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Some considerations on the dielectrophoretic manipulation of nanoparticles in fluid media

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The manipulation of nanoparticles is becoming an important issue as they are massively generated in combustion or material synthesis processes are highly toxic to human health because they can readily enter the human body through inhalation and their toxicity is relatively high. Therefore, their filtration represents an important technological challenge, which makes the object of a very active research. In many scientific and technical areas, a considerable interest is also shown to the separation of nanoparticles in accordance with their physical or chemical characteristics using dielectrophoresis. Dielectrophoretic (DEP) force is exerted when a neutral particle is polarized in a non-uniform electric field, and depends on the dielectric properties of the particle and the suspending medium. This paper investigates the behavior of a suspension of nanometric particles under the action of DEP force. A theoretical model is proposed and a set of numerical results is provided. In particular, the trajectories required to achieve a steady-state pattern are theoretically modeled and computed for a planar electrode array configuration.

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1. Introduction

Nanosized particles have received considerable interest in the past two decades. Their toxicity for human health is relatively high because they can readily enter the human body through inhalation and have a large specific surface area. Their filtration is an important technological challenge, as they are produced in large numbers from material synthesis and combustion emission [1]. In many scientific and technical areas, a considerable interest is also shown to the separation of nano-particles in accordance with their physical or chemical characteristics. As technology is moving towards the nano-scale, several new methods of particle manipulation are being explored. Mechanical devices of controlling particle movement are less effective at this scale. Flotation separation methods are usually slow and may contaminate the particles under manipulation. Optical techniques sometimes used in trapping nano-particles have the major disadvantage that they produce significant heating of the fluid in which the targeted bodies are suspended. They also require the use of optical equipment that is often large in size and difficult to integrate on a micro- or nano-analysis device. The methods utilizing electric fields are emerging as the most promising techniques for nano-particle manipulation. Indeed, the electrical forces can act both on particles and on the suspending fluid. In spatially non-uniform ac electric fields, dielectric particles move as a consequence of the interaction of the dipole induced in the particle and the applied field gradient. This movement was termed dielectrophoresis (DEP) by Pohl [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 (CNT) and biological particles such as viruses, DNA, bacteria and cells of various kinds [3], [4].

The aim of the present paper is to analyze dielectrophoresis, in order to reveal their potential for novel applications in the field of nanoparticles manipulation.

2. Theoretical background

Motion of particles suspended in a fluid is due to electrophoresis and dielectrophoresis phenomena. Electrophoresis occurs due to the action of the electric field on charged particles, while dielectrophoresis involves polarized bodies only (Fig. 1).

The utilization of the difference between dielectrophoretic forces exerted on different particles in nonuniform electric fields is known as DEP separation. DEP migration uses DEP forces that exert opposite signs of force on different particle types to attract some of the particles and repel others [1]. DEP retention uses the balance between DEP and fluid-flow forces. Particles experiencing repulsive and weak attractive DEP forces are eluted by fluid flow, whereas particles experiencing strong attractive DEP forces are trapped at electrode edges against flow drag [4].

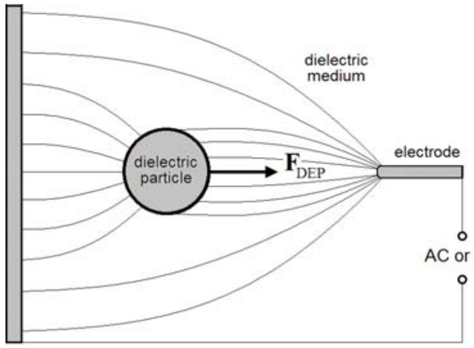


Fig. 1. Electrically neutral particle in the presence of a spatially non-uniform electric-field. The dipole moment induced within the particle results in a translational force and the dielectric spherical particle undergoes a DEP motion.

The total force on a polarizable particle in a nonuniform AC field can be written as the sum of a number of independently acting forces [3], [5], [7], as in Figure 2:

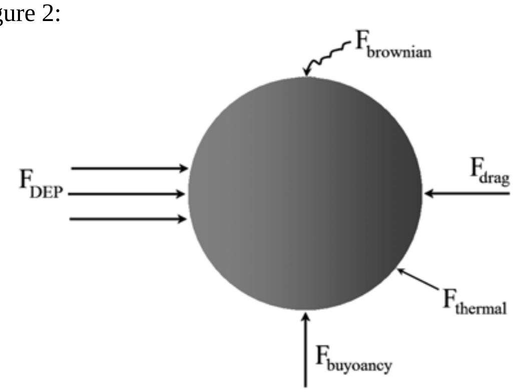


Fig. 2. Forces exerted on a particle moving in fluid, under the influence of dielectrophoresis

$$\mathbf{F} = \mathbf{F}_{DEP} + \mathbf{F}_{\text{drag}} + \mathbf{F}_{\text{buyoancy}} + \mathbf{F}_{\text{thermal}} + \mathbf{F}_{\text{brownian}} \quad (1)$$

Where: $\mathbf{F}_{DEP}$ is the dielectrophoretic force, $\mathbf{F}_{\text{drag}}$ is the hydrodynamic drag force, $\mathbf{F}_{\text{thermal}}$ the thermal force and $\mathbf{F}_{\text{brownian}}$ is the force due to the brownian motion of the particles. The dielectrophoretic force can be written as:

$$\mathbf{F}_{DEP} = (\tilde{\mathbf{p}} \cdot \nabla)\tilde{\mathbf{E}} \quad (2)$$

where $\tilde{\mathbf{E}} = -\nabla\tilde{V} = -\nabla(V_R + jV_I)$ is the electric field, $\tilde{\mathbf{p}}(\omega)$ is the induced dipole moment of the particle, V_R, V_I are the real and imaginary part of the electrical potential, respectively. For a homogeneous dielectric sphere, the induced dipole moment is given by:

$$\tilde{\mathbf{p}}(\omega) = 4\pi a^3 \varepsilon_m k(\omega)\tilde{\mathbf{E}} \quad (3)$$

where ω is the angular field frequency, a the particle radius and $k(\omega)$ the Clausius–Mossotti factor given by [6], [7]:

$$k(\omega) = \frac{\tilde{\varepsilon}_p - \tilde{\varepsilon}_m}{\tilde{\varepsilon}_p + 2\tilde{\varepsilon}_m} \quad (4)$$

where $\tilde{\varepsilon}_p$ and $\tilde{\varepsilon}_m$ are the absolute complex permittivity of the particle and the medium respectively. The complex permittivity is $\tilde{\varepsilon} = \varepsilon - j\sigma/\omega$ where $j = (-1)^{1/2}$, ε is the permittivity and σ the conductivity of the dielectric. The time averaged DEP force is found by substituting equation (4) into (3) and is given by:

$$\langle \mathbf{F}_{DEP} \rangle = 2\pi a^3 \varepsilon_m \operatorname{Re}\{k(\omega)\}\nabla|\mathbf{E}_{rms}|^2 = 2\pi a^3 \varepsilon_m \operatorname{Re}\{k(\omega)\}\nabla\left(|\nabla V_R|^2 + |\nabla V_I|^2\right) \quad (5)$$

where Re{} indicates the real part of the equation (2) and $\nabla|\mathbf{E}_{rms}|^2$ is the gradient of the square of the rms (root mean square) electric field.

The Clausius–Mossotti factor determines the direction of the dielectrophoretic force. When the sign of Re$\{k\}$ is positive, the particle is more polarizable than its surrounding medium and it undergoes what is known as positive dielectrophoresis (pDEP), the force vector being directed along the gradient of electric field. In this case, the net movement of particles is oriented towards regions of highest field strength, whereas particles with polarizability less than that of the medium move towards the region of lowest field gradient. The last situation occurswhen Re$\{k\}$ is negative, the phenomenon being known as negative dielectrophoresis (nDEP). Because the particle's polarization is frequency dependent, the net force is also frequency dependent. Dielectrophoresis techniques work for both AC and DC excitations of the electric field. By substituting the complex permittivity in equation (4), the high and low frequency limits for Re$\{k\}$ are found to be [3], [7]:

$$\lim_{\omega\to 0} \operatorname{Re}\{k\} = \frac{\sigma_p - \sigma_m}{\sigma_p + 2\sigma_m} \quad (6)$$

$$\lim_{\omega\to \infty} \operatorname{Re}\{k\} = \frac{\varepsilon_p - \varepsilon_m}{\varepsilon_p + 2\varepsilon_m} \quad (7)$$

Equations (6) and (7) show that the relative differences in ohmic losses dominates the low frequency behavior of, while dielectric polarization effects are more significant at high frequencies. For particles whose polarisability is greater than the medium the net movement is to regions of highest field strength, whereas particles whose polarisability is less than the medium move to the region of lowest field gradient. Because the particle's polarization is frequency dependent, the net force is also frequency dependent. A disadvantage to use of DEP is that the DEP forces are inherently transient and disappear when the field is removed.

3. Numerical results

The proposed model 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 two important aspects of the dielectrophoresis: first we investigated the dielectrophoretic force for an interdigitated electrode array, as in Figure 3 [7], and then we computed the particles trajectories for a typical system for experiments. All the numerical simulations were performed using a finite element code, FreeFEM [8].

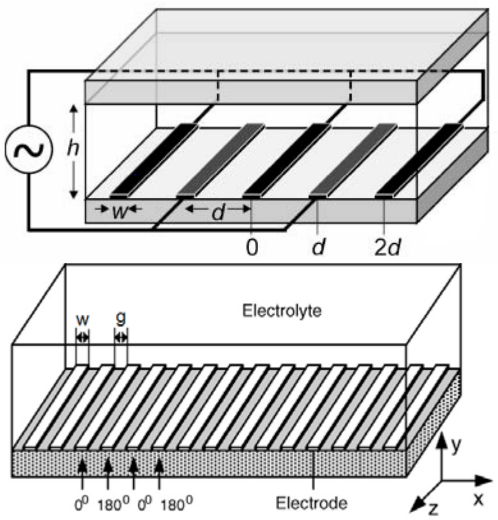


Fig. 3. Schematic of the DEP patterning chamber with interdigitated bar electrodes at bottom surface with 2-phases.

For the computation of the dielectrophoretic force we solved the Laplace equation 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 considered to be two dimensional. The computational domain and the boundary conditions can be assumed as shown in Fig. 4 [3], [7].

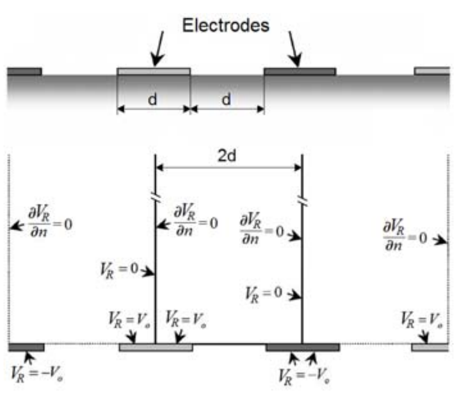


Fig. 4. Boundary conditions for the real part of electric potential in the DEP.

The vertical lines mark the period over which the system repeats. Also shown are the values for the potential on each electrode. The solid lines indicate this unit cell with a line of even symmetry on the left and even symmetry on the right and the single half-electrode required. The dotted lines indicate the images of the unit cell demonstrating that the problem is completely described.

In order to avoid extreme numbers in numerical calculations, the variables are usually scaled according to typical values. In this paper, the potential is scaled with V_0, the amplitude of the applied signals, and the distances are scaled with d, the distance between the center of the electrode and the center of the adjacent gap. In terms of dimensionless variables $V'_R=V_R/V_0$, $V'_I=V_I/V_0$ and $\mathbf{x'}=\mathbf{x}/d$, the time-averaged DEP force becomes:

$$\langle \mathbf{F}_{DEP} \rangle = \left[2\pi a^3 \varepsilon_m \operatorname{Re}\{k(\omega)\} \frac{V_0^2}{d^3} \right] \nabla' \left(\left| \nabla' V'_R \right|^2 + \left| \nabla' V'_I \right|^2 \right) \tag{8}$$

where the term before the differential operator represents a characteristic force constant, K. The dimensionless DEP force:

$$\langle \mathbf{F}'_{DEP} \rangle = \frac{\langle \mathbf{F}_{DEP} \rangle}{K} = \nabla' \left(\left| \nabla' V'_R \right|^2 + \left| \nabla' V'_I \right|^2 \right) \tag{9}$$

is obtained by solving the dimensionless Laplace equations for the real and the imaginary components of the electric potential together with the associated boundary conditions. The simplified boundary conditions require the height h of the solution space is required to be much greater than d and was set to 10 in dimensionless units.

The results obtained for the magnitudes of the dimensionless vector $\nabla'\left(\left|\nabla' V'_R\right|^2 + \left|\nabla' V'_I\right|^2\right)$ of the dimensionless DEP force given by Equation 9 in a 1x1 region are presented in Fig. 5.

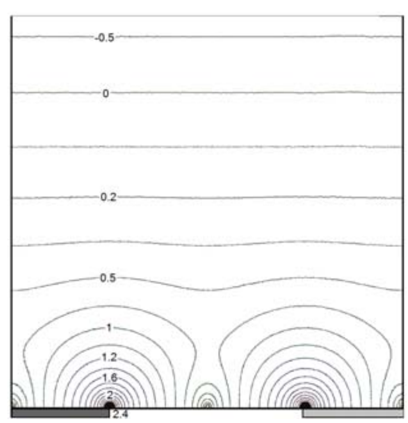
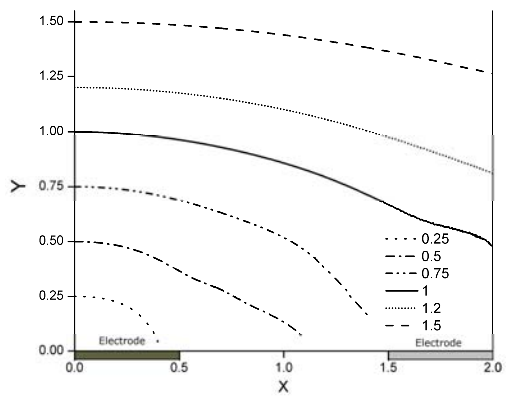


Fig. 5. Calculated values for the magnitudes of dimensionless vector $\nabla'\left(\left|\nabla' V'_R\right|^2 + \left|\nabla' V'_I\right|^2\right)$ of dimensionless DEP force (logarithmic scale).

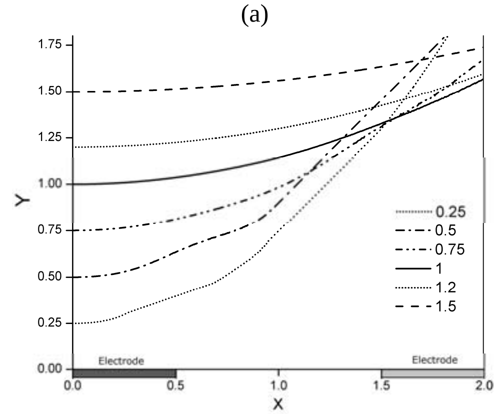
A more refined study of the behavior of the suspension subject to DEP forces is provided by the analysis of particles trajectories. The dimensionless movement equation:

$$\mathbf{x}' = \mathbf{x}'_0 + \mathbf{v}'_0\, t' + \frac{1}{2}\mathbf{a}'\, t'^2 , \qquad (10)$$

where the time is nondimensionalized by defining a time constant in order to obtain $\mathbf{a}' = \langle \mathbf{F}'_{DEP} \rangle$, is solved for different initial positions (x'_0, y'_0) of particles, with a constant time step $t'=10^{-3}$.
The computed trajectories for particles entering the computational domain at $x'_0=0$ and different values of y'_0 (0.5, 0.75, 1, 1.2) in the case of positive and negative DEP are shown in as in Figures 6, (a) and (b):



(a)



(b)

Fig. 6. Calculated values of particles trajectories in case of positive DEP (a) and negative DEP (b).

The initial velocity of the particle is considered parallel to the electrodes and equal to unity. The trajectories are strongly influenced by the DEP force in the vicinity of the electrode.

When the distance particle-electrode is large, the influence of the DEP force is very week. For particles entering in the domain at $y'_0>3$, there is practically no effect of the DEP force, so is important to use very thin devices in order to control the trajectories using electric field. The analysis of the effects device's geometry (height, distance between electrodes, and shape of electrodes) could lead to the improvement of the separation process.

6. Conclusions

The paper presents a set of numerical results obtained for the description of the particle behavior in a two-phase system under the action of DEP.

Numerical computations deals with two important aspects of DEP: dielectrophoretic force for an interdigitated electrode array and computation of the particles' trajectories for a planar electrode array configuration, in a typical system for experiments on positive and negative DEP.

The results clearly show the repulsive and respectively attractive effects of the dielectrophoretic force on the suspension’s concentration distribution. By adjusting the applied voltage at the command electrodes, a mixture of nanoparticles of different sizes can be continuously separated and different collected.

DEP seems to be a promising technique for nanoparticles separation, function of their physical properties (nature, dimensions).

References

[1] S. Shklyaev, A. V. Straube, New Journal of Physics **10**, 063030 (2008).
[2] Herbert A. Pohl H.A., Dielectrophoresis, Cambridge University Press, Cambridge, UK, (1978).
[3] N. G. Green, A. Ramos, H. Morgan, Journal of Electrostatics **56**, 235 (2002).
[4] N. G. Green, H. Morgan, J. Phys. D: Appl. Phys. **31** (1998).
[5] A. Castellanos, A. Ramos, N. Gonzales, N.G. Green, H. Morgan, J. Phys. D: Appl. Phys., Vol. 36, (2003).
[6] M.P. Hughes, AC electrokinetics: applications for nanotechnology, Nanotechnology, Vol. 11, (2000).
[7] M. Lungu, A. Neculae, M. Bunoiu, Proceeding of the Physics Conference TIM-08 AIP 1131164-168, pag. 164-168, (2009).
[8] www.freefem.org