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Forces acting on multilayer dielectric particle in DC dielectrophoresis

***Abstract**. Dielectrophoresis has become a common method in biotechnology and other areas civil engineering for a wide range of applications dealing with sorting of single cells, centrifugation-free exposure of cells to different media or candidate drugs, accumulation of bacteria and viruses for improved detection, transient contact formation between two cells for signal transduction experiments and controlled fusion after individual characterization of two cells. In this publication numerical method of computation of force acting on multilayer particle is given.*

Streszczenie.** Dielektroforeza staje się powszechną metodą sortowania cząstek dielektrycznych takich jak, komórki, bakterie czy wirusy, w biotechnologii oraz innych dziedzinach. W publikacji tej została podana numeryczna metoda obliczania siły, jak działa na cząstkę o dowolnym kształcie oraz dowolnej budowie wewnętrznej składającej się z wielu warstw dielektrycznych o zadanych parametrach. **(Siły oddziaływania na cząsteczki o budowie warstwowej w dielektroforezie stałoprądowej)

Keywords: *dielectrophoresis, finite element method, multilayer particles.*
Słowa kluczowe: *dielektroforeza, metoda elementów skończonych, cząsteczki wielowarstwowe.*

Introduction

Dielectrophoresis phenomenon (DEP) arises from the interaction between a polarized dielectric particle and a non-uniform constant or alternating electric field [1]. The non-uniformity of the electric field in dielectric fluid originates from the static field spatial variation (DC-DEP), the sinusoidal time variation (AC-DEP), or the by the coupling time with space what gives as electro-rotation or travelling-wave DEP. Because the electric field can be scaled down to microscale, a highly non-uniform electric field can be generated at relatively lower voltages. The induced by external field charge separation inside the dielectric particle or at the interface between the particle and the suspending fluid produces unbalanced Coulombic force, which influences the dynamic behaviour of the particles by forcing translational motion or spatial reorientation. With the rapid development of lab-on-a-chip technologies in the recent decades, dielectrophoresis has been extensively applied for on-chip manipulation of artificial or biological particles.

The underlying mechanism of dielectrophoresis was described by Pohl [1] as a process where an external electric field induces a dipole moment or higher electric moments in any object that differs in permitivity from the medium that surrounds it. These induced moments interact with the generating electric field, resulting in either an attractive force towards regions of high electric field strength or a repulsive force .

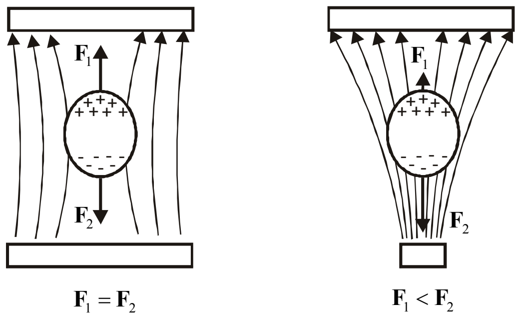

Fig. 1. Forces acting on electrically neutral particle. Polarized particle in uniform field (left) and in inhomogeneous field (right).

The study of the response of polarisable particles, particularly biological cells, to electric fields has gained considerable attention in recent years, because of several important reasons. First, different applications of modern technology in electronic, food, pharmaceutical or metallurgical industries, involve the electric processing of particles. In particular, the introduction of microelectrode technology has facilitated the development of sophisticated methods for manipulating, trapping and separating bio-particles, from bacteria to viruses and ma-cromolecules such as nucleic acids and proteins.

In praxis knowledge of mechanism for the micro-fluidic transport and separation of small biological samples such as cells, proteins, and DNA is very important.

For practical problems interdigitated electrodes are commonly used to generate the non-uniform electric fields. This field induces dipole moment and next the force resulting from this is the cause of particle movement. Among other factors, the magnitude of the dielectropho-retic force depends upon the gradient of the square of the magnitude of electric field that is generated by such electrodes.

In comparison to electrophoresis, by which we understand particle motion due to the force resulting from coupling between an applied external electric field and a charge particle, dielectrophoresis has the disadvantage that the polarization forces acting on polarized particle are quite weak. In general, efficient particle manipulation in microelectrode arrangement requires taken into account other factors, such as viscous, buoyancy, and electrohydrodynamic forces. This constitutes complicated system of mathematically coupled different physical fields, which results in mutually coupled system partial differential equations. From practical point of view only numerical methods can give from practical point of view satisfactory results.

This paper presents results of the numerical solution of the potential, electric field and the DEP force in the dielectrophoretic electrode arrays using the finite element method. The force equations are re-written to obtain expressions for the force in terms of the real and imaginary components of the field phasor. This approach permits the solution of the time-averaged DEP force in a single step.

Main equations

Let us consider electric dipole consisting of two charges of equal values q placed in distance d. If in unit volume we have such dipoles with number density N, then the polarization force density is

$$\mathbf{f} = N\mathbf{f}_d = N\left(\mathbf{p}\cdot\nabla\right)\mathbf{E}\left(\mathbf{r}\right) = \left(\mathbf{P}\cdot\nabla\right)\mathbf{E}\left(\mathbf{r}\right) \tag{1}$$

Let us now place a sphere in external AC electric field. Starting with Maxwell's equation

(2) $$\nabla \times \mathbf{H} = \mathbf{J} + \frac{\partial \mathbf{D}}{\partial t}$$

taking divergence of both side we get

(3) $$\nabla \cdot \left(\mathbf{J} + \frac{\partial \mathbf{D}}{\partial t} \right) = 0$$

But $\mathbf{J} = \sigma \mathbf{E} = -\sigma \nabla V$ and $\mathbf{D} = \varepsilon\, \mathbf{E} = -\varepsilon \nabla V$, so

(4) $$\nabla \cdot \left(\sigma \nabla V \right) + \nabla \cdot \left(\varepsilon \nabla \frac{\partial V}{\partial t} \right) = 0$$

Let us now define

(5) $$V(\mathbf{r},t) = \mathrm{Re}\left[V_m e^{j(\omega t + \varphi)} \right] = \sqrt{2}\, \mathrm{Re}\left[\hat{V} e^{j\omega t} \right]$$

where phasor $\hat{V}$ depends from spatial coordinates and is given by

(6) $$\hat{V}(\mathbf{r}) = \frac{V_m(\mathbf{r})}{\sqrt{2}} e^{j\varphi}$$

Substituting (6) into (4)we get

(7) $$\sqrt{2}\, \mathrm{Re}\left[\nabla \cdot \left(\sigma \nabla \hat{V} \right) e^{j\omega t} \right] + \sqrt{2}\, \mathrm{Re}\left[\nabla \cdot \left(j\omega\varepsilon \nabla \hat{V} \right) e^{j\omega t} \right] = 0$$

There exists lemma, which says, that if

(8) $$\mathrm{Re}\left[\hat{A} e^{j\omega t} \right] = \mathrm{Re}\left[\hat{B} e^{j\omega t} \right]$$

for all t, then $\hat{A} = \hat{B}$. It can be readily shown this by first taking $t = 0$, obtaining $\mathrm{Re}\left[\hat{A} \right] = \mathrm{Re}\left[\hat{B} \right]$, and then taking $\omega t = \pi/2$, giving $\mathrm{Im}\left[\hat{A} \right] = \mathrm{Im}\left[\hat{B} \right]$. Thus, $\hat{A} = \hat{B}$. Using this lemma we have

(9) $$\nabla \cdot \left(\sigma \nabla \hat{V} \right) + \nabla \cdot \left(j\omega\varepsilon \nabla \hat{V} \right) = 0$$

Assuming that conductivity σ and permittivity ε do not depend from spatial coordinates we get

(10) $$\nabla^2 \hat{V} = 0$$

Let us now consider a sphere of radius r_0 with permittivity ε_2, placed within a medium of permittivity ε_1. Both medium and sphere are nonconducting. A uniform DC electric field $\mathbf{E} = E_0\mathbf{e}_z$ is applied at infinity along the positive z-axis. Because of symmetry in spherical coordinates, Laplace's equation is

(11) $$\nabla^2 V = 0$$

(12) $$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial V}{\partial r} \right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial V}{\partial \theta} \right) = 0$$

Solution to this equation can be found as

(13) $$V_1(r,\theta) = \left(A_1 r + \frac{B_1}{r^2} \right)\cos\theta + \sum_{n=2}^{\infty} \frac{B_n}{r^{n+1}} P_n(\cos\theta)$$

(14) $$V_2(r,\theta) = C_0 + C_1 r\cos\theta + \sum_{n=2}^{\infty} C_n r^n P_n(\cos\theta)$$

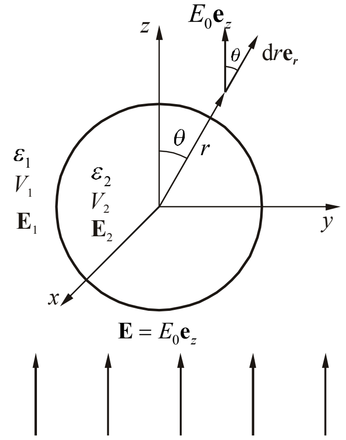

Fig. 1. Torque and force acting on single dipole.

On the boundary $r = r_0$, following boundary conditions has to be fulfilled:
– for tangential component of electric field strength

(15) $$\mathbf{E}_1 \times \mathbf{n} = \mathbf{E}_2 \times \mathbf{n}$$

– for normal component of electric flux density (displacement vector)

(16) $$\mathbf{D}_1 \cdot \mathbf{n} = \mathbf{D}_2 \cdot \mathbf{n}$$

It can be shown using above boundary conditions that relations (12) and (12) can be fulfilled if $B_n = 0$ and $C_n = 0$ for all $n > 1$. The only equations which rest are for $n = 1$

(17) $$\begin{cases} -E_0 r_0 + \dfrac{B_1}{r_0^2} = C_1 r_0 \\ \varepsilon_1\left(-E_0 - \dfrac{2B_1}{r_0^3} \right) = \varepsilon_2 C_1 \end{cases}$$

Solution of the above set of equations gives

(18) $$B_1 = \frac{(\varepsilon_2 - \varepsilon_1) r_0^3}{\varepsilon_2 + 2\varepsilon_1} E_0 \quad \text{and} \quad C_1 = -\frac{3\varepsilon_1}{\varepsilon_2 + 2\varepsilon_1} E_0$$

In this way we have solutions for potentials in dielectric fluid and in particle itself

(19) $$V_1(r,\theta) = \left(\frac{(\varepsilon_2 - \varepsilon_1)}{\varepsilon_2 + 2\varepsilon_1}\frac{r_0^3}{r^2} - r \right) E_0 \cos\theta$$

(20) $$V_2(r,\theta) = -\frac{3\varepsilon_1}{\varepsilon_2 + 2\varepsilon_1} E_0 r \cos\theta$$

Comparison this value with potential from electric dipole

(21) $$\mathbf{p} = 4\pi\varepsilon_1 \frac{(\varepsilon_2 - \varepsilon_1)}{\varepsilon_2 + 2\varepsilon_1} r_0^3 \mathbf{E}_0$$

The above equation (10) is the same as (11), so the solution defined by (17) is also the same, with exception that all coefficient are now complex. Boundary conditions for this complex case are

(22) $$\left(\mathbf{J}_1 - \mathbf{J}_2 \right) \cdot \mathbf{n}_{12} = -\frac{\partial \rho_s}{\partial t}$$

(23) $$\left(\mathbf{D}_1 - \mathbf{D}_2 \right) \cdot \mathbf{n}_{12} = \rho_s$$

where $\mathbf{n}_{12}$ is a unit vector pointing from region 1 to region 2 and in our case is equal $\mathbf{e}_r$. Taking into account that

(24) $\mathbf{J} = \sigma\mathbf{E} = -\sigma\nabla V \qquad \mathbf{D} = \varepsilon\mathbf{E} = -\varepsilon\nabla V$

and after transformation these relations to complex domain

(25) $$-\sigma_1\frac{\partial\hat{V}_1}{\partial r} + \sigma_2\frac{\partial\hat{V}_2}{\partial r} = -j\omega\left(-\varepsilon_1\frac{\partial\hat{V}_1}{\partial r} + \varepsilon_2\frac{\partial\hat{V}_2}{\partial r}\right)$$

or

(26) $$\hat{\varepsilon}_1 = \varepsilon_1 - j\frac{\sigma_1}{\omega} \qquad \hat{\varepsilon}_2 = \varepsilon_2 - j\frac{\sigma_2}{\omega}$$

boundary condition have the same form as in direct current case, but with complex coefficients

(27) $$\hat{\varepsilon}_1\frac{\partial\hat{V}_1}{\partial r} = \hat{\varepsilon}_2\frac{\partial\hat{V}_2}{\partial r}$$

so the dipole moment has now the value

(28) $$\hat{\mathbf{p}} = 4\pi\varepsilon_1\hat{K}\left(\hat{\varepsilon}_1,\hat{\varepsilon}_2\right)r_0^3\hat{\mathbf{E}}_0$$

where $\hat{K}\left(\hat{\varepsilon}_1,\hat{\varepsilon}_2\right)$ is the well known Clausius-Mossotti complex factor defined as

(29) $$\hat{K}\left(\hat{\varepsilon}_1,\hat{\varepsilon}_2\right) = \frac{\left(\hat{\varepsilon}_2 - \hat{\varepsilon}_1\right)}{\hat{\varepsilon}_2 + 2\hat{\varepsilon}_1}$$

Surface charge density is given by

(30) $$\sigma_{pol} = 3\varepsilon_0\frac{\varepsilon_2 - \varepsilon_1}{\varepsilon_2 + 2\varepsilon_1}E_0\cos\theta$$

In the case of two-layer particle this equation can be modified by substitution particle permeability ε_2 by an expression

(31) $$\hat{\varepsilon}_2' = \hat{\varepsilon}_2\frac{\left(\frac{r_1}{r_2}\right)^3 + 2\left(\frac{\hat{\varepsilon}_3 - \hat{\varepsilon}_2}{\hat{\varepsilon}_3 + \hat{\varepsilon}_2}\right)}{\left(\frac{r_1}{r_2}\right)^3 - \left(\frac{\hat{\varepsilon}_3 - \hat{\varepsilon}_2}{\hat{\varepsilon}_3 + \hat{\varepsilon}_2}\right)}$$

where r_1 and r_2 are outer and inner radius of the dielectric layers and ε_2 and ε_3 are inner and outer permittivity of the layers as in fig.2.

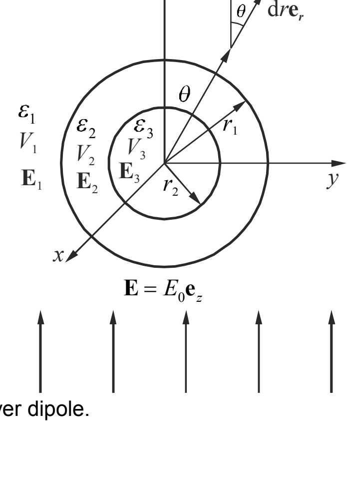

Fig. 2. Two-layer dipole.

Complex domain force calculation in AC steady state electrical field

Let us calculate the mean value of force acting on particle when all fields are sinusoidal in steady state. The force in time domain is given by

(32) $$\mathbf{f}(t) = \left(\mathbf{p}(t)\cdot\nabla\right)\mathbf{E}(t)$$

where electric dipole moment can be written in complex form as

(33) $$\mathbf{p}(t) = \mathbf{P}_{\mathrm{m}}\cos(\omega t + \varphi) = \frac{1}{2}\left(\hat{\mathbf{P}}_{\mathrm{m}}e^{j\omega t} + \hat{\mathbf{P}}_{\mathrm{m}}^{*}e^{-j\omega t}\right)$$

also

(34) $$\mathbf{E}(t) = \frac{1}{2}\left(\hat{\mathbf{E}}_{\mathrm{m}}e^{j\omega t} + \hat{\mathbf{E}}_{\mathrm{m}}^{*}e^{-j\omega t}\right)$$

Thus, force acting on particle in time domain has the value

(35) $$\mathbf{f}(t) = \frac{1}{4}\Big(\left(\hat{\mathbf{P}}_{\mathrm{m}}\cdot\nabla\right)\hat{\mathbf{E}}_{\mathrm{m}}e^{2j\omega t} + \left(\hat{\mathbf{P}}_{\mathrm{m}}^{*}\cdot\nabla\right)\hat{\mathbf{E}}_{\mathrm{m}} + \left(\hat{\mathbf{P}}_{\mathrm{m}}\cdot\nabla\right)\hat{\mathbf{E}}_{\mathrm{m}}^{*} + \left(\hat{\mathbf{P}}_{\mathrm{m}}^{*}\cdot\nabla\right)\hat{\mathbf{E}}_{\mathrm{m}}^{*}e^{-2j\omega t}\Big)$$

where $\hat{\mathbf{P}}_{\mathrm{m}}$ and $\hat{\mathbf{E}}_{\mathrm{m}}^{*}$ are complex amplitudes of electric dipole moment and electric field, respectively.

Integrating the first and last term over one time period T we get zero value. The mean square value of this expression has the form

(36) $$\left\langle\mathbf{f}(t)\right\rangle = \frac{1}{2}\mathrm{Re}\left[\left(\hat{\mathbf{P}}_{\mathrm{m}}\cdot\nabla\right)\hat{\mathbf{E}}_{\mathrm{m}}^{*}\right] = \frac{1}{2}\mathrm{Re}\left[\left(\hat{\mathbf{P}}_{\mathrm{m}}^{*}\cdot\nabla\right)\hat{\mathbf{E}}_{\mathrm{m}}\right]$$

Let us now calculate the value in brackets

(37) $$(\hat{\mathbf{p}}\cdot\nabla)\hat{\mathbf{E}}^{*} = 4\pi\varepsilon_1 r_0^3\left[\left(K_{\mathrm{R}} + jK_{\mathrm{I}}\right)\left(\mathbf{E}_{\mathrm{R}} + j\mathbf{E}_{\mathrm{I}}\right)\cdot\nabla\right]\cdot \cdot\left(\mathbf{E}_{\mathrm{R}} + j\mathbf{E}_{\mathrm{I}}\right)^{*}$$

After some manipulations it can be shown that in complex domain the force acting on particle is given by

(38) $$\left\langle\mathbf{f}\left(t\right)\right\rangle = 2\pi\varepsilon_1 r_0^3\left\{K_{\mathrm{R}}\nabla\left|\hat{\mathbf{E}}\right|^2 + 2K_{\mathrm{I}}\left[\nabla\times\left(\mathbf{E}_{\mathrm{I}}\times\mathbf{E}_{\mathrm{R}}\right)\right]\right\}$$

where K_{R} and K_{I} are real and imaginary parts of Clausius-Mossotti complex factor and E_{R} and E_{I} are real and imaginary parts of electric field strength.
This can be further transform to the end form as

(39) $$\left\langle\mathbf{f}\left(t\right)\right\rangle = 2\pi\varepsilon_1 r_0^3\Big[K_{\mathrm{R}}\nabla\left(E_{\mathrm{rms}}\right)^2 + +2K_{\mathrm{I}}\left(\left(E_{x,\mathrm{rms}}\right)^2\nabla\varphi_x + \left(E_{y,\mathrm{rms}}\right)^2\nabla\varphi_y + \left(E_{z,\mathrm{rms}}\right)^2\nabla\varphi_z\right)\Big]$$

where E_{rms} is the root mean square amplitude of the total electric field strength $\mathbf{E}(t)$ and, for example, $E_{x,\mathrm{rms}}$ is the root mean square amplitude of the x component of the $\mathbf{E}(t)$.

Computational results

The finite element calculations was done for following geometrical dimensions: A–B = 60 μm, A–C = 160 μm, *a* = 40 μm, *b* = 40 μm, *h* = 4 μm. Spherical dielectric particle has radius *r* = 4 μm and relative permittivity ε_2 = 80. The fluid, where particle moves has permittivity ε_1 = 4. First electric potential φ was calculated and next electric field strength $\mathbf{E}$ (Fig.2).

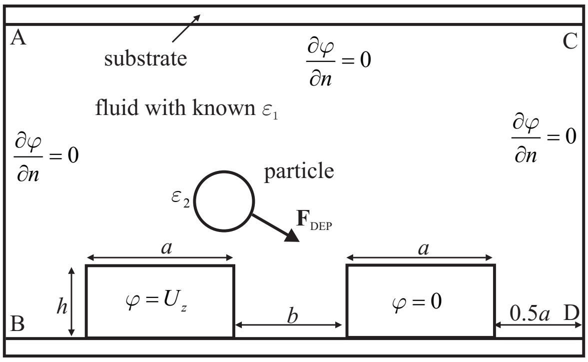

Fig.3. Cross section of the electrode arrangement with one pair of electrodes and moving biological particle is depicted.

The simulated chamber is modeled as a two-dimensional model, where we need to consider only a single pair of electrodes, one with positive $Uz = 4$ V and one with zero voltage. The extension of the interdigitated electrode array beyond the considered region can be simulated by applying periodic boundary conditions to the left and right of the problem boundary model.

Boundary conditions on the computational problem boundary are Neuman's or Dirichlet's type. On the bottom and top insulating substrate current cannot flow into this boundary, so Neuman's conditions here apply. Periodic boundary conditions are present on the left and right sides A-B and C-D of the model boundary to simulate the presence of neighboring electrodes. It is assumed that all computational cells are of the same type. Using typical fabrication procedures, the thickness of the deposited metal that forms the interdigitated electrodes is in most cases less than 1μm.

The main purpose of this article is to give general method of computation forces acting on multilayer particles of any shape. As test problem two-dimensional and two-layer particle is considered. For spherical dielectric particle has radius $r_1 = 4$ μm and $r_2 = 3$ μm and relative permittivities $\varepsilon_2 = 40$ and $\varepsilon_3 = 80$ placed in vacuum the force have the value

(40) $$\mathbf{F}_{DEP} = \left(0.26\mathbf{a}_x - 0.82\mathbf{a}_y\right)\left[\mu\text{N/m}\right]$$

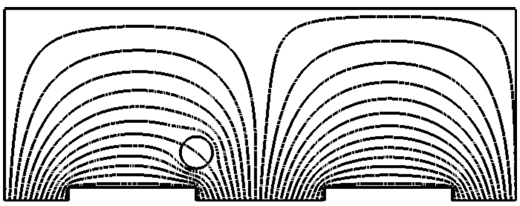

Fig.4. Equipotential lines in dielectric fluid.

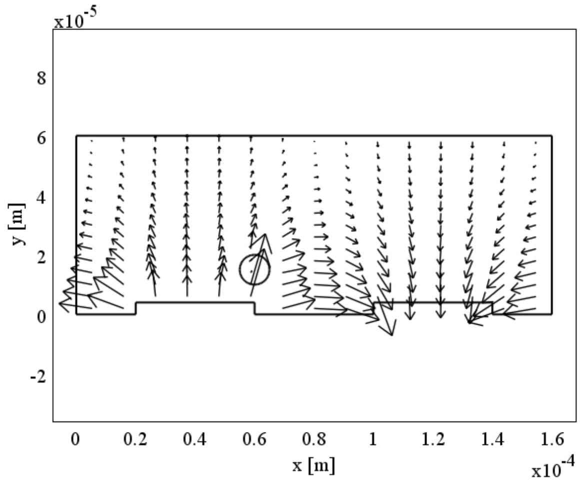

Fig. 5. Current density vector. in arrow form.

Summary

In this article computation of dielectrophoretic force acting on dielectric particle immersed in dielectric fluid and utilizing finite element method is presented. It was shown how to compute dependence of the $\mathbf{F}_{DEP}$ from fluid and particle permittivitis and particle dimensions.

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