Numerical simulation of the dielectrophoretic concentration of DNA particles and the effect of AC electroosmosis

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Abstract. The dielectrophoretic concentration of DNA particles suspended in a solution is investigated in a system of parallel electrodes, where the particles are attracted to the edges of the electrodes by positive dielectrophoresis. The AC electroosmotic motion of the fluid is also considered, as well as the diffusion of the particles, using the solution of the Smoluchowski equation. The results examine the effect of AC electroosmosis in steady state dielectrophoretic concentration of particles, by demonstrating that AC electroosmosis significantly reduces the dielectrophoretic concentration at the edges and moves the particles towards the electrode centres.

1. Introduction
The manipulation of DNA particles is a subject of increasing interest, due to applications in lab-on-chip systems [1]. A very useful method for DNA manipulation utilises the dielectrophoretic (DEP) force. This force is caused by the interaction of the dipole formed when a particle is placed in a non-uniform electric field with the field.

Experimental investigations of DEP particle concentration suggest a difference between experimental and numerical results, which is attributed to other factors, such as the AC electroosmotic (ACEO) flow [2], caused by the interaction of the ions in the electrical double layer with the tangential electric field on the electrode surface. The manipulation problem therefore becomes more complicated by the fact that ACEO fluid flow is induced in the system, which disturbs the DEP concentration of particles. As a result the inclusion of the ACEO effect is required to more accurately simulate the behaviour of the system.

For this reason, a significant number of investigations has been carried out on ACEO as a phenomenon coexistent with DEP [3]. ACEO flow has also proved to be a useful phenomenon on its own, with a most useful application in solid state devices for pumping fluid [4] with low power consumption. Such pumping devices are expected to be very valuable in lab-on-chip systems where low power and solid state operation will be crucial. Furthermore, the operation of DEP systems where ACEO is inherently existent has exhibited useful side effects such as the stretching of DNA on an electrode edge [5]. These suggest that carefully designed DEP systems may use ACEO to their advantage. The significance of ACEO flow has led to the proposition of mathematical models to describe the ACEO flow, such as the one presented in [6], which has been validated with experimental results.
It has also been shown that the ACEO flow can be characterised by a non-dimensional frequency, which can provide important information about the nature of the flow at one particular frequency [6]. There have also been investigations about the scaling issues of ACEO and other effects associated with DEP [7]. These investigations have led to useful information on the range of device sizes, particle sizes and frequencies where each of these phenomena is dominant.

In this investigation, the Smoluchowski form of the Fokker-Planck equation [8], [9], [10] is used in order to study the steady state concentration of dsA5 DNA in a sample under both DEP and ACEO. The ACEO and DEP induced velocities are used as the convective terms in the equation, whilst the diffusion of DNA is also taken into account [11]. It is assumed that the particles do not affect the electric field or the fluid flow and that the particles do not interact with each other. The results from this investigation clearly indicate the significant effect of ACEO. The fluid flow caused by ACEO effectively carries the particles from the electrode edges towards the electrode centre, therefore reducing the DEP concentration at the edges. This observation is consistent with experimental observations.

2. Theory
2.1. Dielectrophoresis
The system in figures 1 and 2 is used as an example of a possible electrode configuration in a lab-on-chip system to manipulate DNA, which is suspended in water with KCl. The combined force from gravity and buoyancy is neglected in this domain since, at this distance from the electrodes, the DEP force is orders of magnitude higher. The DEP force is given by

$$F_{DEP} = \frac{Re(a_m) \times \nabla E^2}{4}$$

where $a_m(Fm^2)$ is the polarisability of the DNA particle and $E$ the peak electric field applied.

Investigations of the diffusion of dsA5 DNA estimate its diffusion coefficient to be $1.07 \times 10^{-10} m^2 s^{-1}$ [11]. Furthermore, studies on the dielectric relaxation of 12kbp plasmid DNA [12] give approximate values for the polarisability of the DNA at several frequencies. A reasonable
assumption for the dsA5 polarisability, which has 20 bases length, would be to consider the ratio of the $a_m$ of the dsA5 to the $a_m$ of the 12kbp plasmid DNA to be equal to the ratio of their volumes. This estimate of $a_m$ is accurate enough to give an order of magnitude value of the DEP force on DNA particles of this scale. The friction factor is found by $f = \frac{6 \pi \eta l}{\ln(\frac{l}{2})} = 4.387 \times 10^{-11} N \text{ms}^{-1}$ [13] and the diffusion coefficient gives $D_1 = \frac{kT}{f} = 9.22 \times 10^{-11} \text{m}^2\text{s}^{-1}$ which is very close to the one used and which was observed experimentally [11]. The Debye length for the system here is approximately $\lambda_{\text{Debye}} = 10 \text{nm}$.

To calculate the DEP force the Poisson equation is solved for the electric potential ($\phi$).

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

This is used to calculate $\nabla E^2$ and therefore the DEP force from equation 1.

### 2.2. AC Electroosmosis

Here Poisson’s equation for the potential is solved with the following boundary condition on the electrode, in order to find the potential at the edge of the double layer [6]

$$\sigma \nabla \phi_{ep} = \frac{\phi_{ep} - V_0}{Z_{DL}} \quad (3)$$

where $\phi_{ep}$ is the potential at the edge of the electrical double layer, $\sigma$ the fluid electrical conductivity, $V_0$ the absolute value of the voltage applied at the electrodes, $Z_{DL} = \frac{1}{\omega C_{DL}}$ the impedance of the double layer, $C_{DL} = \frac{\epsilon}{\lambda_{\text{Debye}}}$ the capacitance of the double layer, $\omega$ the angular frequency of the electric field and $\lambda_{\text{Debye}}$ the Debye length. The physical meaning of this boundary condition is that for low frequencies all the voltage is dropped across the double layer, whilst for very high frequencies the potential drop across the double layer goes to zero.

A coupled Navier Stokes model is solved to find the resulting fluid flow (under no external forces on the fluid)

$$\eta \nabla^2 u - \nabla p = 0 \quad (4)$$

where $\eta$ is the fluid viscosity, $u$ the fluid velocity and $p$ the fluid pressure. This has the following boundary condition for the fluid velocity on the surface of the electrode [6] equal to

$$U_{\text{slip}} = -\frac{\epsilon}{4\eta} \Lambda \frac{\partial |\phi - V_0|^2}{\partial x} \quad (5)$$

where $\Lambda$ is the ratio of the total diffuse layer potential drop over the double layer potential drop. The parameter $\Lambda$ is given by the ratio between the total capacitance and the diffuse double layer capacitance and was found experimentally to be approximately 0.25 [6].

### 2.3. Stochastic motion

The concentration or probability density function for the particles in two dimensions $C(x,y,t)$ is given by the Smoluchowski equation, as described in [10], [14]

$$\frac{\partial C}{\partial t} = -\frac{\partial}{\partial x}(v_{\text{DEP}}(x) + v_{\text{fluid}}(x)) + D \frac{\partial^2}{\partial x^2} - \frac{\partial}{\partial y}(v_{\text{DEP}}(y) + v_{\text{fluid}}(y)) + D \frac{\partial^2}{\partial y^2} C(x,y,t) \quad (6)$$

where $D$ is the diffusion coefficient, $f$ the friction factor and the other variables have the meaning stated before. Here the diffusion constant $D = 1.07 \times 10^{-10} \text{m}^2\text{s}^{-1}$ found experimentally [11] is used. For the solution of the Smoluchowski equation, all boundaries are set to be reflective.
**Table 1.** Electrolyte and particle properties used in the simulations.

| Property                                      | Value                                              |
|-----------------------------------------------|----------------------------------------------------|
| Fluid Viscosity ($\eta$)                      | $1 \times 10^{-3} Pa.s$                           |
| Diffusion coefficient for dsA5 DNA (D)         | $1.07 \times 10^{-10} m^2 s^{-1}$                 |
| Relative permittivity of medium ($\varepsilon_r$) | 80                                                |
| Electrode peak potential ($V_0$)              | 4.5V                                               |
| $\Lambda$                                     | 0.25                                               |
| Permittivity of free space ($\varepsilon_0$)  | $8.8542 \times 10^{-12} Fm^{-1}$                   |
| Debye length ($\lambda_{Debye}$)              | $1 \times 10^{-8} m$                              |
| Conductivity ($\sigma$)                       | 8.6$m Sm^{-1}$                                    |
| Friction factor (f)                           | $4.387 \times 10^{-11} Nms^{-1}$                  |
| Real part of Dipole moment (Re($a_m$))        | varied from 0.1667 to $5.333 \times 10^{-33} Fm^2$ |

3. Results

3.1. Steady state simulations

The interest here lies in the relationship between the dipole moment (or equivalently frequency) and the steady state DNA concentration under DEP. This will allow the investigation of how ACEO flow affects the final distribution of particles in the device when ACEO is also considered. It is predicted by theory that the relationship is exponential [8], however the relationship indicated by experimental results is a linear one [2]. It is also found experimentally that the concentration is much lower than the one predicted by DEP theory alone. The main issue of interest is the relation between the dipole moment and steady state concentration, which is why the concentration is plotted as the nondimensional ratio $\frac{C}{C_0}$, the ratio of the steady state concentration $C$ to the initially uniform concentration $C_0$. The point tested is $(1.499 \times 10^{-5}, 3 \times 10^{-7})$, which is close to the electrode edge. By using the properties in table 1 and the boundary conditions in figure 2, the system shown in figure 1 is simulated. A $4.5$ V peak voltage is applied and equation 1 is used for the DEP force.

It can be seen in figure 3 that the steady state concentration with DEP alone is of exponential form, as predicted by theory (the logarithmic plot is linear) [8]. The concentration due to ACEO and DEP is simulated using the Smoluchowski equation, by using the DEP and ACEO induced velocities as the convective terms. The effect of ACEO flow (which is the induced fluid velocity) is superimposed to the DEP-induced particle velocity and then it is incorporated in the Smoluchowski equation. The steady state concentration is clearly disturbed by the ACEO flow, as seen by the circular patterns of the concentration isocontours formed by the DNA in figure 4. Figure 4 is a side view of one of the electrodes shown in figure 1, of length equal to one periodic length of the array.

When ACEO flow is introduced, it can be seen in figure 5 that the concentration dramatically decreases, which agrees with experimental observations [2], where very modest collections of DNA on the array were observed in comparison to the concentrations predicted experimentally by DEP. It can be seen that the induced velocity due to ACEO is of the same order of magnitude or larger than the particle velocity induced by DEP. That means that ACEO is strong enough to distort the exponential relationship predicted by theory and is expected to be significantly modified and very dependent on ACEO flow. More specifically, ACEO flow is maximum at the electrode edges, where DEP is also maximum. The ACEO flow effectively removes the particles from the edges and carries them towards the electrode centre. Furthermore it can be observed that the effect of ACEO is at its highest at a dipole moment of $5.3 \times 10^{-33} Fm^2$ or equivalently at a frequency of about $10kHz$, as shown in figures 5 (the minimum concentration is at dipole...
Figure 3. Natural logarithm of the steady state concentration due to DEP alone vs dipole moment($Fm^2$)

Figure 4. Concentration of DNA (in nondimensional units $\frac{C}{C_0}$) in steady state over the electrodes, taking both DEP and ACEO into account

moment $5.3 \times 10^{-33} Fm^2$ for the combined ACEO and DEP case) and 6 (the maximum ACEO velocity magnitude is at $10kH_z$). This frequency corresponds to a non-dimensional frequency of 8, which agrees with the literature [6].

Figure 5. Logarithm of the steady state concentration due to DEP alone and joint DEP and ACEO vs dipole moment($Fm^2$)

Figure 6. Fluid speed at the point ($1.499 \times 10^{-5}, 3 \times 10^{-7}$) over the electrode surface as a function of frequency (Hz)

4. Conclusions

The DEP manipulation of dsA5 DNA particles in a suspension was investigated numerically. ACEO fluid motion was also simulated and the results with and without ACEO were compared. These indicate a strong decrease in the concentration at the edges and subsequent movement of particles towards the centre of the electrode, a fact verified by experimental observations.
Finally, the ability of the Smoluchowski equation to simulate combined diffusion, ACEO and DEP to describe the evolution of particle concentrations in such a system has been verified.

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