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EFFECTS OF FLUID FLOW VELOCITY UPON NANOPARTICLE DISTRIBUTION IN MICROFLUIDIC DEVICES UNDER DIELECTROPHORESIS

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Abstract. This paper presents some numerical results concerning the influence of fluid flow velocity on the concentration distribution of nanoparticles suspended in a dense and viscous fluid inside a microfluidic channel under dielectrophoresis (DEP). DEP induces spatial movement of polarizable particle suspended in a fluid medium, placed in a nonuniform electric field. The numerical study uses a 2D mathematical model, the equations being solved using a code based on finite element method. This type of analysis leads to the optimization of the control parameters, being crucial in designing of an experimental microfluidic device with application in the separation of nanoparticles.

Key words: flow velocity, dielectrophoresis, nanoparticles, microfluidic, concentration profile, finite element method.

1. INTRODUCTION

Dielectrophoresis is a phenomenon in which, under spatially non-uniform AC or DC electric fields, dielectric particles move because of interaction of the dipole induced in the particle with the applied field gradient [1]. This interaction does not require the particle to be charged and its strength depends strongly on the medium and particles' electrical properties, on the particles' shape and size, as well as on the frequency of the electric field. In classical dielectrophoresis, the positive DEP force attracts particles into the regions of strong electric field gradients, while negative DEP force repels them from those regions [2]. DEP methods can be used in many forms (electrorotation, traveling wave DEP, negative and positive DEP) to manipulate and, more generally, control the position, orientation and velocity of micro- and nanometer scale particles, including carbon nanotubes and biological particles such as viruses, DNA, bacteria and cells of various kinds [3, 4].

This paper is a study regarding the behavior of a suspension of nanoparticles under the action of dielectrophoretic force in a system consisting of a micro-channel controlled with an interdigitated electrode array. The reported results focus on the influence of the fluid flow velocity on the concentration field of suspended nanoparticles inside a separation device for the cases of positive and negative DEP, respectively.

2. THEORETICAL BACKGROUND

When an electrically neutral dielectric particle is subjected to a spatially non-uniform electric field, the induced dipolar moment results in a translational force and the particle undergoes a DEP motion as shown in Fig. 1. The force does not require the particle to be charged, the interaction strength depending strongly on the medium and particle electrical properties, on the particle shape and size, as well as on the frequency of the electric field [1, 5].

The time averaged DEP force, characteristic to non-uniform in magnitude but no variation in phase electric field, is given by [6]:

$$\langle \mathbf{F} \rangle = \frac{3}{4} \varepsilon_m k_R \nabla |\mathbf{E}|^2 , \tag{1}$$

where **E** is the electric field, k_R is the real part of the so-called Clausius-Mossotti (CM) factor, $\tilde{k}(\omega) = k_R + \mathrm{j}k_I$, which for a spherical particle can be expressed as [4,7]:

$$\tilde{k}(\omega) = \frac{\tilde{\varepsilon}_p - \tilde{\varepsilon}_m}{\tilde{\varepsilon}_p + 2\tilde{\varepsilon}_m} . \tag{2}$$

ω is the angular frequency of the electric field, while $\tilde{\varepsilon}_p$ and $\tilde{\varepsilon}_m$ are the absolute complex permittivities of the particle and the medium, respectively.

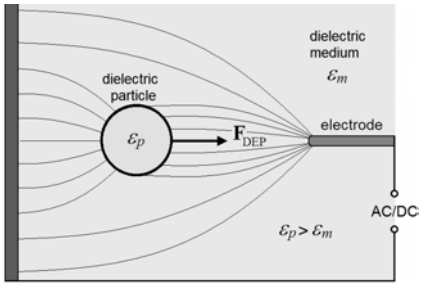


Fig. 1 – Electrically neutral particle in the presence of a spatially non-uniform electric field. The dipole moment induced within the particle results in a translational force and the dielectric spherical particle undergoes a DEP motion.

The complex permittivity is $\tilde{\varepsilon} = \varepsilon - \mathrm{j}\sigma/\omega$, where $\mathrm{j}=(-1)^{1/2}$, ε being the permittivity and σ the conductivity of the dielectric. The Clausius-Mossotti factor is a measure of relative permittivity of the particle and the surrounding medium. It determines the direction of the dielectrophoretic force depending on the dielectric properties of the particle and medium and the frequency of the applied field. When the sign of $k_R(\omega)$ is positive, the particle is more polarizable than its surrounding medium and is attracted to the locations of electric field intensity maxima, phenomenon known as positive dielectrophoresis (pDEP). The opposite situation occurs when $k_R(\omega)$ is negative, and is referred to as negative dielectrophoresis (nDEP). Consequently, particles are attracted to regions of stronger electric field when their permittivity ε_p exceeds that of suspension medium ε_m, *i.e.*, when $\varepsilon_p > \varepsilon_m$, and are repelled from regions of stronger electric field when $\varepsilon_p < \varepsilon_m$ [6]. The electric field can be written as $\mathbf{E}(\mathbf{x},t) = \mathrm{Re}\{\tilde{\mathbf{E}}(\mathbf{x})\mathrm{e}^{\mathrm{j}\omega t}\}$, where $\tilde{\mathbf{E}} = -\nabla\tilde{V} = -\nabla\left(V_R + \mathrm{j}V_I\right)$ represents the corresponding phasor. For a homogeneous medium, the electrical potentials satisfy the Laplace's equation:

$$\nabla^2 V_R = 0 \quad \text{and} \quad \nabla^2 V_I = 0 . \tag{3}$$

In terms of electrical potentials, the DEP force from equation (1) can be expressed as [6]:

$$\left\langle \mathbf{F}_{DEP} \right\rangle = \frac{3}{4}\varepsilon_m k_R \nabla\left(\left|\nabla V_R\right|^2 + \left|\nabla V_I\right|^2\right). \tag{4}$$

If the potential is scaled with the amplitude of the applied signals V_0, and the distances are scaled with a characteristic length d (for example the width of an electrode), one obtain the dimensionless electric potentials $V'_R=V_R/V_0$, $V'_I=V_I/V_0$ and displacement $\mathbf{x'} = \mathbf{x}/d$. The corresponding dimensionless form of the DEP force is:

$$\left\langle \mathbf{F}_{DEP} \right\rangle = F_{0DEP}\nabla'\left(\left|\nabla' V'_R\right|^2 + \left|\nabla' V'_I\right|^2\right), \tag{5}$$

where we noted $F_{0DEP} = \frac{3}{4}\varepsilon_m k_R \frac{V_0^{\,2}}{d^3}$.

The macroscopic behavior of a suspension of spherical particles in a dense and viscous fluid can be modeled considering the mechanical equilibrium between an external spatially dependent force $\mathbf{F}$ and the Stokes drag. When the size of the particles relative to the length L of the microchannel and the volume fraction C of particles are small, the dynamics of the two-phase system can be expressed by the following system of equations [4]:

$$\mathbf{v} = \mathbf{u} + \frac{2a^2}{9\eta}\mathbf{F}\text{, where: } \nabla\mathbf{u} = 0\text{,} \tag{6a}$$

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{j} = 0\text{, where: } \mathbf{j} = C\mathbf{v} - D\nabla C\text{.} \tag{6b}$$

Here **u** and **v** are the fluid and particle velocities, respectively, a the particle radius, η the viscosity of the fluid, t the time, **j** the particle flux, D the diffusion coefficient of the particles and $\mathbf{F}$ denotes the dielectrophoretic external force.

Using the scales of $d, d^2/D, D/d$ and C_0 (the initial average volume fraction) for the length, time, velocity and particle volume fraction, respectively, the problem is expressed in terms of dimensionless variables by the following system of equations:

$$\mathbf{v}' = \mathbf{u}' + Q\mathbf{F}'\text{, where: } \nabla\mathbf{u}' = 0\text{,} \tag{7a}$$

$$\frac{\partial C'}{\partial t'} + \nabla \cdot \mathbf{j}' = 0\text{, where: } \mathbf{j}' = C'\mathbf{v}' - D\nabla C'\text{.} \tag{7b}$$

The prime symbol above denotes the dimensionless quantities and $Q = 2a^2F_0d/9\eta D$ with F_0 a measure of the intensity of the external field, for example the quantity F_{0DEP} from equation (5).

3. NUMERICAL RESULTS AND DISCUSSIONS

The mathematical model presented above describes the behavior of a suspension of spherical particles in a dense and viscous fluid, subject to an imposed non-uniform external force. Our numerical study deals with the computation of the concentration field for positive and negative DEP and the analysis of concentration profiles at different positions, inside an interdigitated electrode array sketched in Fig. 2. More precisely, the influence of the fluid flow velocity field at the entrance of the device on the particle concentration profile is investigated.

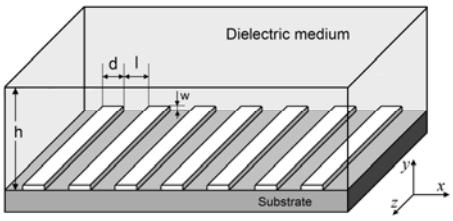


Fig. 2 – Schematic representation of the dielectrophoretic patterning chamber with interdigitated bar electrodes at bottom surface used for DEP nanoparticles separation.

All the numerical simulations were performed using a partial differential equations solver, FreeFEM++ [8, 9], based on the finite element method. For the computation of the DEP force, we solved the Laplace equations (3) for the real and imaginary components of the electric potential, together with the associated boundary conditions. Due to the symmetry of the problem and considering the electrodes long compared to their width, the problem can be treated as two-dimensional. In order to have a realistic description of the device's geometry, the shape and the height of the electrodes is taken into account. The computational domain and the boundary conditions can be assumed as shown in Fig. 3, where the particular case $d = 1 = 50\mu m$, $w = 0.2d$ and $h = 2d$ is considered. The vertical lines mark the period over which the system is repeated (the basic unit cell). Each electrode was assigned its corresponding value for the real part of the potential phasor. For the case of the electrode array with 2-phases applied, as in most of dielectrophoresis experiments, the imaginary part of the potential phasor is zero everywhere [3].

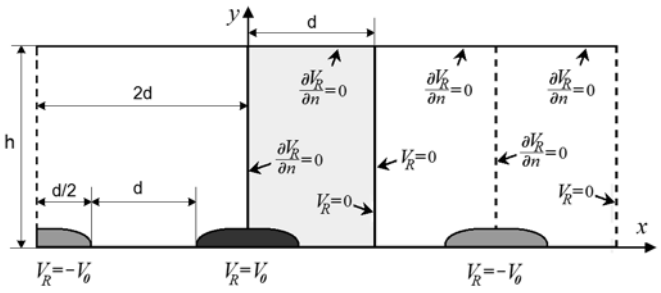


Fig. 3 – The geometry of the computational domain and the boundary conditions for the real part V_R of the electric potential. The solid lines indicate the basic unit cell.

Details on the validation procedure of the program and an analysis of the dielectrophoretic force distribution are given in [6]. We present here only a set of numerical results concerning the concentration field inside the separation device.

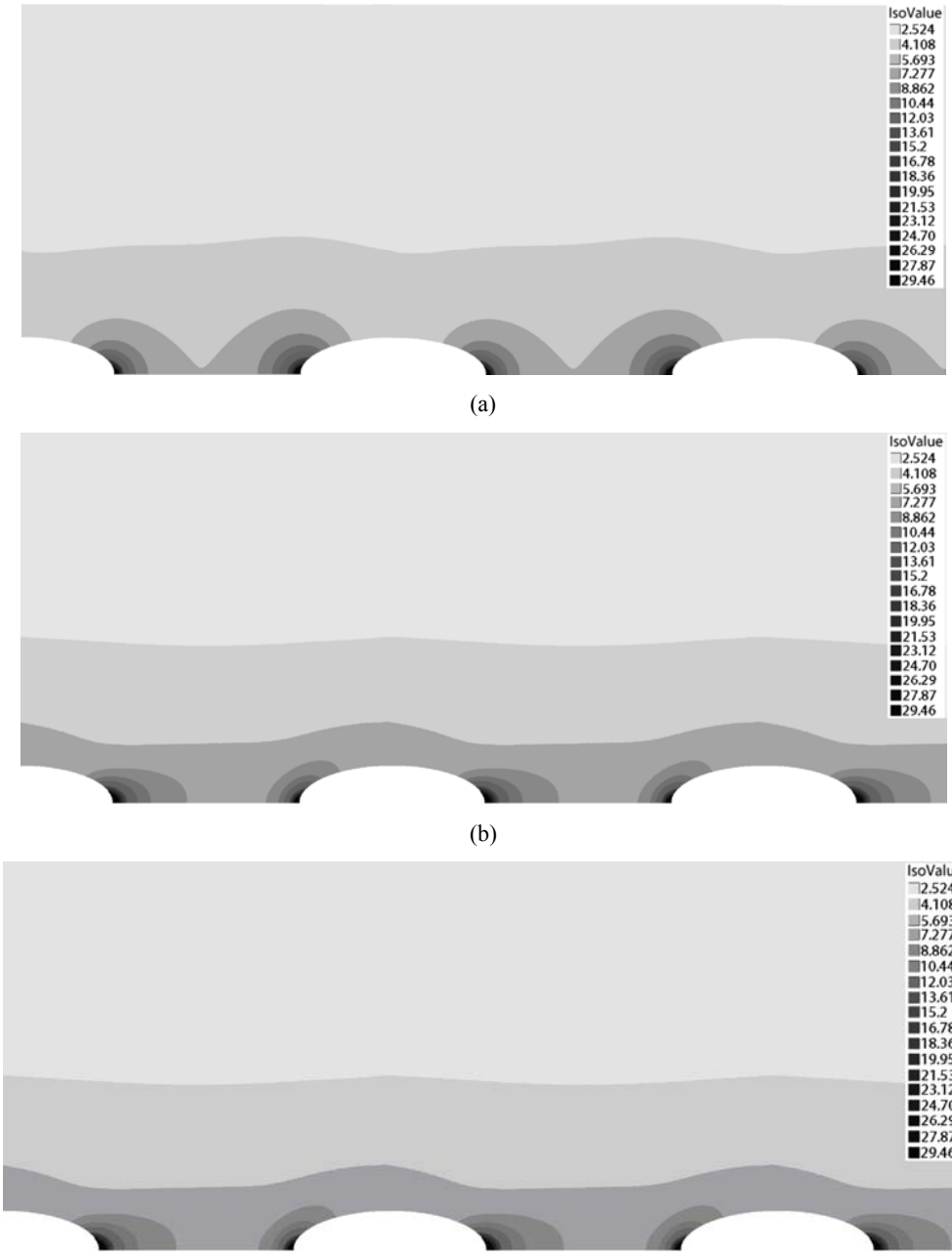
The simulations were performed for a suspension of particles with characteristic size $a = 200\,\text{nm}$ in water ($\eta = 10^{-3}\,\text{kgm}^{-1}\text{s}^{-1}$, $\rho = 10^{3}\,\text{kgm}^{-3}$, $D \approx 10^{-12}\,\text{m}^2\text{s}^{-1}$, $\varepsilon_r \simeq 80$ with $\varepsilon_m = \varepsilon_0 \varepsilon_r$, where ε_0 is the absolute permittivity of vacuum). The characteristic length of the device is $d = 50\,\mu\text{m}$. For a real part of the Clausius-Mossotti factor $k_R \approx 0.6$, an amplitude of the electric potential $V_0 \simeq 1\text{V}$ and a traveling wave with $\lambda = 400\,\mu\text{m}$, one obtains for the dimensionless parameter in equation (7a) a typical value of $Q \approx 0.2$.

Due to the geometry of electrodes, the fluid flow inside micro channel is not described by the classical Poiseuille profile any more, but requires solving the Navier-Stokes equation for the computational domain shown in Figure 3. The calculated values of velocity field and dielectrophoretic force are used in the transport equations (7a,b) in order to obtain the concentration distribution inside the separation device. Computations were performed for values of the parameter Q ranging from – 0.5 to 0.5, in order to describe the repulsive (negative values of Q) and respectively attractive (positive values of Q) behavior. We remind here that the key parameter of the problem Q can be practically varied by modifying the applied signal. Thus, by increasing or decreasing the voltage, Q increases or decreases corresponding to a square law. In addition, by shifting the frequency of the input potential, the sign of Q can be changed from positive to negative and vice-versa, according to the Clausius-Mossotti formula. The influence of the fluid flow is analyzed by computing the concentration field at different flow intensities, having maximum values of the dimensionless velocity ranging from 1 to 500, corresponding, for a device with $h = 200\ \mu\text{m}$ and $L = 1000\ \mu\text{m}$, to physical values ranging from 1 to 500 $\mu\text{m/s}$.

For simplicity, we drop the prime symbol, even the analysis is performed in terms of dimensionless quantities. Figures 4a-c and 5a-c respectively show the calculated concentration field at three different dimensionless values of the velocity ($v = 1$, $v = 10$ and $v = 100$) for $Q = 0.2$ (p-DEP) and $Q = -0.2$ (n-DEP), respectively. The results reveal that the nanoparticles in suspension tend to concentrate on the channel walls (positive DEP) or in the center of the channel (negative DEP) depending on their dielectric properties and geometry. On the other hand, the modifications in concentration profile symmetry, especially for $v = 100$, clearly outline the effect of the flow on the particle dispersion.

Furthermore, a set of more refined numerical results concerning the variation of the stationary concentration field for different positions inside the considered separation device is provided. The numerical calculations were performed for a computational domain corresponding to the basic unit cell presented in Fig. 2. The dimensionless coordinates $x/d = 0$, $x/d = 0.5$ and $x/d = 1$ respectively, correspond to the left margin of the computational domain, the margin of the left electrode and the middle of the distance between electrodes, respectively.

Figures 6a and 6b show the vertical variation of the concentration for different horizontal coordinates in the case of positive dielectrophoresis. For both presented cases ($v = 1$ and $v = 100$) the profiles are similar. The concentration slightly increases while approaching the electrode. Only at the margin of the electrode ($x/d = 0.5$) the concentration increases suddenly, reaching values with one order of magnitude larger then the average value.

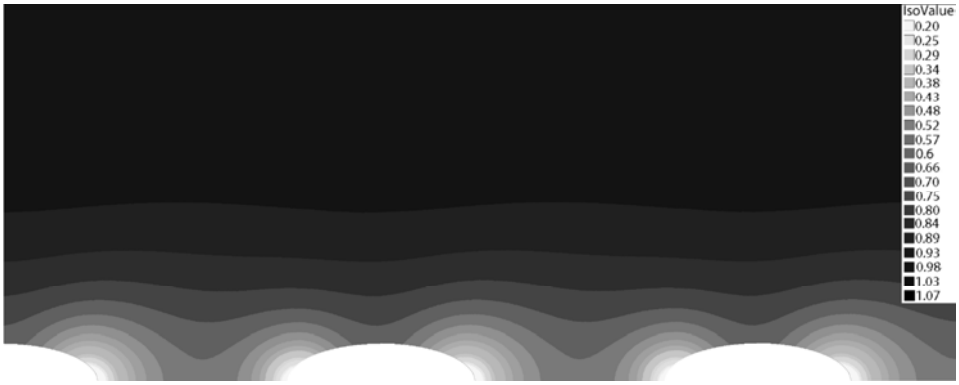


(a)

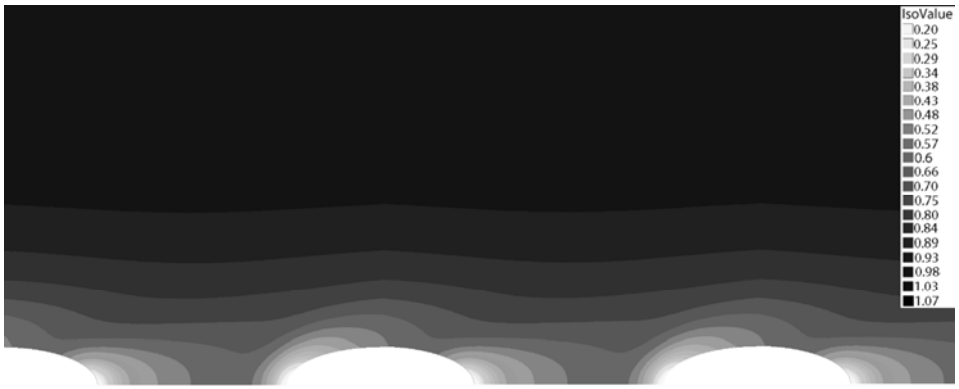
(b)

(c)

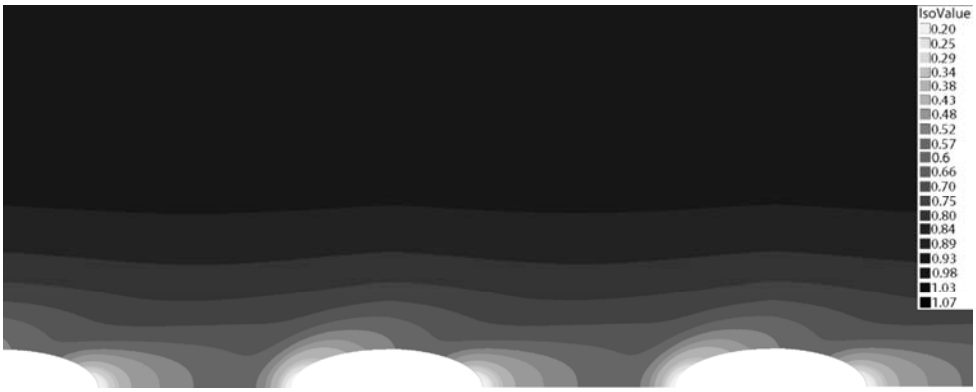
Fig. 4 – Calculated concentration fields for positive DEP ($Q = 0.2$) for: a) $v = 1$; b) $v = 10$; c) $v = 100$, respectively.



(a)



(b)



(c)

Fig. 5 – Calculated concentration fields for negative DEP ($Q = –0.2$) for: a) $v = 1$; b) $v = 10$; c) $v = 100$, respectively.

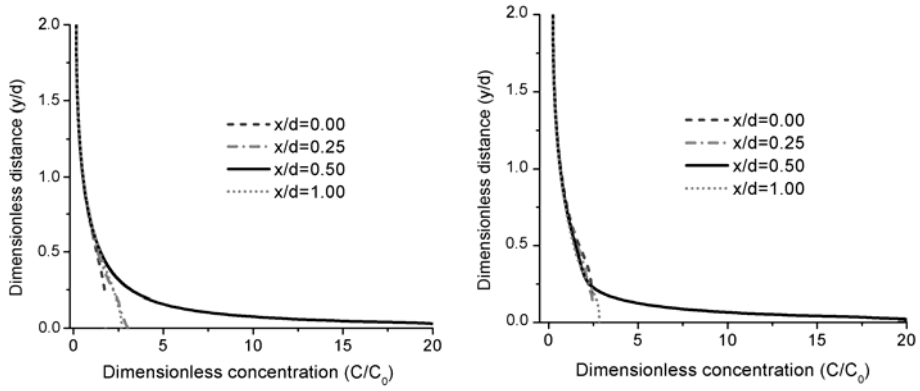


Fig. 6 – Calculated concentration profiles for positive DEP at: a) $v = 1$; b) $v = 100$.
The dimensionless coordinates $x/d = 0$, $x/d = 0.25$, $x/d = 0.5$ and x/d=1 respectively, correspond to the left margin of the computational domain, the middle of the left electrode, the margin of the left electrode and the middle of the distance between electrodes, respectively.

Figures 7a and 7b present the effect of the flow velocity on the p-DEP concentration field at the margin of the electrode and in the middle of the distance between electrodes, respectively. For weak fluid flow intensities, practically there is no influence on the concentration field. In the region between the electrodes there is a trend to homogenize the particle distribution, especially at important fluid flow rates ($v = 100$).

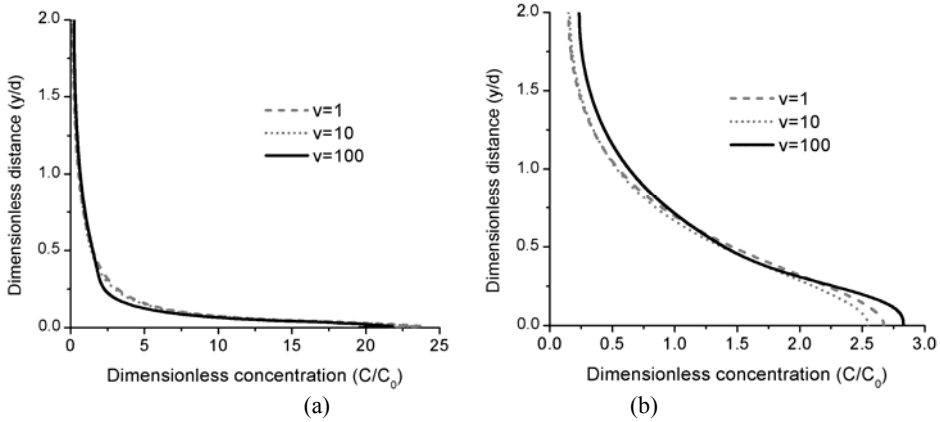


Fig. 7 – Calculated concentration profiles for positive DEP at: a) $x/d = 0.5$; b) $x/d = 1.0$.
The dimensionless coordinates $x/d = 0.5$ and $x/d = 1$ respectively, correspond to the margin of the left electrode and the middle of the distance between electrodes, respectively.

In the case of negative dielectrophoresis, the particles are expelled from the electrodes. As shown in Figures 8a and 8b, the vertical variation of the

concentration field has a weak dependence on horizontal coordinate, excepting the margin of the electrodes where the concentration diminish rapidly. Figures 9a and 9b present the effect of the fluid flow velocity on the n-DEP concentration field at the margin of the electrode and in the middle of the distance between electrodes, respectively. Like in the p-DEP case, for weak fluid flow intensities practically there is no influence on the concentration field. In the region between the electrodes, for important fluid flow rates (v = 100) the concentration diminishes because particles are "washed-out" towards the center of the separation device.

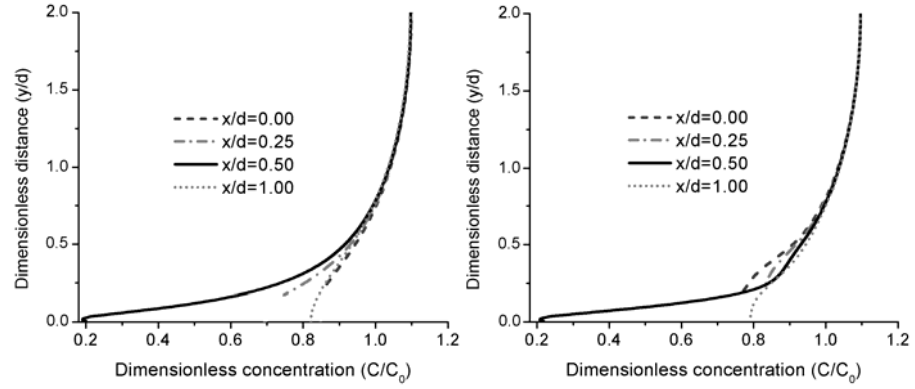


Fig. 8 – Calculated concentration profiles for negative DEP at: a) v = 1; b) v = 100. The dimensionless coordinates x/d = 0, x/d = 0.25, x/d = 0.5 and x/d = 1 respectively, correspond to the left margin of the computational domain, the middle of the left electrode, the margin of the left electrode and the middle of the distance between electrodes, respectively.

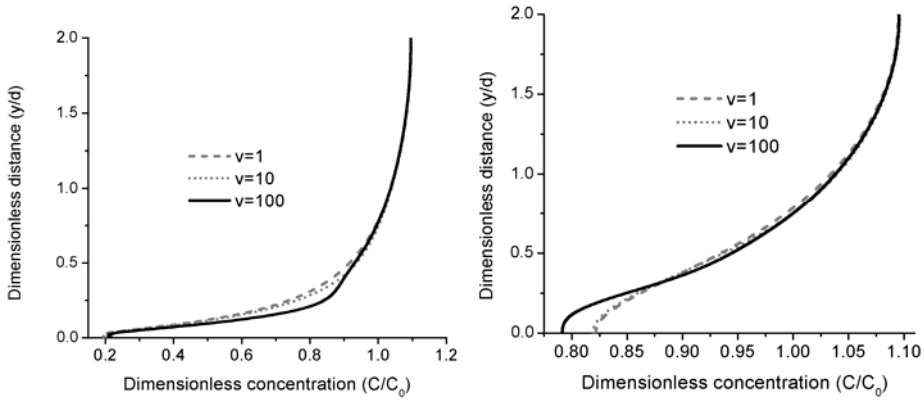


Fig. 9 – Calculated concentration profiles for negative DEP at: a) x/d = 0.5; b) x/d = 1. The dimensionless coordinates x/d = 0.5 and x/d = 1 respectively, correspond to the margin of the left electrode and the middle of the distance between electrodes, respectively.

In order to conclude, one can say that the numerical results obtained in the frame of the proposed mathematical model reveal the influence of some fundamental parameters (nature and size of particles, geometry of device, fluid flow debit) on the nanoparticles manipulation in a fluid suspension. This type of analysis leads to the optimization of experimental devices with potential applications in both particles filtering and sorting.

4. CONCLUSIONS

The study presented in this paper concerns the description of nanoparticles behavior in a suspension under the action of DEP forces. More precisely, the concentration profile of the particles exposed to DEP forces was numerically computed and the influence of the suspension's flow velocity on this profile was analyzed. Both the cases of repulsive and respectively attractive effects of the dielectrophoretic force are considered. Furthermore, a set of more refined numerical results concerning the variation of the stationary concentration field for different positions inside the separation device is provided. The mathematical model and the numerical simulations can help us both understand the physics and behavior of dielectrophoresis as well as allow us to design new and more efficient devices for nanoparticles sorting and tracking. The numerical analysis of the influence of specific parameters on the dielectrophoretic process can lead to further advancements, improved designs and new applications of DEP force as an important tool for nano-scale research and engineering.

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