Mutual Forces Acting on Chains of Particles

Eugeniusz Kurgan and Piotr Gas

Abstract This paper describes a method to determine mutual forces acting between dielectric particles, which form chains. The Maxwell stress tensor method together with finite element method are used. It is shown that particles placed in inhomogeneous field, because of dielectrophoretic forces acting between them, have a tendency to collect one by one giving in effect even long particles chains. In this article, Maxwell stress tensors are integrated over particle surfaces to give total mutual forces interacting between molecules.

Keywords Dielectrophoresis · Maxwell stress tensor · Forces · Particle chains · Finite element method

1 Introduction

Dielectrophoresis (DEP) phenomenon is increasingly used in a variety of cheap fabricated devices, where micro-scale fluid flow is observed. Such small apparatus may easily interact with larger electronic devices, which results in a great reduction for complex and expensive methods of macro-fluid manipulations by mechanical valves and complex pumps. DEP techniques are also very useful in purifying, enriching and characterizing a large amount of various biological, clinical, environmental and industrial ingredients. Recently, significant development of these and many accompanied technologies have been made [1]. It should be emphasized that dielectrophoretic phenomenon enables voltage trapping, concentrating, translating as well as fractionating of minerals, biological and chemical molecules of suspending liquid medium. Dielectrophoretic forces make possible to investigate

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different fluid properties including dielectric and conducting properties of individual particles since they depend not only on frequency of the exciting source, but also on both its structure and composition. Many different effects appear when dielectric particles such as, for example, biological cells are subjected to an electric field generated in dielectric fluid. In practice, dielectrophoresis occurs in micropatterned electrodes immersed in dielectric fluid. When the electrodes are subjected to applied external voltages, they generate nonuniform electric field, which next produces dielectrophoretic forces [2]. Next, such forces induce effective dipole moment and force resulting in specific molecule movement. What is important, the magnitude of dielectrophoretic force depends mainly on the gradient of the square of the magnitude of electric field strength produced around the interdigitated electrodes.

The dielectrophoretic force calculations are essential during the modelling of complex electrical and mechanical systems. In the case of stiff materials, only the total effective force is necessary, while for non-rigid system with deformable structure the local force distribution is required. This is especially important during separation processes of various biological particles, such as bacteria, cells, proteins and so on. Usually, to calculate DEP force one uses equivalent dipole method, which is computationally very effective because there is no need to consider particles together with surrounding medium [3]. It is enough to compute electric field strength distribution in points of particle's positions and by adequate equations compute force acting on the particle. In the case of one or two particles, this method can be without difficulties applied; but in multi-particles structures, it gives force values with unacceptable error levels. This is caused by mutual interaction of particles placed between two distant particles. Moreover, this method does not permits force density calculations on particle boundary. This is especially important when particles are made from little coherent material, which by high field gradient can undergo total destruction. Another important approach for evaluating DEP forces is based on so-called Maxwell stress tensor (MST) method [4]. It should be stressed that such tensor is calculated by integration over whole molecule surface. Moreover, this method is the most general approach to calculate DEP forces acting on particles.

The methodology presented in this paper is similar to that described by other authors [5]. In this work, two different techniques are used to calculate the same force on both sides of surrounding particle surface. Theoretically, both forces should be equal but often some unexpected differences can occur. At the beginning, in order to estimate the electric potential distribution within the fluid and particles, the Laplace equation is solved. In the next step, the electric field strength is determined. All calculations are based on analysis with the finite element method [6]. MST method allows fast computing of the electromagnetic field around electrodes with complex geometries as well as the DEP forces acting on particles immersed in fluid with inhomogeneous electric properties. However, many papers have reported that both force and torque values obtained from FEM analysis could be not precise in the case of particularly complex models, including DEP traps with multiple molecules [7].

In the Maxwell's stress method, the total force, which acts on particle, is computed by surrounding an object by closed surface and integrating Maxwell stress tensor over the entire surface. In application of the ordinary Maxwell stress method, the integration surface should be closed, and located completely in the linear part of the material. Inhomogeneous domains should be treated with special care. In this paper [8], the authors discuss particle chain formation using a reaction-diffusion approach. Jones [5] extensively has been considered different interaction collections of various particles. In article [9], the authors describe known DC dielectrophoretic particle interactions as well as their mutual motions through equivalent dipole method. In papers [10–12], the authors propose a new method based on iterative moment method for computing dielectrophoretic forces, which does not need to solve electromagnetic field by the finite element method. In the current paper, the authors have successfully shown in which way the particles immersed in fluid and placed in the strongly inhomogeneous field can collect to form chains. Some important application of particle manipulation can be found in similar numerous publications [13–20].

2 Main Equations

Let us consider longitudinal cross section of the flow channel with two electrodes and two particles, as in the following Fig. 1.

There are two electrodes: one connecting to ground potential and another to potential U_z, which is equal usually several volts. Because distance between electrodes is very small, thus the gradient of the electric field can attain very big value. This results, as consequence, with very high mutual forces acting between particles. In order to derive surface force density, we assume that unit vector is normal to given surface. Maxwell stress tensor T_{ij} for electric field $\mathbf{E}$ has the following formula [3]:

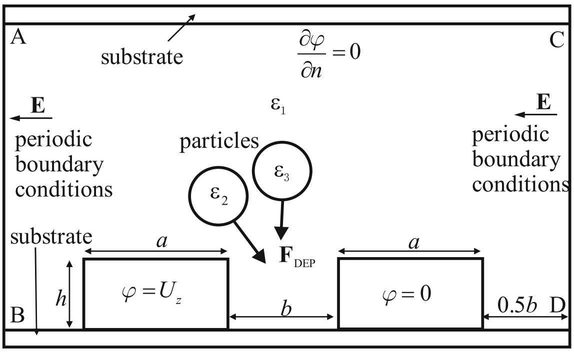


Fig. 1 Schematic representation of the electrode arrangement with one pair of electrodes and moving biological particle (periodic boundary conditions mean that the potentials at the inlet and outlet of the subsequent periodic computational cells are the same, e.g. $\varphi_{A-B} = \varphi_{C-D}$)

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

The surface force density **f** can be computed by

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

In this formula, the indexes $i, j, k = 1, 2, 3$ should be replaced, conveniently, by 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]:

$$\mathbf{f} = \varepsilon \sum_{j=1}^{3}\sum_{k=1}^{3} E_j E_k n_k \mathbf{a}_j - \frac{1}{2}\varepsilon \sum_{j=1}^{3}\sum_{k=1}^{3} E^2 \delta_{jk} n_k \mathbf{a}_j \tag{3}$$

In the last expression only these terms are nonzero, when $k = j$, but in our case:

$$\mathbf{E} = \sum_{j=1}^{3} E_j \mathbf{a}_j \quad \text{and} \quad \mathbf{n} = \sum_{j=1}^{3} n_j \mathbf{a}_j \tag{4}$$

gives

$$\mathbf{f} = \varepsilon\left(\sum_{k=1}^{3} E_k n_k\right)\mathbf{E} - \frac{1}{2}\varepsilon E^2 \mathbf{n} \tag{5}$$

The terms in parenthesis are identical to scalar product **E** and **n**, therefore:

$$\mathbf{f} = \varepsilon(\mathbf{E} \cdot \mathbf{n})\mathbf{E} - \frac{1}{2}\varepsilon E^2 \mathbf{n} \tag{6}$$

This is the fundamental equation, which enables us to compute force densities on particle surfaces. Because dielectric in fluid and particles undergo mutual polarization, force densities will occur on both sides of the boundaries. When we assume that liquid has number 1 and particle has number 2, then formula (6) on both sides of the boundary give us suitable force densities values [7]:

$$\mathbf{f}_1 = \varepsilon_1(\mathbf{E}_1 \cdot \mathbf{n}_1)\mathbf{E}_1 - \frac{1}{2}\varepsilon_1 E_1^2 \mathbf{n}_1 \tag{7}$$

$$\mathbf{f}_2 = \varepsilon_2(\mathbf{E}_2 \cdot \mathbf{n}_2)\mathbf{E}_2 - \frac{1}{2}\varepsilon_2 E_2^2 \mathbf{n}_2 \tag{8}$$

External field induces surface charge density which can be integrated to obtain total force acting on the particle. One can assume that we have no free electric charges in particle. The resulting force density is equal to the sum of both components:

$$\mathbf{f} = \mathbf{f}_1 + \mathbf{f}_2 \tag{9}$$

Let us now relate force densities with normal and tangential components of electric field strength acting on boundaries of the particle. On both sides of the suspension-particle boundary, unit vectors have opposite sign. In this way: $\mathbf{n}_1 = \mathbf{n}$ and $\mathbf{n}_2 = -\mathbf{n}$, therefore in end effect we get:

$$\mathbf{f}^{(2)} = \varepsilon_1(\mathbf{E}_1 \cdot \mathbf{n})\mathbf{E}_1 - \varepsilon_2(\mathbf{E}_2 \cdot \mathbf{n})\mathbf{E}_2 - \frac{1}{2}\left(\varepsilon_1 E_1^2 - \varepsilon_2 E_2^2\right)\mathbf{n} \tag{10}$$

Now both vectors $\mathbf{E}_1$ and $\mathbf{E}_2$ can be split into two components: one perpendicular and another tangential to the surface:

$$\mathbf{E}_1 = E_{1n}\mathbf{n} + E_{1t}\mathbf{t} \tag{11}$$

$$\mathbf{E}_2 = E_{2n}\mathbf{n} + E_{2t}\mathbf{t} \tag{12}$$

and after some further manipulation we obtain:

$$\begin{aligned}\mathbf{f}^{(2)} = &\left(\frac{1}{2}\varepsilon_1 E_{1n}^2 - \frac{1}{2}\varepsilon_2 E_{2n}^2 - \frac{1}{2}\varepsilon_1 E_{1t}^2 + \frac{1}{2}\varepsilon_2 E_{2t}^2\right)\mathbf{n} \\ &+ \left(\varepsilon_1 E_{1n} E_{1t} - \varepsilon_2 E_{2n} E_{2t}\right)\mathbf{t}\end{aligned} \tag{13}$$

Boundary conditions on both sides of the particle surface give:

$$E_{1t} = E_{2t} \tag{14}$$

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

or finally

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

This is the force density acting between fluid and particle. After calculation of the electric field $\mathbf{E}$ inside of the particle, the total force acting on the whole particle can be computed by following formula:

$$\mathbf{F}^{(2)} = \frac{1}{2}(\varepsilon_2 - \varepsilon_1)\oint_S \left(\frac{\varepsilon_2}{\varepsilon_1}E_{2n}^2 + E_{2t}^2\right)\mathbf{n}\,\mathrm{d}s \tag{17}$$

In quite analogous, we can derive similar relation using fields from fluid side. The boundary condition gives:

$$E_{2n} = \frac{\varepsilon_1}{\varepsilon_2} E_{1n} \tag{18}$$

and after introduction (18) into (16) we have [14]:

$$\mathbf{f}^{(1)} = \frac{1}{2}(\varepsilon_1 - \varepsilon_2)\left(\frac{\varepsilon_1}{\varepsilon_2} E_{1n}^2 + E_{1t}^2\right)\mathbf{n} \tag{19}$$

When we use electric field in suspension to calculate force acting on particle and integrate it over whole boundary, we get

$$\mathbf{F}^{(1)} = \frac{1}{2}(\varepsilon_1 - \varepsilon_2)\oint_S \left(\frac{\varepsilon_1}{\varepsilon_2} E_{1n}^2 + E_{1t}^2\right)\mathbf{n}\,\mathrm{d}s \tag{20}$$

In accordance with the Newton's third law, both forces $\mathbf{F}^{(1)}$ and $\mathbf{F}^{(2)}$ acting on particle should have the same value. It should be emphasized, that this form of equations can be used both in two and three-dimensional problems.

3 Illustrative Example

One section of the separating structure in two dimensions can be modelled by one electrode with voltage $U_z = 4$ V and one the electrode with zero potential. The presence of another parts of the interdigitated electrode array outside the analyzed region can be taken into account using periodic boundary conditions on both sides of the given section. The periodic boundary condition relates potential and electric field values on these parts of the boundary, which are neighbouring with left and right sections with the same field distribution. In our, case it was assumed that

$$\varphi(a, y) = \varphi(a + d_{\mathrm{A-C}}, y) \text{ and } \frac{\partial\varphi(a, y)}{\partial n} = \frac{\partial\varphi(a + d_{\mathrm{A-C}}, y)}{\partial n} \tag{21}$$

In Fig. 1, we can see cross section, which consists of the isolating base and channel covering, the interdigitated electrodes and a suspension. The finite element has been used to calculate field in geometry given by: $d_{\mathrm{A-B}} = 60$ μm, $d_{\mathrm{A-C}} = 160$ μm, $a = 40$ μm, $b = 40$ μm and $h = 4$ μm. Dielectric cylindrical particles have radiuses $r_2 = r_3 = 5$ μm and relative permittivity $\varepsilon_2 = \varepsilon_3 = 80$. The suspension with the particle, has relative permittivity $\varepsilon_1 = 5$. On the bottom and top of the substrate, we have the Neumann's conditions. We also have periodic boundary conditions on the left and right sides of boundary parts: A–B and C–D. Moreover, the Laplace equation div(ε grad φ) = 0, for electric potential φ, where ε is dielectric permittivity, should be solved to obtain the electric field strength **E** in simulated chamber section. In Fig. 1 two particles are shown and our goal is to compute Maxwell tensor, force densities and total forces acting on particles by means of Eqs. (16) and (19). Let us now consider two particles as depicted in Fig. 1 and compute Maxwell tensor, force densities as well as total forces acting on particles using Eqs. (17) and (20). Force densities acting between two particles are given in Fig. 2.

One can easily see that we have greatest forces in the neighborhood of both particles. Figure 3 shows the real values of force density calculated along each particle perimeter.

Let us now compute total forces acting on both particles by means of Eqs. (17) and (20), namely:

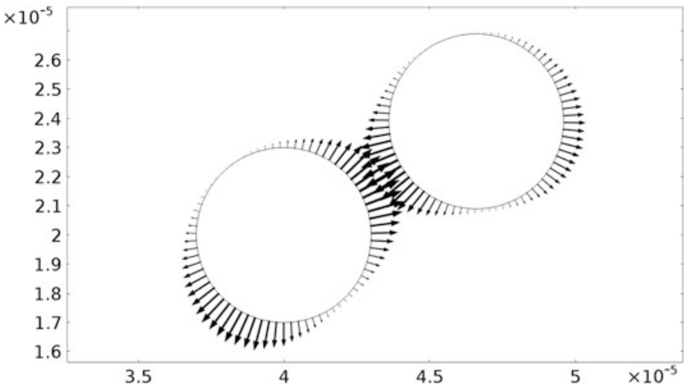
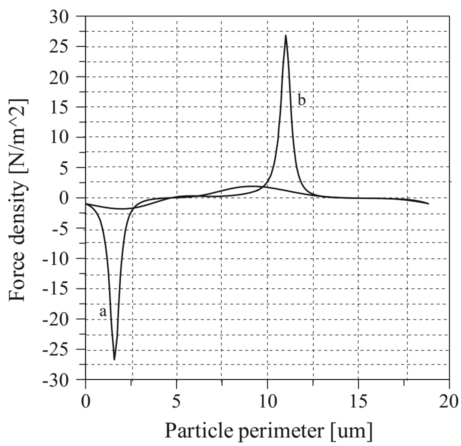


Fig. 2 Force densities distribution on particle-fluid boundaries

Fig. 3 Force densities on particle perimeters: **a** particle on the *right* side and **b** particle on the *left* side as depicted in Fig. 1



$$\begin{aligned} \mathbf{F}^{(1)} &= \quad 3.144\mathbf{a}_x - 2.600\mathbf{a}_y \ \left(\mu\ \mathrm{N/m^2}\right) \\ \mathbf{F}^{(2)} &= -1.561\mathbf{a}_x - 4.415\mathbf{a}_y \ \left(\mu\ \mathrm{N/m^2}\right) \end{aligned} \tag{22}$$

It is easy to seen that both forces are directed towards electric trap occurring between electrodes. This force can be calculated by simple projection forces $\mathbf{F}^{(1)}$ and $\mathbf{F}^{(2)}$ on the stride line connecting centers of both particles and labelled as $\mathrm{F}_s^{(1)}$ and $\mathrm{F}_s^{(2)}$. From geometrical relations, required angles can be calculated. After some manipulations we finally get the following values:

$$\begin{aligned} \mathrm{F}_s^{(1)} &= 1.3938\ \left(\mu\ \mathrm{N/m^2}\right) \\ \mathrm{F}_s^{(2)} &= 3.5944\ \left(\mu\ \mathrm{N/m^2}\right) \end{aligned} \tag{23}$$

They are not equal because additional force resulting from electrodes influences both forces. In Fig. 4, we can see the example when two particles touch each other. Maxwell stress tensor assumes substantial values in the vicinity of both particles. Mutual forces acting between both particles also assume much greater values than in the previous case.

$$\begin{aligned} \mathbf{F}^{(1)} &= \quad 17.663\mathbf{a}_x + 5.168\mathbf{a}_y \ \left(\mu\ \mathrm{N/m^2}\right) \\ \mathbf{F}^{(2)} &= -15.537\mathbf{a}_x - 13.830\mathbf{a}_y \ \left(\mu\ \mathrm{N/m^2}\right) \end{aligned} \tag{24}$$

One can easily see that now forces acting between particles are almost on order greater and directed almost parallel each other. In Figs. 5, 6 and 7, collections of four particles are shown. It can be observed that distribution of Maxwell stress tensor given as resultant forces which attract each other. This process leads to the formation of specific particle chains. This was confirmed experimentally by several authors [8, 9, 20].

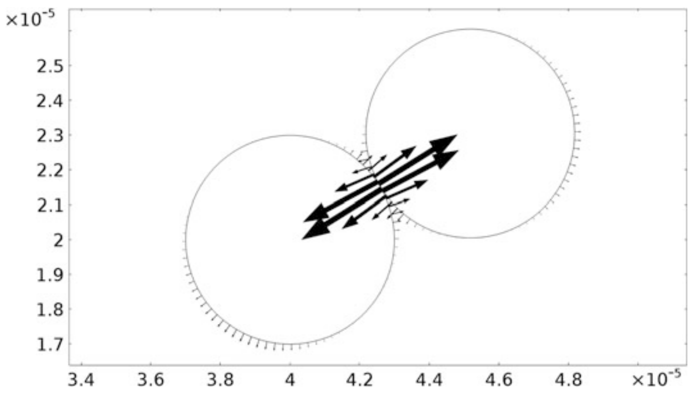


Fig. 4 Force densities on particle perimeters for two contacting particles

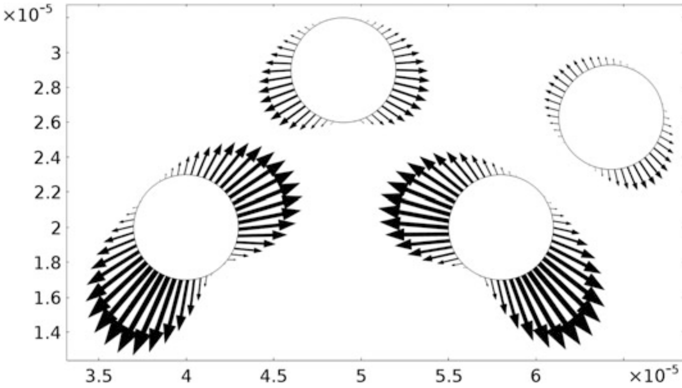


Fig. 5 Force densities on particle perimeters for distant particles

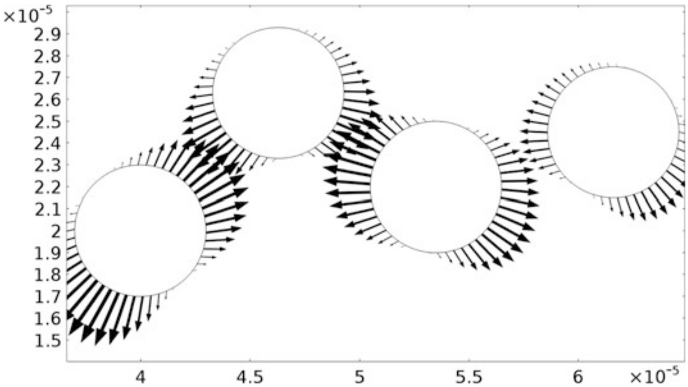


Fig. 6 Force densities on particle perimeters for molecules at shorter distances than in Fig. 5 (the acting forces are much higher than in Fig. 5)

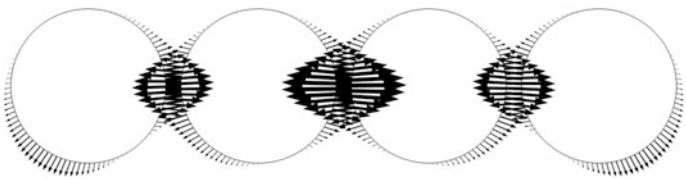


Fig. 7 Force densities on particle perimeters for molecules connected in one chain as a result of acting DEP forces

4 Conclusions

Various dielectrophoretic techniques are greatly useful in enriching, purifying and describing of various environmental, biological, industrial and clinical ingredients. In this paper, it has been demonstrated that with an appropriate electrode array and a suitable electric field, separation of particles can be accomplished. Unfortunately, this phenomenon of mutual force interaction has negative influence on particle separation process. Because dielectrophoresis is mainly utilized to separate different micro-particles, aggregation of particles can substantially hinder separation process of various molecules. The mutual interaction of particles by surface densities forces can be minimalised by according selection suspension permittivity and interdigitated electrode potentials. Therefore, any theoretical considerations, leading to better understanding of this phenomenon, have great practical value.

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