

NANOPARTICLE MANIPULATION BY DIELECTROPHORESIS

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Abstract. In the last decades, non-uniform electric field proved to be the most promising technique for nanoparticles manipulation with applications in fields such as medicine, biology, physics or nanotechnology. The paper presents a set of numerical results concerning the influence of the dielectrophoretic (DEP) forces on a nanoparticle suspension. The DEP force depends on the electric properties of the nanoparticles, as well as their shape, size and mass, and the properties of the surrounding medium. The numerical study was performed in the frame of a mathematical model describing the electric field distribution and the suspended nanoparticle movement in a dense and viscous fluid. The equations are solved, together with the appropriate boundary conditions using a code based on the finite element method. The dielectrophoretic force distribution, the particle trajectories and the nanoparticle concentration profile are computed. This type of analysis leads to the optimization of the control parameters and is crucial in the designing process of an experimental microfluidic device with application in the separation of submicronic particles.

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1. INTRODUCTION

Dielectrophoresis (DEP) is a phenomenon in which, under spatially non-uniform AC or DC electric fields, dielectric particles move because of the interaction of the dipole induced in the particle and 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 fields, 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].

This paper represents a numerical study on the behavior of a suspension of submicron particles under the action of dielectrophoretic force in a system consisting of a micro-channel controlled with an interdigitated electrode array. The reported results concern the influence of the geometry and experimental parameters on the dielectrophoretic force, particle trajectories and concentration field.

2. THEORETICAL CONSIDERATIONS

To compute the electric field and the dielectrophoretic forces, the electric potential is solved for a defined space and set of boundary conditions (that represent the electrode array). In this paper phasor notation is used, with an arbitrary potential oscillating at frequency ω defined as [4]:

$$V(\mathbf{x}, t) = \text{Re}\{\tilde{V}(\mathbf{x})e^{j\omega t}\}, \quad (1)$$

where $j = (-1)^{1/2}$, \mathbf{x} is the coordinate, $\text{Re}\{\}$ indicates the real part and the tilde indicates the phasor $\tilde{V} = V_R + jV_I$, with V_R and V_I the real and respectively imaginary part of the electric potential.

For a homogeneous medium, the electrical potentials satisfy the Laplace's equation:

$$\nabla^2 V_R = 0 \quad \text{and} \quad \nabla^2 V_I = 0, \quad (2)$$

and the time-averaged dielectrophoretic force can be expressed as [6]:

$$\langle \mathbf{F}_{DEP} \rangle = \frac{3}{4} \epsilon_m \tilde{k}_r(\omega) \nabla (|\nabla V_R|^2 + |\nabla V_I|^2), \quad (3)$$

where $\tilde{k}(\omega)$ is the Clausius–Mossotti (CM) factor: $\tilde{k}(\omega) = \tilde{\epsilon}_p - \tilde{\epsilon}_m / \tilde{\epsilon}_p + 2\tilde{\epsilon}_m$, with $\tilde{\epsilon}_p$ and $\tilde{\epsilon}_m$ the absolute complex permittivity of the particle and the medium, respectively, and depends on the dielectric properties of the particles and medium and on the geometry of the particles. The complex permittivity is $\tilde{\epsilon} = \epsilon - j\sigma / \omega$, where ϵ represents the electric permittivity and σ the conductivity of the dielectric. The real part $\tilde{k}_r(\omega)$ of CM factor gives the DEP force in the vertical direction. In a dielectric medium, the direction of the DEP force is influenced by the polarizability of the particle, which depends on the permittivities of the particle and the suspending medium. When the sign of $\tilde{k}_r(\omega)$ is positive, the particle is more polarizable than its surrounding medium and its movement is oriented towards regions of highest field strength, known as positive dielectrophoresis (pDEP). When $\text{Re}\{k\}$ is negative, particles with polarizability less than that of the medium move towards the region of lowest field gradient, known as negative dielectrophoresis (nDEP).

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 of the microchannel and the volume fraction ϕ of particles is small, the dynamics of the two-phase system can be expressed by the following system of equations [6]:

$$\begin{aligned} \mathbf{v} &= \mathbf{u} + \frac{2a^2}{9\eta} \mathbf{F}, \quad \text{where} \quad \nabla \mathbf{u} = 0 \\ \frac{\partial \phi}{\partial t} + \nabla \cdot \mathbf{j} &= 0, \quad \text{where} \quad \mathbf{j} = \phi \mathbf{v} - D \nabla \phi. \end{aligned} \quad (4)$$

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

In order to avoid extreme numbers in the numerical calculations, the potential is scaled with V_0 , the amplitude of the applied signal, and the distances are scaled with d , the width of the electrode.

In terms of dimensionless electric potentials $V'_R=V_R/V_0$, $V'_I=V_I/V_0$ and displacement $\mathbf{x}'=\mathbf{x}/d$, the time-averaged expression for the dielectrophoretic force becomes:

$$\langle \mathbf{F}_{DEP} \rangle = F_{0DEP} \nabla' \left(|\nabla' V'_R|^2 + |\nabla' V'_I|^2 \right), \quad \text{where} \quad F_{0DEP} = \frac{3}{4} \varepsilon_m \tilde{\kappa}_r \frac{V_0^2}{d^3}. \quad (5)$$

Using the scales of $d, d^2/D, D/d$ and φ_0 (the initial average volume fraction) for the length, time, velocity and particle volume fraction, respectively, the macroscopic transport is expressed in terms of dimensionless variables by the following system of equations:

$$\begin{aligned} \mathbf{v}' &= \mathbf{u}' + Q\mathbf{F}', & \text{where} & \quad \nabla \mathbf{u}' = 0 \\ \frac{\partial \varphi'}{\partial t'} + \nabla \cdot \mathbf{j}' &= 0 & \text{where} & \quad \mathbf{j}' = \varphi' \mathbf{v}' - D \nabla \varphi' \end{aligned} \quad (6)$$

The prime symbol above denotes the dimensionless quantities, $Q = 2a^2 F_0 d / 9\eta D$ with F_0 a measure of the intensity of the external field.

3. NUMERICAL RESULTS AND DISCUSSIONS

All the numerical simulations were performed using a finite element code, FreeFEM++ [7]. Figure 1 presents a typical DEP array of rectangular shape electrodes. We noted with d the electrode width, l the distance between two adjacent electrodes, w the electrodes height and h the dielectrophoretic chamber height.

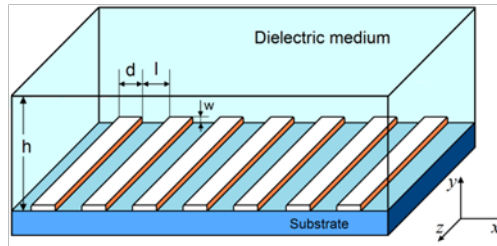


Fig. 1: Schematic of the dielectrophoretic chamber with interdigitated bar electrodes at bottom surface used for DEP separation.

For the computation of the dielectrophoretic force, we solved the Laplace's equations (2) for the real and imaginary components of the potential, together with the associated boundary conditions. Due to the symmetry of the problem and considering the electrodes long compared to their width, problem can be treated as two-dimensional. The computational domain

and the boundary conditions can be assumed as in Figure 2, where the particular case $l = d$ and $h=2d$ was considered.

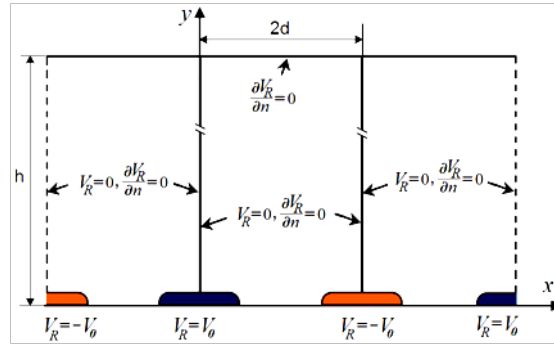


Fig. 2: Computational domain with boundary conditions for the real part V_R of the electric potential.

The numerical analyses were performed for a computational domain with electrodes of dimensionless width $d' = 1$ and different shapes. The calculated values of the magnitude of dimensionless dielectrophoretic force $\langle \mathbf{F}_{DEP} \rangle / F_{0DEP}$ in the case of electrodes with negligible height and with elliptic shape, respectively, are presented in Figures 3(a) and 3(b) respectively. In both cases, the magnitudes of the computed quantities, and consequently the effect of the DEP force, increase to a maximum value at the electrode edge and diminish rapidly with the distance on vertical direction.

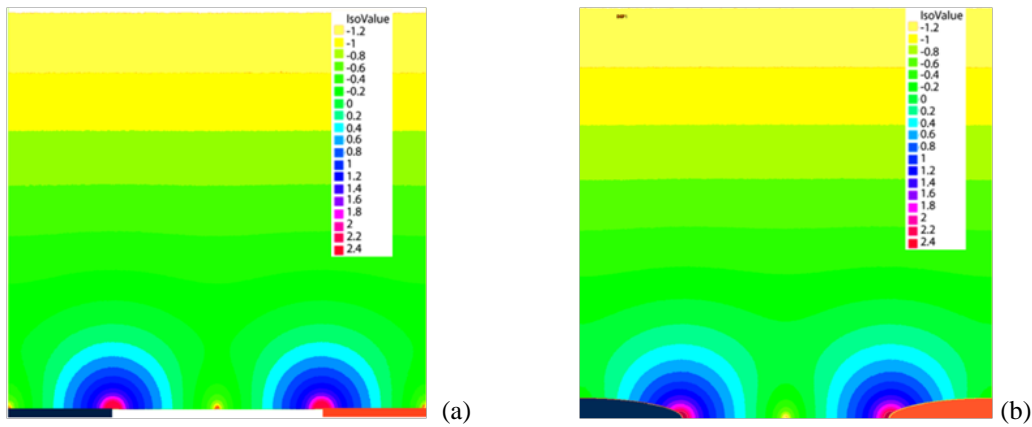


Fig. 3: Calculated values for the magnitudes of the dimensionless DEP force $\langle \mathbf{F}_{DEP} \rangle / F_{0DEP}$, plotted on logarithmic scale; (a) plane electrodes, (b) elliptic electrodes.

The analysis of particles trajectories is performed by integrating the dimensionless movement equation (6a) and considering a Poiseuille flow profile for the fluid, with a maximum value of dimensionless velocity equal to unity. The computed trajectories for particles entering the computational domain at $x'_0=0$ and different values of y'_0 in the case of positive and negative DEP are shown in Figures 4 (a) and (b) respectively. As it can be seen, the trajectories are strongly influenced by the DEP force in the vicinity the electrode. When the distance particle-electrode is large, the influence of the DEP force is very weak. This analysis reveals that the

nanoparticles in suspension tend to concentrate to the channel walls for positive DEP or to the channel center for negative DEP.

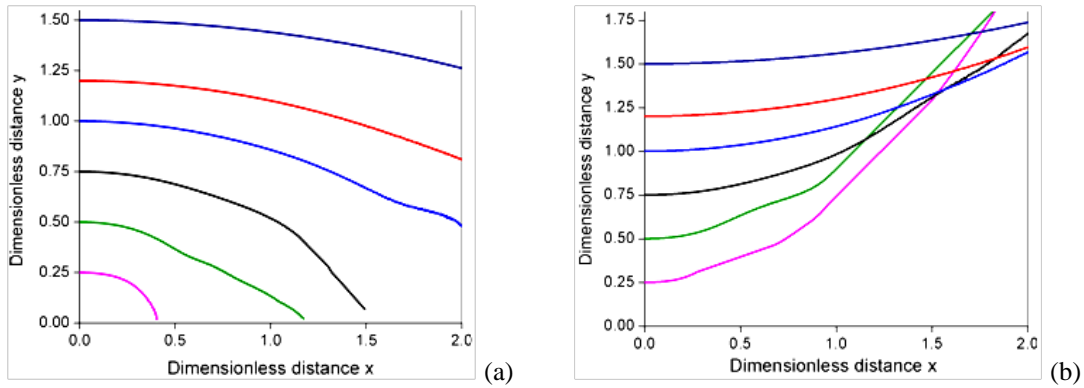


Fig. 4: Calculated particle trajectories in case of positive DEP (a), negative DEP (b).

The global concentration field is influenced both by the DEP force and the velocity of the fluid flow. In figures 5a,b we present two examples of computed stationary concentration field in the case of a typical force parameter $Q=0.2$ (positive DEP) and two different flow velocity values.

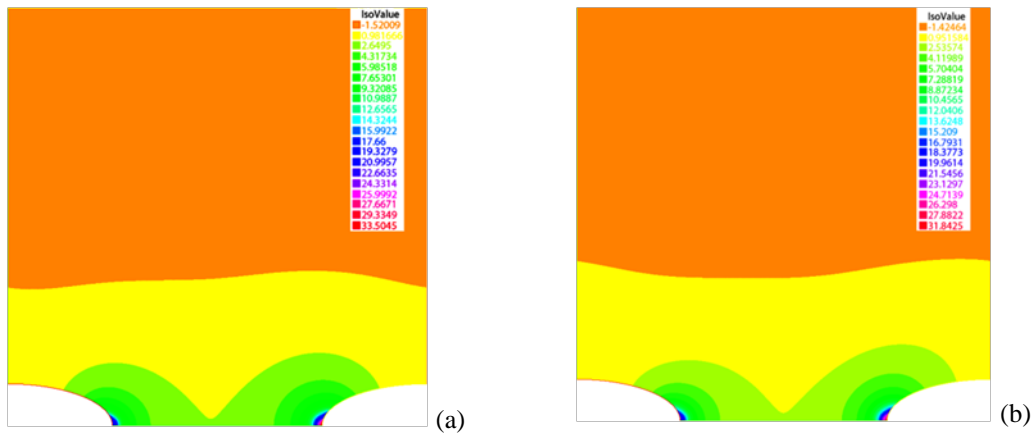


Fig. 5: Positive DEP for $Q=0.2$ and $\nu=1$ (a), and $\nu=10$ (b).

The assembly of numerical results shows that in the case of positive DEP the nanoparticles in suspension tend to concentrate on electrodes edge. Depending on their properties (nature, size), the concentration profile can be controlled by adjusting the applied voltage at the command electrodes and the fluid flow.

4. CONCLUSIONS

The paper presents a set of numerical results concerning the description of the nanoparticles behavior in a suspension under the action of DEP force. As $\tilde{k}_r(\omega)$ is a complex function of particle and fluid properties (permittivity, conductivity) and frequency of the applied field, a particle can experience both positive and negative DEP forces at different combinations of the above variables. The results reveal the influence of the main experimental parameters on the dielectrophoretic effect on the suspension's concentration field and provide an important tool in the particle manipulation within microfluidic systems.

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