

Comparison of different force calculation methods in DC dielectrophoresis

Abstract In this paper two-dimensional dielectrophoresis is described. First electric field distribution in particle and surrounding fluid is calculated and next stresses acting from both sides suspension-particle boundary are calculated. These values are fundamental for force calculation in two-dimensional dielectrophoresis and in simulation velocity distribution in interdigitated electrodes.

Streszczenie. W tej publikacji omówiono zjawisko dielektroforezy w dwóch wymiarach. Najpierw odpowiednie równania pola zostaną analitycznie rozwiązane, a następnie zostaną wyprowadzone wzory na wartość tensora naprężeń Maxwella działającego na obie strony cząsteczki. Wielkości te mają podstawowe znaczenie w obliczaniu sił i momentów działających na cząsteczkę oraz na wyznaczanie rozkładu prędkości w urządzeniach do separacji cząstek. (Porównanie różnych metod obliczania sił w DC dielektroforezie)

Keywords: dielectrophoresis, Maxwell stress tensor calculation

Słowa kluczowe: dielektroforeza, tensor naprężeń Maxwella.

Introduction

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. Based on the measurement of electric and dielectric properties, a further study of selective segregation and purposeful manipulation of micro- or nanostructures of living organisms can be achieved.

The phenomenon of dielectrophoresis (DEP) was first defined by Pohl [1] as the motion of neutral but polarizable particles subjected to nonuniform electric fields. DEP provides an increased measurement precision and sensitivity in the detection of cells with different dielectric properties, without any need for labeling them. Two different methods electric force computation in dielectrophoresis is presented. The first is based on equivalent dipole method, which is easy to use, but in some situations not accurate [2, 3]. The second one is based on Maxwell stress tensor and gives in all possible situations accurate results, but is much more cumbersome in implementation.

All materials from electrical point of view is composed of positive and negative charges which experience an electrostatic force when is placed in an electric field. In a uniform electric field, electrically neutral particles experience a dielectric polarization, but no net force. In a nonuniform electric field, however, forces acting on polarized charges are not balanced, and a motion called dielectrophoresis (DEP) occurs. There are actually two types of dielectrophoresis involving particles suspended in a medium: positive DEP – where the particles move toward the region of stronger electric field, and negative DEP – where the fluid surrounding the particles experience a stronger attractive force than the particles, which causes the suspended particles to be pushed toward the area of weaker electric field

There are many reasons for studying a behavior of particles and fluid globules immersed fluid suspension and placed in electric fields. Among different the chemical engi-

neering applications [2] are the determination of forces acting on droplets exiting electrospray nozzles, the enhancement of heat and mass transfer in emulsions by the imposition of electric fields [3], electrically driven separation of particles techniques [4], dielectrophoretic and electrorotational manipulation of living and death cells [5], and the control of electrorheological fluids [6].

Despite this growing importance of dielectrophoresis is, little attention has been paid to the theoretical and analysis. Although dielectrophoresis is only possible in strong divergent electric fields, theoretical analyses are usually based on equations derived from uniform field behavior. The calculation of DEP force acting on particle has been reported as a difficult task unless in many cases simplifying assumptions and very simple geometries are considered [8] and is usually based on the dipole approximation first introduced by Pohl [1]

The Finite Element Method (FEM) is useful method for analyzing electromagnetic fields in devices, because these can model complicated geometries and non-linear electric properties with relatively short computing time. In spite of these advantages, in many papers have been proved that obtaining an accurate force or torque from FEM computation can be inaccurate, particularly when geometry is enough complex, such as in the case of dielectrophoretic traps with multiple particles. Unfortunately, force and torque calculations are influenced by the approximate nature of the discretisation used in FEM meshes. In the Maxwell's stress method of calculating the force and torque the stress distribution occurs from meshes used for field solution.

In the Maxwell's Stress Tensor (MST) method, it is suggested that the total force acting can be calculated by surrounding a given object by closed surface around the field sources and integrating the MST over the whole surface. The use of the standard Maxwell stress approach requires that the integration path or surface should be fully closed, and situated entirely in linear material.

In this publication Maxwell's stress method is used to evaluation of force acting on both sides of dielectric particle immersed in dielectric fluid. Comparative study of computational inaccuracies is considered.

Equivalent dipole method

The simulated chamber is modeled as a two-dimensional model, where we need to consider only a single pair of electrodes, one with positive $U_z = 10$ V and one with zero voltage. The extension of the interdigitated elec-

trode array beyond the considered region can be simulated by applying periodic boundary conditions to the left and right of the problem boundary model. Fig. 1 shows a cross-sectional geometry, which includes the substrate and channel covers, the interdigitated electrodes, and a fluid.

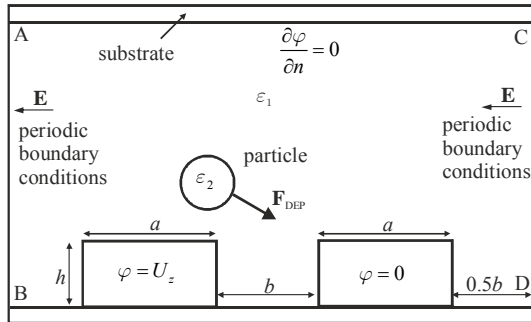


Fig. 1. Computational domain together with geometrical dimensions.

Let us assume that two dimensional cylinder with permittivity ϵ_2 is immersed in external medium with permittivity ϵ_1 . Moreover in the region number one exists uniform electric field with electric field strength E_0 directed perpendicular to z axis and extending from minus to plus infinity. Let V_1 denotes potential in surrounded dielectric with permittivity ϵ_1 and V_2 in the cylinder. Potential outside the cylinder, when $r \rightarrow \infty$, can be calculated along r axis as

$$(1) \quad V_1(r, \phi) = -\int \mathbf{E} \cdot d\mathbf{r} = -\int E_0 \cos \phi dr = -E_0 r \cos \phi$$

The Laplace equation in polar coordinates is given by

$$(2) \quad \frac{1}{r} \frac{\partial}{\partial r} (rV) + \frac{1}{r^2} \frac{\partial^2 V}{\partial \phi^2} = 0$$

If the geometry does not depend on z , we can choose a solution that is a product of functions which only depend on the radius r and angle ϕ

$$(3) \quad V(r, \phi) = R(r)\Phi(\phi)$$

what when introduced in (2) gives

$$(4) \quad \frac{r}{R(r)} \frac{d}{dr} \left(r \frac{dR(r)}{dr} \right) + \frac{1}{\Phi(\phi)} \frac{d^2 \Phi(\phi)}{d\phi^2} = 0$$

This equation can be solved by variable separation method giving as a result

$$(5) \quad V_1(r, \phi) = \left(-r + \frac{r_0^2}{r} \frac{\epsilon_2 - \epsilon_1}{\epsilon_2 + \epsilon_1} \right) E_0 \cos \phi$$

$$(6) \quad V_2(r, \phi) = -r \frac{2\epsilon_1}{\epsilon_2 + \epsilon_1} E_0 \cos \phi$$

where $V_1(r, \phi)$ and $V_2(r, \phi)$ are potentials in surrounding dielectric and in particle, respectively. Potential generated by dielectric cylinder is equal $V_1(r, \phi)$ minus exciting field

$$(7) \quad V_{\text{diel}}(r, \phi) = \frac{r_0^2}{r} \frac{\epsilon_2 - \epsilon_1}{\epsilon_2 + \epsilon_1} E_0 \cos \phi$$

The above equation describes potential distribution generated by single dipole, so dielectric cylinder in external uniform field one can replace by equivalent dipole with electric moment value

$$(8) \quad p = \frac{2\pi r_0^2 \epsilon_1 (\epsilon_2 - \epsilon_1)}{\epsilon_2 + \epsilon_1} E_0$$

The force acting on two-dimensional dipole has the same form as for three-dimensional one. The force acting on two-dimensional dipole is thus given by

$$(9) \quad \mathbf{f}_d = (\mathbf{p} \cdot \nabla) \mathbf{E}(\mathbf{r}) = \frac{\pi r_0^2 \epsilon_1 (\epsilon_2 - \epsilon_1)}{\epsilon_2 + \epsilon_1} \nabla E^2$$

This is the force density which falls on one unit length in z direction. Expression of the ∇E^2 is function of potential V and its derivative

$$(10) \quad E^2 = \left(\frac{\partial V}{\partial x} \right)^2 + \left(\frac{\partial V}{\partial y} \right)^2$$

so after some manipulations we have

$$(11) \quad \nabla E^2 = 2 \left(\frac{\partial V}{\partial x} \frac{\partial^2 V}{\partial x^2} + \frac{\partial V}{\partial y} \frac{\partial^2 V}{\partial x \partial y} \right) \mathbf{a}_x + 2 \left(\frac{\partial V}{\partial x} \frac{\partial^2 V}{\partial y \partial x} + \frac{\partial V}{\partial y} \frac{\partial^2 V}{\partial y^2} \right) \mathbf{a}_y$$

In end effect the components of the force acting on particle have the values:

$$(12) \quad \mathbf{f}_1 = 2C \left[\frac{\partial V}{\partial x} \frac{\partial^2 V}{\partial x^2} + \frac{\partial V}{\partial y} \frac{\partial^2 V}{\partial x \partial y} \right] \mathbf{a}_1$$

$$(13) \quad \mathbf{f}_2 = 2C \left[\frac{\partial V}{\partial x} \frac{\partial^2 V}{\partial x \partial y} + \frac{\partial V}{\partial y} \frac{\partial^2 V}{\partial y^2} \right] \mathbf{a}_2$$

where constant C is given by

$$(14) \quad C = \pi \epsilon_1 \frac{(\epsilon_2 - \epsilon_1)}{\epsilon_2 + \epsilon_1} r_0^2$$

Maxwell stress tensor method

Let us now derive close form of surface force density \mathbf{f} acting on unit area when unit normal vector to the surface is given. Maxwell stress tensor T_{ij} for electric field is given by

$$(15) \quad T_{ij} = \epsilon \left(E_i E_j - \frac{1}{2} E^2 \delta_{ij} \right)$$

The surface force density \mathbf{t} is given by

$$(16) \quad \mathbf{f} = \vec{\mathbf{T}} \cdot \mathbf{n} = \sum_{j=1}^3 \sum_{k=1}^3 \sum_{r=1}^3 T_{jk} n_r \mathbf{a}_j (\mathbf{a}_k \cdot \mathbf{a}_r)$$

In the above equations indexes $i, j, k = 1, 2, 3$ replace, for convenience, coordinates x, y and z . Because

$$(17) \quad \mathbf{E} = \sum_{j=1}^3 E_j \mathbf{a}_j \quad \mathbf{n} = \sum_{j=1}^3 n_j \mathbf{a}_j$$

then

$$(18) \quad \mathbf{f} = \varepsilon \left(\sum_{k=1}^3 E_k n_k \right) \mathbf{E} - \frac{1}{2} \varepsilon E^2 \mathbf{n}$$

The expression in parenthesis is equal to the scalar product \mathbf{E} and \mathbf{n} , thus the surface force density has value

$$(19) \quad \mathbf{f} = \varepsilon (\mathbf{E} \cdot \mathbf{n}) \mathbf{E} - \frac{1}{2} \varepsilon E^2 \mathbf{n}$$

One needs to calculate force densities on both sides of the particle-suspension boundary. Let us assume that suspension has number 1 and particle as number 2. Then equation (19) gives us for both sides of the boundary:

$$(20) \quad \mathbf{f}_1 = \varepsilon_1 (\mathbf{E}_1 \cdot \mathbf{n}_1) \mathbf{E}_1 - \frac{1}{2} \varepsilon_1 E_1^2 \mathbf{n}_1$$

$$(21) \quad \mathbf{f}_2 = \varepsilon_2 (\mathbf{E}_2 \cdot \mathbf{n}_2) \mathbf{E}_2 - \frac{1}{2} \varepsilon_2 E_2^2 \mathbf{n}_2$$

The force is obtained by calculating surface integral around surface charge density induced in the particle by external field. It is assumed that there are not volume induced charges inside particle. Apparently unit normal vectors on both sides of the particle-suspension boundary have opposite sign, so because $\mathbf{n}_1 = \mathbf{n}$ and $\mathbf{n}_2 = -\mathbf{n}$ we have

$$(22) \quad \mathbf{f}^{(2)} = \varepsilon_1 (\mathbf{E}_1 \cdot \mathbf{n}) \mathbf{E}_1 - \varepsilon_2 (\mathbf{E}_2 \cdot \mathbf{n}) \mathbf{E}_2 - \frac{1}{2} (\varepsilon_1 E_1^2 - \varepsilon_2 E_2^2) \mathbf{n}$$

Now, both vectors \mathbf{E}_1 and \mathbf{E}_2 can be resolved into two components: perpendicular and tangential to the boundary.

$$(23) \quad \mathbf{E}_1 = E_{1n} \mathbf{n} + E_{1t} \mathbf{t} \quad \mathbf{E}_2 = E_{2n} \mathbf{n} + E_{2t} \mathbf{t}$$

where \mathbf{n} is a normal and \mathbf{t} tangential vectors to the boundary. Boundary conditions on both side the boundary have following form

$$(24) \quad E_{1t} = E_{2t} \quad \varepsilon_1 E_{1n} = \varepsilon_2 E_{2n}$$

This allows us to eliminate components of electric field in suspension. In this case \mathbf{E}_{1n} .

$$(25) \quad \mathbf{f}^{(2)} = \frac{1}{2} (\varepsilon_2 - \varepsilon_1) \left(\frac{\varepsilon_2}{\varepsilon_1} E_{2n}^2 + E_{2t}^2 \right) \mathbf{n}$$

and total force acting on particle and described by the field obtained in particle and calculated on particle-suspension boundary is given by

$$(26) \quad \mathbf{F}^{(2)} = \frac{1}{2} (\varepsilon_2 - \varepsilon_1) \oint_S \left(\frac{\varepsilon_2}{\varepsilon_1} E_{2n}^2 + E_{2t}^2 \right) \mathbf{n} ds$$

This is the force acting on particle, where under integration sign field in particle is taken into account. This equation one can apply both in two-and three-dimensional problems.

Let us now eliminate in (22) not field in suspension with index 1 but instead field in particle with number 2. The force is obtained by calculating surface integral around surface charge density induced in the particle by external field. The boundary condition gives

$$(27) \quad E_{2n} = \frac{\varepsilon_1}{\varepsilon_2} E_{1n}$$

This allows us to eliminate components of electric field in suspension. In this case \mathbf{E}_{2n} . After some manipulation we have finally

$$(28) \quad \mathbf{f}^{(1)} = \frac{1}{2} (\varepsilon_1 - \varepsilon_2) \left(\frac{\varepsilon_1}{\varepsilon_2} E_{1n}^2 + E_{1t}^2 \right) \mathbf{n}$$

and total force acting on particle described by field calculated in suspension and evaluated on suspension-particle boundary is given by

$$(29) \quad \mathbf{F}^{(1)} = \frac{1}{2} (\varepsilon_1 - \varepsilon_2) \oint_S \left(\frac{\varepsilon_1}{\varepsilon_2} E_{1n}^2 + E_{1t}^2 \right) \mathbf{n} ds$$

According with Newton's third law both forces $\mathbf{F}^{(1)}$ and $\mathbf{F}^{(2)}$ should be equal.

Illustrative example

The simulated chamber is modeled as a two-dimensional model, where we need to consider only a single pair of electrodes, one with positive $U_z = 10$ 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. Figure 2 shows a cross-sectional geometry, which includes the substrate and channel covers, the interdigitated electrodes and a fluid.

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 . Cylindrical dielectric particle has radius $r_1 = 3$ μm and relative permittivity $\varepsilon_2 = 50$. The fluid, where particle moves, has permittivity $\varepsilon_1 = 5$.

Computed electric field distribution is shown in Fig.2. Both x -component and y -component are given in logarithmic scale. The force acting on dielectric particle is not proportional to modulus of electric field, but instead to gradient of this field.

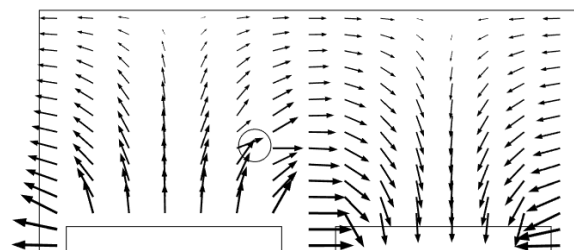


Fig. 2. Electric field strength \mathbf{E} in computational domain. The length of the vectors are in logarithmic scale

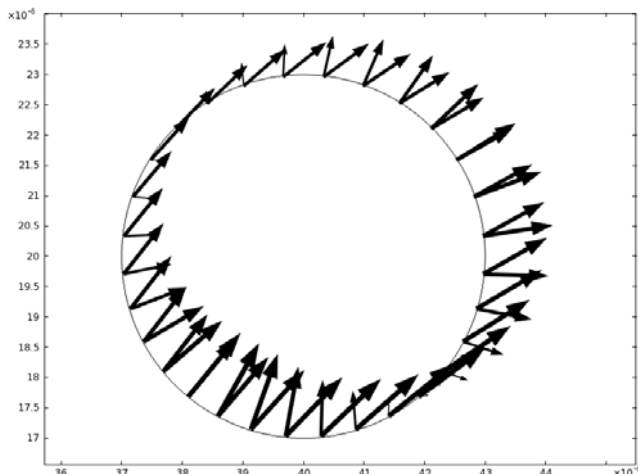


Fig. 3. Electric field strength on both sides of suspension-particle boundary

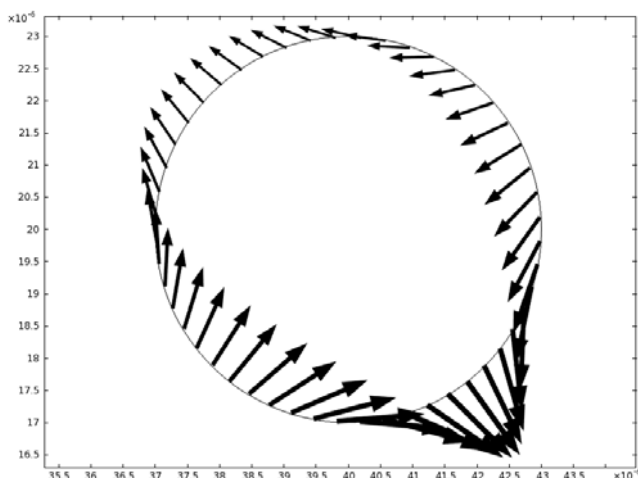


Fig. 4. Electric stress acting on suspension throughout particle on suspension-particle boundary

In Figure 3 electric field strength on both sides of the suspension-particle boundary is given. These values directly are used in equations for Maxwell stress tensor, which acts on both sides of the boundary.

In Figure 4. Electric stress acting on suspension throughout particle on suspension-particle boundary is presented. Figure 5 shows electric stress x -component acting on suspension throughout particle on suspension-particle boundary. The total force acting on particle computed from (26) formula has value

$$(30) \quad \mathbf{F}^{(2)} = 1.114\mathbf{a}_x - 3.460\mathbf{a}_y, \quad [\mu\text{N}]$$

and from equation (29)

$$(31) \quad \mathbf{F}^{(1)} = 1.157\mathbf{a}_x - 3.483\mathbf{a}_y, \quad [\mu\text{N}]$$

Force calculating from equivalent dipole method is given by

$$(32) \quad \mathbf{f}_d = 1.120\mathbf{a}_x - 3.288\mathbf{a}_y, \quad [\mu\text{N}]$$

For particle radius $r_1 = 5 \mu\text{m}$ this forces have following values:

$$(33) \quad \mathbf{F}^{(2)} = 3.496\mathbf{a}_x - 10.242\mathbf{a}_y, \quad [\mu\text{N}]$$

$$(34) \quad \mathbf{F}^{(1)} = 3.535\mathbf{a}_x - 10.410\mathbf{a}_y, \quad [\mu\text{N}]$$

$$(35) \quad \mathbf{f}_d = 3.113\mathbf{a}_x - 9.135\mathbf{a}_y, \quad [\mu\text{N}]$$

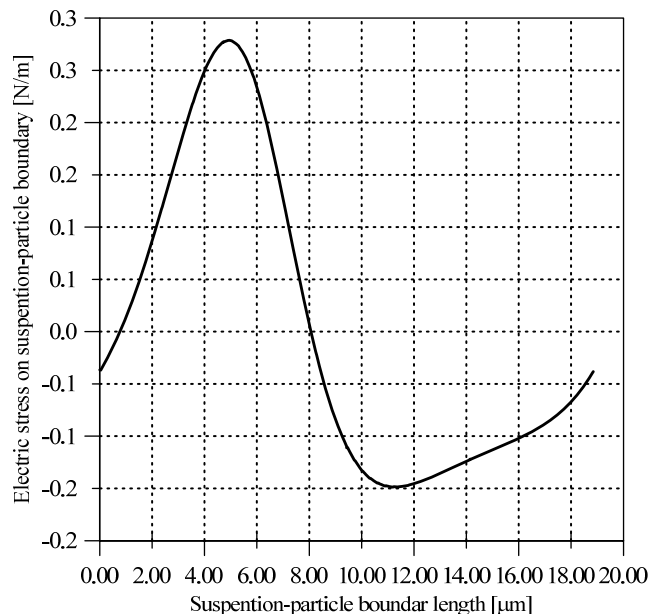


Fig. 5. Electric stress x -component acting on suspension throughout particle on suspension-particle boundary

Conclusions

In this article, cylindrical particle in uniform electric field perpendicular to the particle was considered. One can see that differences in calculation of forces acting on dielectric particle immersed in dielectric fluid are comparable. The error is not greater than 5%. Maxwell stress method can be applied to particles of any shape but equivalent dipole method only for cylindrical or spherical particles. For greater values of particle radius the difference between stress calculated on Maxwell stress tensor method and equivalent dipole method is greater. This is caused by the fact that bigger particle disturbs the field in greater degree.

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