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Stress Calculation in Two-Dimensional 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 pole 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. (**Obliczenia naprężeń w dwuwymiarowej DC dielektroforezie**)*

Keywords: *dielectrophoresis, Maxwell stress tensor calculation*
Słowa kluczowe: *dielektroforeza, tensor naprężeni Maxwella.*

Introduction

It is well-known that an electrically neutral but polarizable particle, suspended in a dielectric or conducting fluid, under the influence of a non-uniform electric field tends to move towards the region of highest electric field intensity. This migration caused by dielectric polarization forces is discovered by Pohl [1] and named as dielectrophoresis. During the past years dielectrophoresis has proved to be of very important in many applications such as, for example, industrial filtration of liquids, dielectric solid - solid separations and biological analyses.

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 engineering 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].

Dielectrophoretic (DEP) traps use the force acting on an induced multipole with a nonuniform steady or alternating electric field to create electric forces that will change position of particles. DEP forces can trap different kind of particles on or between special electrodes – among others including micron and submicron polymer beads, cells, viruses, and bacteria. With the appropriate electrode geometry design and careful control of the potentials conditions, single particle trapping can be attained.

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]. Pohl derived an expression for the dielectrophoretic force acting on cells by modeling the cell as a solid spherical dielectric particle placed in a fluid medium. A more realistic geometries for biological particles has been used by a number of scientists, which includes a spherical dielectric shell employed usually for the dielectric properties of the plasma-membrane [8].

The Pohl approach is a acceptable approximation only under a first order dipole approximation and can be used only if the radius of a particle is very small compared with the spatial dimensions of the electrode system. This yields difficulties when applied to modeling biological cells, when their dimensions are often comparable to the trap array. A more general approach for calculating the dielectrophoretic forces is based on the Maxwell stress tensor (MST) formulation [9], where the stress tensor is integrated over a particle surface S surrounded the cell. This method is regarded as the most general and rigorous approach to the calculation of field-induced forces. Although in many instances the value of the force derived from MST more or less agrees with those obtained from the effective moment method, some substantial differences have been reported even in a loss-free medium and steady electric fields. These differences arise simply because the approximations in the two methods were taken to different orders rather than fundamental differences between the two methods [9]. Although the method for calculating the MST force presented in this article is similar to that given in [9] and other authors, in this work the MST technique is employed to calculate the same force in two different ways integrating on both sides surrounding surface. Thou theoretically this forces should be the same, some unexpected differences can occur. The complex Laplace equation is solved to obtain a value for the voltage everywhere within a structure. The electric field is then obtained by a simple finite element approach [7].

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 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.

Theoretically, this path is arbitrary. In practice, the location of the path has a very strong influence on the computed force or torque. In [10] authors have proposed to chose the integration path as: (i) a path joining the centroids of neighbouring elements, (ii) a path crossing elements by joining the midpoints of two of their sides, and (iii) a path crossing perpendicularly each element boundary.

In electromagnetic field computation it is pointed out in [10], that two boundary conditions are governing:
1. the normal components of the electric flux density must be continuous,
2. the tangential component of the electric field strength on either side of the boundary must be equal.

In FEM with Lagrangian low order elements only the first condition is fulfilled if the solution is based on the electric scalar potential V [10]. The Maxwell stress method is popular, but is also known to be very prone to numerical errors. Near a sharp corner of the metallic and dielectric objects, the field intensity can be very large. In order to reduce such errors it is necessary to use the high number of finite elements for a field solution

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.

Main equations

The simulated chamber is modeled as a two-dimensional model, where we need to consider only a single pair of electrodes, one with positive $U_z = 4$ 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. Fig. 1 shows a cross-sectional geometry, which includes the substrate and channel covers, the interdigitated electrodes, and a fluid.

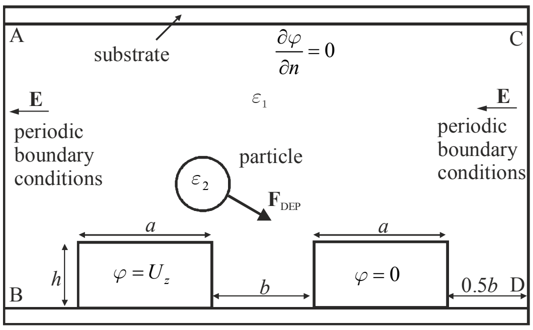

Fig. 1. Computational domain together with geometrical dimensions.

Let us now derive close form of surface force density **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

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

The surface force density **t** is given by

(2) $$\mathbf{f} = \overleftrightarrow{\mathbf{T}}\cdot\mathbf{n} = \left(\sum_{j=1}^{3}\sum_{k=1}^{3}T_{jk}\mathbf{a}_j\mathbf{a}_k\right)\cdot\left(\sum_{r=1}^{3}n_r\mathbf{a}_r\right) = \\ = \sum_{j=1}^{3}\sum_{k=1}^{3}\sum_{r=1}^{3}T_{jk}n_r\mathbf{a}_j\left(\mathbf{a}_k\cdot\mathbf{a}_r\right)$$

In the above equations indexes $i, j, k = 1, 2, 3$ replace, for convenience, coordinates x, y and z. Only these terms under summation signs remain nonzero, where scalar product ($\mathbf{a}_k\cdot\mathbf{a}_r$) is nonzero. This will occur for $r = k$. Thus we have

(3) $$\mathbf{f} = \sum_{j=1}^{3}\sum_{k=1}^{3}T_{jk}n_k\mathbf{a}_j = \\ = \varepsilon\sum_{j=1}^{3}\sum_{k=1}^{3}E_jE_kn_k\mathbf{a}_j - \frac{1}{2}\varepsilon\sum_{j=1}^{3}\sum_{k=1}^{3}E^2\delta_{jk}n_k\mathbf{a}_j$$

But in the last expression only these terms are nonzero, when $k = j$. In the first term we can separate the summations, so

(4) $$\mathbf{f} = \varepsilon\left(\sum_{k=1}^{3}E_kn_k\right)\left(\sum_{j=1}^{3}E_j\mathbf{a}_j\right) - \frac{1}{2}\varepsilon E^2\left(\sum_{j=1}^{3}n_j\mathbf{a}_j\right)$$

But now

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

yields

(6) $$\mathbf{f} = \varepsilon\left(\sum_{k=1}^{3}E_kn_k\right)\mathbf{E} - \frac{1}{2}\varepsilon E^2\mathbf{n}$$

The expression in parenthesis is equal to the scalar product **E** and **n**

(7) $$\mathbf{E}\cdot\mathbf{n} = \sum_{k=1}^{3}\sum_{r=1}^{3}E_kn_r\left(\mathbf{a}_k\cdot\mathbf{a}_r\right) = \sum_{k=1}^{3}E_kn_k$$

Thus the surface force density has value

(8) $$\mathbf{f} = \varepsilon\left(\mathbf{E}\cdot\mathbf{n}\right)\mathbf{E} - \frac{1}{2}\varepsilon E^2\mathbf{n}$$

Derivation of force density on both sides of boundary

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 (8) gives us for both sides of the boundary:

(9) $$\mathbf{f}_1 = \varepsilon_1\left(\mathbf{E}_1\cdot\mathbf{n}_1\right)\mathbf{E}_1 - \frac{1}{2}\varepsilon_1E_1^2\mathbf{n}_1$$

(10) $$\mathbf{f}_2 = \varepsilon_2\left(\mathbf{E}_2\cdot\mathbf{n}_2\right)\mathbf{E}_2 - \frac{1}{2}\varepsilon_2E_2^2\mathbf{n}_2$$

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

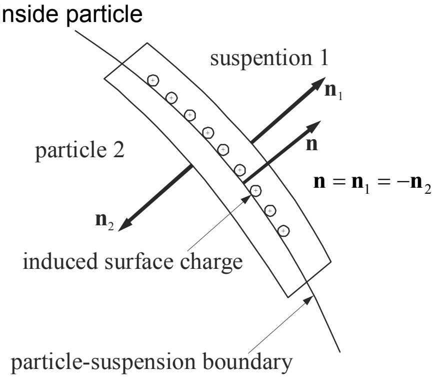

Fig. 2. Normal vectors in Maxwell stress tensor integration.

$$\mathbf{f} = \mathbf{f}_1 + \mathbf{f}_2 = \varepsilon_1\left(\mathbf{E}_1 \cdot \mathbf{n}_1\right)\mathbf{E}_1 - \frac{1}{2}\varepsilon_1 E_1^2 \mathbf{n}_1 + \tag{11}$$
$$+\varepsilon_2\left(\mathbf{E}_2 \cdot \mathbf{n}_2\right)\mathbf{E}_2 - \frac{1}{2}\varepsilon_2 E_2^2 \mathbf{n}_2$$

Particle-suspension boundary is shown in Fig.2, where also all normal vectors needed in derivation are presented. 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

$$\mathbf{f}^{(2)} = \varepsilon_1\left(\mathbf{E}_1 \cdot \mathbf{n}\right)\mathbf{E}_1 - \varepsilon_2\left(\mathbf{E}_2 \cdot \mathbf{n}\right)\mathbf{E}_2 - \frac{1}{2}\left(\varepsilon_1 E_1^2 - \varepsilon_2 E_2^2\right)\mathbf{n} \tag{12}$$

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

$$\mathbf{E}_1 = E_{1n}\mathbf{n} + E_{1t}\mathbf{t} \qquad \mathbf{E}_2 = E_{2n}\mathbf{n} + E_{2t}\mathbf{t} \tag{13}$$

where $\mathbf{n}$ is a normal and $\mathbf{t}$ tangential vectors to the boundary. After introduction into equation for force we have

$$\mathbf{f}^{(2)} = \left(\frac{1}{2}\varepsilon_1 E_{1n}^2 - \frac{1}{2}\varepsilon_2 E_{2n}^2 - \frac{1}{2}\varepsilon_1 E_{1t}^2 + \frac{1}{2}\varepsilon_2 E_{2t}^2\right)\mathbf{n} + \tag{14}$$
$$+\left(\varepsilon_1 E_{1n} E_{1t} - \varepsilon_2 E_{2n} E_{2t}\right)\mathbf{t}$$

Boundary conditions on both side the boundary have following form

$$E_{1t} = E_{2t} \qquad \varepsilon_1 E_{1n} = \varepsilon_2 E_{2n} \tag{15}$$

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

$$\mathbf{f}^{(2)} = \left(\frac{1}{2}\frac{\varepsilon_2^2}{\varepsilon_1} E_{2n}^2 - \frac{1}{2}\varepsilon_2 E_{2n}^2 - \frac{1}{2}\varepsilon_1 E_{2t}^2 + \frac{1}{2}\varepsilon_2 E_{2t}^2\right)\mathbf{n} + \tag{16}$$
$$+\left(\varepsilon_2 E_{2n} E_{2t} - \varepsilon_2 E_{2n} E_{2t}\right)\mathbf{t} =$$

or finally

$$\mathbf{f}^{(2)} = \frac{1}{2}\left(\varepsilon_2 - \varepsilon_1\right)\left(\frac{\varepsilon_2}{\varepsilon_1} E_{2n}^2 + E_{2t}^2\right)\mathbf{n} \tag{17}$$

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

$$\mathbf{F}^{(2)} = \frac{1}{2}\left(\varepsilon_2 - \varepsilon_1\right)\oint_S \left(\frac{\varepsilon_2}{\varepsilon_1} E_{2n}^2 + E_{2t}^2\right)\mathbf{n}\, ds \tag{18}$$

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 (14) 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

$$E_{2n} = \frac{\varepsilon_1}{\varepsilon_2} E_{1n} \tag{19}$$

This allows us to eliminate components of electric field in suspension. In this case $\mathbf{E}_{2n}$

$$\mathbf{f}^{(1)} = -\left(\frac{1}{2}\varepsilon_1 E_{1n}^2 - \frac{1}{2}\frac{\varepsilon_1^2}{\varepsilon_2} E_{1n}^2 - \frac{1}{2}\varepsilon_1 E_{1t}^2 + \frac{1}{2}\varepsilon_2 E_{1t}^2\right)\mathbf{n} + \tag{20}$$
$$+\left(\varepsilon_1 E_{1n} E_{1t} - \varepsilon_1 E_{1n} E_{1t}\right)\mathbf{t}$$

After some manipulation we have finally

$$\mathbf{f}^{(1)} = \frac{1}{2}\left(\varepsilon_1 - \varepsilon_2\right)\left(\frac{\varepsilon_1}{\varepsilon_2} E_{1n}^2 + E_{1t}^2\right)\mathbf{n} \tag{21}$$

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

$$\mathbf{F}^{(1)} = \frac{1}{2}\left(\varepsilon_1 - \varepsilon_2\right)\oint_S \left(\frac{\varepsilon_1}{\varepsilon_2} E_{1n}^2 + E_{1t}^2\right)\mathbf{n}\, ds \tag{22}$$

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 = 5 μm and relative permittivity $\varepsilon_2 = 50$. The fluid, where particle moves, has permittivity $\varepsilon_1 = 5$.

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. Laplace equation $\nabla(\varepsilon\nabla V) = 0$ for potential V, where ε is dielectric permittivity, is solved in order to obtain electric field strength in simulated chamber. Electric distribution is shown in Fig.3.

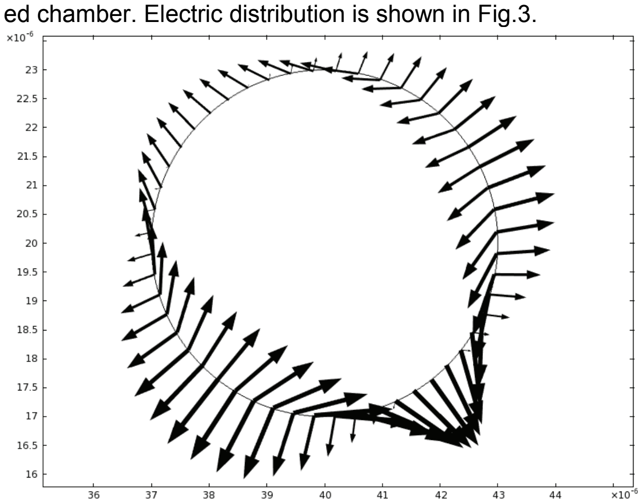

Fig. 3. Electric stress acting on suspension-particle boundary from suspension and particle side.

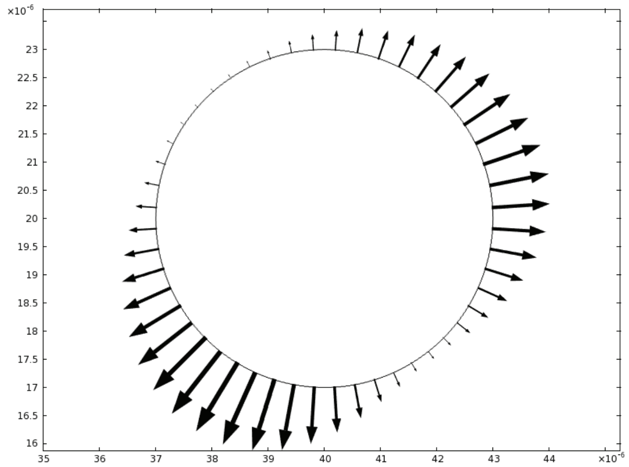

Fig. 4. Total stress acting on suspension-particle boundary.

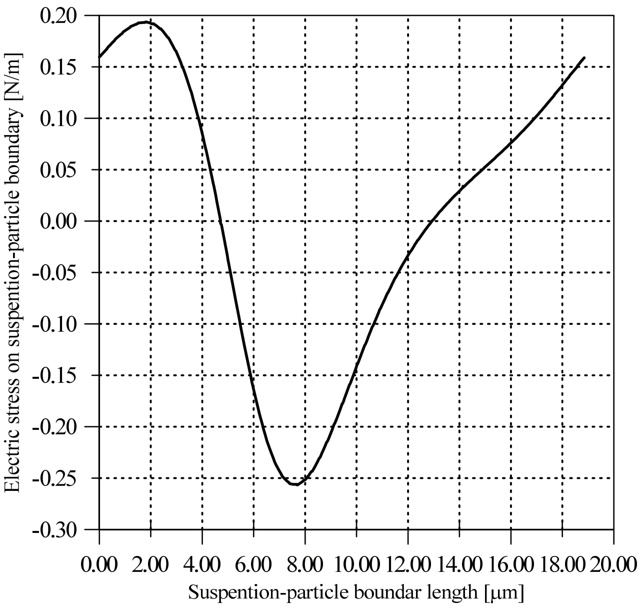

Fig. 5. Electric stress y-component acting on suspension throughout particle on suspension-particle boundary.

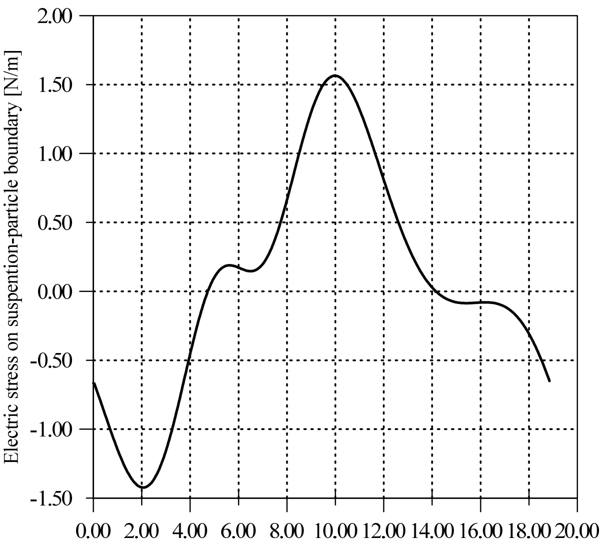

Fig. 6. Total x-component stress acting on suspension-particle boundary when to calculations was taken electric field in particle.

In Fig 4. total stress computed from equations (17) and (21) are presented. The difference is not noticeable in this figure. Figures 5 and 6 presents y and x components stresses on particle perimeters.
The total force acting on particle computed from (18) formula has value

(23) $$F^{(2)} = 1.162\mathbf{a}_x - 3.487\mathbf{a}_y \quad [\mu\text{N}]$$

and from equation (22)

(24) $$F^{(1)} = 1.169\mathbf{a}_x - 3.497\mathbf{a}_y \quad [\mu\text{N}]$$

Conclusions

In this article, cylindrical particle in uniform electric field perpendicular to the particle was considered.

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