensors to improve the time of response. The phenomenon relies on the apparition of electrical double layers (EDL) at the surface of electrically charged electrodes. These layers can be displaced with the action of a transverse electric field. Their characteristic dimensions are so thin compared to the other dimensions that the displacement of the layers acts like a slip velocity at the surface of the electrodes. These fluid displacements create then bulk fluid movements. In our case, the charged electrodes create both the EDL and the electric field necessary to move the layers. Particles in suspension follow the bulk flow and are transported through the fluid. Other forces like dielectrophoresis (DEP) or electrophoresis can attract the particles on the electrodes forcing them to artificially concentrate.

To apply this phenomenon to different geometry of sensors, we propose here a dedicated model and numerical simulations for concentration of particles on patterned electrodes.

2 MODEL

Our electrohydrodynamic model is similar to that of Ramos *et al* [4] and to Ajdari *et al* [5]. It is based on the following classical approximations: (i) The bulk fluid is charge neutral with uniform ionic concentration. (ii) The Debye layer is assumed to be in local equilibrium, and is thickness is small compared to other dimensions. (iii) The bulk fluid motion is described by Navier-Stokes equations with a slip condition on the electrodes. (iv) We assume that the electrochemical reactions are negligible. (v) The potential drop is supposed to be small. Therefore the electrokinetic problem can be linearized. (vi) Finally the influence of the particles in suspension is supposed to be small compared to other phenomena. (vii) The electrolyte is monovalent and symmetric (1:1).

Upon these approximations, theoretical expressions of the electric potential and of the bulk fluid flow are written. Then the different forces can be described. This part focuses on the theoretical model and on the phenomena which explain the behavior of the fluid.

2.1 Debye layer and electric potential

When a potential ($\pm V_0 \cos(wt)$) is applied to the electrodes, the electric equilibrium of the bulk electrolyte is broken in a thin layer called the Debye layer above the charged electrodes. In the Debye-Hückel limit (small potential drop across the layer), the total charge in this layer can be linearized and simply written. In addition to the

Debye layer, the compact (Stern) layer gives rise to an additional capacitance C_s in series with the Debye Layer. This capacitance can also model a thin layer of isolating oxide. Once the physical properties of the layer are described, we can describe the electric potential φ just outside this layer:

$$\varphi = \frac{V_0}{2} + \frac{1}{C_T}\frac{\partial \varphi}{\partial y} \tag{1}$$

This equation coupled to the classical Poisson equation lead to the electric potential in the whole electrolyte. Thus we can compute both electric potential and field. Then the tangential slip velocity u_S of the Debye layer induced by the electric field E is classically written as $u_S = -\frac{\varepsilon\zeta}{\eta}E_t$, based on the Helmholtz-Smoluchovski slip velocity calculations (where η is the viscosity of the fluid, ζ the potential drop and ε the dielectric permittivity).

Using the different equations leads to the following result for the mean velocity slip flow:

$$< u_S > = -\frac{1}{4}\frac{C_T\lambda_D}{\eta}\frac{\partial}{\partial x}\left|V_{ext} - \varphi\right|^2 \tag{2}$$

Thus we have the necessary expressions to determine the bulk fluid flow and the forces that act on particles, where λ_D is the classical Debye length.

2.2 Fluid Dynamics

The fluid dynamics is described by the classical Navier-Stokes equations.

$$\begin{aligned} \nabla\vec{u} &= 0 \\ \rho\nabla p &= \mu\Delta\vec{u} \end{aligned} \tag{3}$$

where $\vec{u}$ is the velocity vector, ρ the fluid density, p the pressure and μ the dynamic viscosity. To simplify the simulations and the numerical considerations, the problem is reduce to one variable ψ, known as the current function. Using this definition, the first equation of (3) is directly verified, and the second one can be simplified to a scalar equation. Moreover as the Reynolds number is small ($\mathrm{Re} \prec 1$) the convection forces are neglected.

2.3 Forces acting on particles

Now both the fluid flow and the electric field (through the electric potential) are calculated. The particles behavior can then be estimated though the different forces applied.

A. Drag force

The circulating fluid exerts a drag force on the particles corresponding to the Stokes law as the Reynolds number is sufficiently small:

$$F_{drag} = \frac{24}{\mathrm{Re}}\frac{\pi}{2}\rho a^2 U^2 \tag{4}$$

where a is the particle radius, and U is the modulus of the fluid velocity.

B. DEP

DEP is often use as a concentrating force. It concentrates or repulses particles from high field zone. The time-average DEP force for a homogenous dielectric spherical particle is written [6]:

$$F_{DEP} = 2\pi\varepsilon a^3 \Re\left[K(\omega)\right]\nabla\left|E_{rms}\right|^2 \tag{5}$$

K is the Clausius-Mossotti factor which depends on frequency.

Positive DEP occurs when R[K]>0, the force is towards points of high electrical field. Negative DEP occurs when R[K]<0.

C. Gravity and lift

Two other forces acting on the particles can be calculated: the gravity and the buoyancy may have an important role.

$$F_g = \frac{4}{3}\pi a^3(\rho_{part} - \rho_{fluide})g \tag{6}$$

D. Other forces

Depending on the experimentations conditions and the frequency of the applied voltage, other forces can play an important role for the particles behavior: (i) electrohermal forces [6]. (ii) Illumination effects [7]. (iii) Electrophoresis. (iv) Brownian motion [6].

2.4 Geometrical aspect

The theoretical development is not based on particular geometrical considerations. To reduce the number of cases, our work focuses in the following on two major geometries: (i) two infinite rectangular parallel electrodes separated by a gap; (ii) One circular electrode surrounded by a ring electrode [3]. In the first case, we calculate all the results in a plane perpendicular to the electrodes using Cartesian coordinates. In the second one we use a cylindrical symmetry centered in the first electrode.

3 NUMERICAL CALCULATIONS

The numerical method use here is the spectral collocation. First of all, the electric potential is evaluated in the whole space. Thus we obtain the slip velocity of the Debye layer. The current function is thus calculated and the velocity vector is deduced for the bulk fluid. Finally using both results the different forces are evaluated for different size of particles, different case of experimentations, and different geometries of concentrators.

3.1 Spectral collocation

Spectral collocation is a classical spectral method in fluid dynamics calculations. Here it is used both for the electric potential and the fluidic parts. The points of collocation are the zero of the Chebychev polynomials on the interval [-1;1]. One major advantage of the spectral collocation is his versatility: (i) the scale in X and Y can be tuned. (ii) The repartition of the points can be also changed on the interval.

The major problem in our problems comes from the boundary conditions. Therefore they are explicated in the following paragraphs.

3.2 Cartesian coordinates

We consider here the first geometrical aspect given in 2.4. The electrical problem (second order) is trivial and the boundary conditions due to the symmetry are simple. There are described in the figure 1.

We focus though on the fluidic problem. The current function is defined as

$$u_x = \frac{\partial \psi}{\partial y} \qquad u_y = -\frac{\partial \psi}{\partial x} \tag{7}$$

Equation 3 simplifies into $\Delta^2 \psi = 0$. Thus we need eight boundary conditions on the current function. The non-slip velocity conditions on the walls and the slip velocity u_S are seven obvious boundary conditions. As u_x is odd in x, we can impose an eighth boundary condition on the (Oy) axis. The calculation is also possible on the whole space without taking into account the symmetry.

The different boundary conditions are resumed on the figure 1.

3.3 Cylindrical symmetry

The boundary conditions are a real problem in these configurations. In fact the Laplace operator is written as:

$$\Delta \equiv \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial y^2} \tag{8}$$

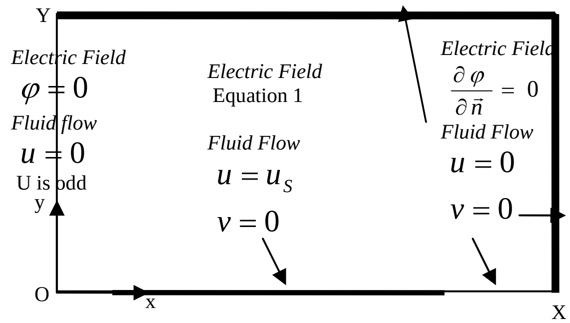

Figure 1: Boundary conditions for Cartesian coordinates.

Then it is singular in r=0 contrary to the Laplacian in Cartesian coordinates. This is quite a paradox, as the new coordinates create singularities. This can be solved by introducing new boundary conditions preventing from infinite results at r=0. In fact, as there are no natural singularities, the result functions have to be smooth at r=0. Thus we can developed them using a Taylor development and put it in the different equations. This way new boundaries conditions can be extracted preventing the system to be singular.

For the electrical calculations this problem is directly solved by the Van Neumann boundary condition ($\frac{\partial \varphi}{\partial r} = 0$). The fluidic part (fourth order) is more problematic. The current function is defined as

$$u_r = -\frac{1}{r}\frac{\partial \psi}{\partial y} \qquad u_y = \frac{1}{r}\frac{\partial \psi}{\partial r} \tag{9}$$

And the development of the equation 3 around r=0 leads to the boundary condition $\frac{\partial^3 \psi}{\partial r^3} = 0$. The different boundary conditions are resumed on the figure 2.

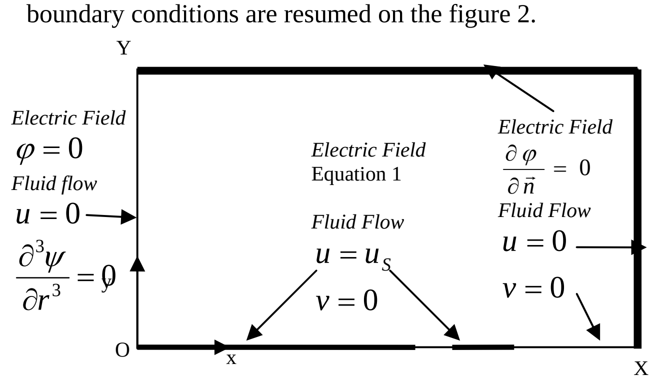

Figure 2: Boundary conditions for Cartesian coordinates.

4 SIMULATION RESULTS

Once both electrical and fluidic problem are fully written, numerical simulations become possible. To obtain better performance of the concentrator, we have to study the variations of different significant parameters: (i) The gap between the electrodes. (ii) The frequency of the signal. (iii) The size of the particles. (iv) Properties of the fluid.

Practically, the gap between the electrodes has not a huge influence. In fact it lowers the value of the electric field between the two electrodes and therefore the velocity of the Debye layer. As it is a fabrication problem and can not be tuned from one experiment to another, smaller gaps are more interesting, as the value of the electric field can also be tuned through the voltage applied to the electrodes.

4.1 Electroosmotic speed

The electroosmotic speed above the electrodes determines the aspect of the bulk flow. Two major properties can be tuned on the electroosmotic speed: (i) the maximum value. (ii) The global shape of the speed.

The first one can be tuned with the potential applied to the electrodes, whereas the frequency of the signal influences both aspects. The figure 3 represents the aspect of the slip velocity in the first geometric case.

This figure shows clearly that at low frequency the particles (through the drag force) will be transported above the whole electrodes, whereas at high frequency, the fluid moves only above the electrodes edge thus the drag force tends to collect on a larger surface on the electrodes.

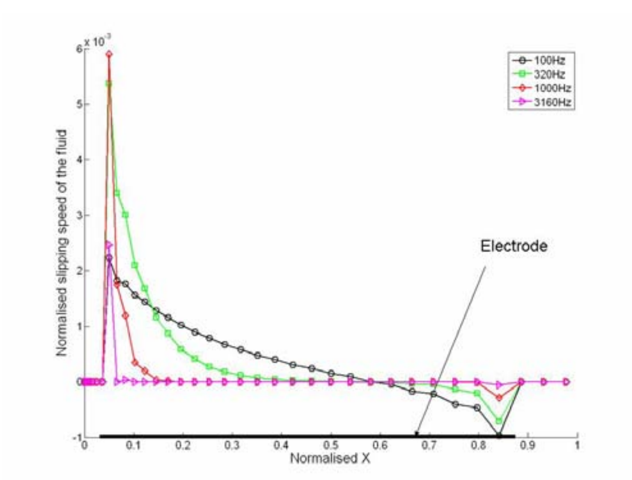

Figure 3: Sleep velocity variations with the frequency.

4.2 Fluidic Flow

A typical fluid flow obtained in a cylindrical symmetry is shown in figure 4. It represents also the aspect of the drag forces on the particles.

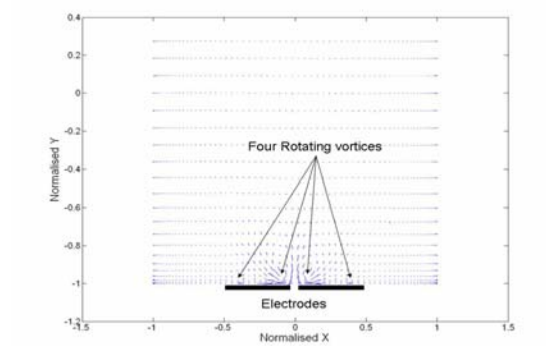

Figure 4: Typical fluid flow obtained @200Hz.

4.3 Other forces

The major force we have to consider is now the DEP. Following the sign of K(w), the particles are attracted or repulsed from the high field region. We are particularly interested in the second case in order to avoid any concentrations between the electrodes. This can be notably tuned by the conductivity of the fluid.

The simulations give us the value of this force and can be compared to the drag force. DEP force has a real influence on big particles (R>10µm). Smaller particles are more influenced by the drag force and can therefore be deposited in the center of the electrodes where the drag force shrinks.

4.4 Conclusions

Our theoretical model provides the major equations to model a particle concentrator based on electroosmotic flows. Using spectral collocation based calculations, we obtained electric potential, fluid flows and DEP forces for different type of concentrators and related experiments. Now a parallel work with experimentations will permit to valid the model and develop concentrators with more complicated shapes dedicated to existing sensors.

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