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Influence of numerical method on computational accuracy in DC dielectrophoresis

***Abstract**: Dielectrophoresis is the translational motion of neutral matter caused by polarization effects in a non-uniform electric field. Dielectrophoresis, arising from spatially nonuniform electric fields, has become one of the more promising tools for particle manipulation in microfluidics and nanofluidics. Because numerical accuracy of computations of force acting on particle is of great importance, the author has been investigating in this paper numerical error analysis in two-dimensional DC dielectrophoresis. Nonuniform field with high gradient has been obtained by assuming nonlinear permittivity what allowed analytical calculation of potential and electric strength and its gradient distribution. Analytical calculation of forces acting on particle is compared with numerical values computed with finite element method.*

***Streszczenie.** W publikacji tej omówiono analizę błędu obliczania siły działającej na cząsteczkę w polu elektrycznym o dużym gradiencie. Ponieważ w ogólnym przypadku jest bardzo trudno obliczyć analitycznie rozkład potencjału oraz pola elektrycznego wraz z jego gradientem, przyjęto bardzo prosty kształt analizowanego obszaru w postaci prostokąta wraz z nieliniową zależnością przenikalności elektrycznej od współrzędnych przestrzennych. Porównano wyniki obliczeń analitycznych z wynikami obliczeń opartych na metodzie elementów skończonych. (**Wpływ metod numerycznych na dokładność dielektroforezy DC**)*

Keywords: dielectrophoresis, dipole force calculations, error calculation
Słowa kluczowe: dielektroforeza, siły działających na dipol, obliczanie błędu.

Introduction

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 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.

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 [2] 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 [3] 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, dielectrophoretic and electrorotational manipulation of living and death cells, and the control of electrorheological fluids.

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 [4].

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 [5]. Unfortunately, force and torque calculations are influenced by the approximate nature of the discretisation used in FEM meshes.

Analytical calculation of forces acting on particle is compared with numerical values computed with finite element method.

Equations describing the electromagnetic field

In practical applications of dielectrophoresis, inhomogeneous electric filed with sufficient gradient is obtained throughout adequate configuration of electrode geometry of the channel, where particles in dielectric fluid are moving and by properly little electrode dimensions. Important role plays here sharp edges of electrodes, where in vicinity of them, as it is commonly known, electric field attains high values and with high gradients. In order to orientate about size of errors, which introduce equivalent dipole method and numerical method used to solve adequate Laplace's equation on size of occurring here errors, it is necessary to know exact solution of the electromagnetic field and its gradients in computational domain [6]. When geometrical shapes of electrodes and fluid flow channel have complicated shapes, it is very difficult to solve analytically Laplace's equation together with, frequently, complicated boundary conditions [7]. Inhomogeneous field with arbitrary shape, can be relatively easy obtained in inhomogeneous medium, with very simple geometrical shape of computational domain.

Let us assume that geometrical form of channel has a cuboid shape with following dimensions: L in direction of x-axis, h in direction in y-axes and L_p in z-axis. Two dimensional cross section of the channel with dielectric fluid, but without a particle, is presented in Fig. 1. On the Fig.9 we have the same medium, but with a particle with the same permittivity coefficient, as dielectric fluid. From physical point of view, both cases are entirely equivalent, but from point of view finite element method, which will be used to solve Laplace's equation, they are not equivalent, because on the fluid-particle border electric field continuity conditions have to be fulfilled, what as we shall see, will cause arising substantial errors by calculation forces acting on particle.

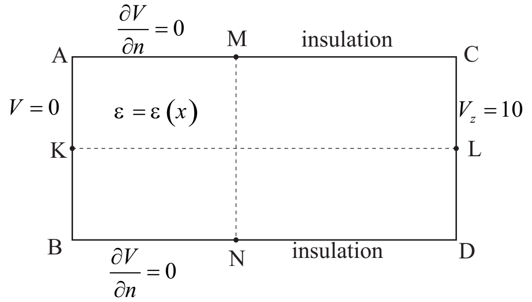

Fig.1. Inhomogeneous medium without a particle

Now we assume following computational data: segment AB = CD = h =40μm, BD = AC = L = 100μm, length L_p = 10μm, the particle radius r_0 = 3μm and is placed in point x_p = 40μm and y_p = 20μm. On side AB there are zero boundary conditions and on side CD potential is constant and is equal V_z = 10V. On segments BD and AC normal derivative of the potential V perpendicular to boundary amounts zero. It was assumed that relative permittivity of the particle ε_2 = 1.5. On the Fig.1 two segments KL and MN are distinguished along which we shell observe analyzed values. S permittivity following function was assumed:

(1) $$\varepsilon(x)=\varepsilon_{\mathrm{w}}\varepsilon_0=\left(a+be^{cx}\right)\varepsilon_0$$

where am b and c are parameters describing permittivity shape, x is coordinate in rectangular coordinate system, which origin is placed in point B. One has to notice that relative dielectric permittivity depends only on coordinate x. Calculations will be made for a = 2, b = 10 and for two parameter values $c=-0.1$[1/m] i $c=-10$[1/m], as in Fig. 2. Let the exact value of potential be V_a. This potential, because of symmetry, depends only on x-coordinate. The field is described by following Laplace's equation [8]:

(2) $$\frac{d}{dx}\left(\varepsilon_{\mathrm{w}}(x)\varepsilon_0\frac{d}{dx}V_{\mathrm{a}}(x)\right)=0$$

After integration we obtain formula for analytical calculation of potential function in computational domain. Knowing nonlinear function of electric permittivity allow us calculate analytical form of solution.

(3) $$V_{\mathrm{a}}(x)=\int\frac{C_1}{\varepsilon_{\mathrm{w}}(x)}dx+C_2$$

where C_1 and C_2 are integrating constants. One should notice that ε_0 in the above equation reduces. After taking into account equation (1) we get

(4) $$V_{\mathrm{a}}(x)=\frac{C_1}{ac}\left(cx-\log\left(a+be^{cx}\right)\right)+C_2$$

From boundary conditions for $x=0$ and $x=L$ we have

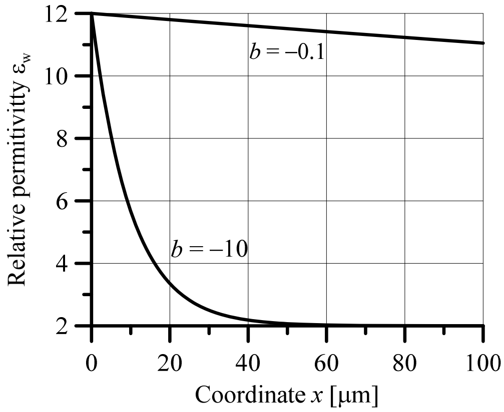

Fig.2. Relative permittivity for two parameter values

(5) $$-\frac{C_1}{ac}\log(a+b)+C_2=0$$

(6) $$\frac{C_1}{ac}\left(cL-\log\left(a+be^{cL}\right)\right)+C_2=V_z$$

Solution of the above set two equations yields

(7) $$C_1=\frac{acV_z}{\log\left(\frac{a+b}{a+be^{cL}}\right)+cL}$$

(8) $$C_2=\frac{V_z\log(a+b)}{\log\left(\frac{a+b}{a+be^{cL}}\right)+cL}$$

Electric field is equal $\mathbf{E}=-\mathrm{grad}(V)$, that is

(9) $$\mathbf{E}_{\mathrm{a}}=-\frac{\partial V}{\partial x}\mathbf{a}_x=\frac{C_1}{a+be^{cx}}\mathbf{a}_x$$

Gradient of the square of electric field strength is given by

(10) $$\mathrm{grad}\left(E_{\mathrm{a}}^2\right)=\frac{\partial}{\partial x}\left(\frac{C_1^2}{\left(a+be^{cx}\right)^2}\right)\mathbf{a}_x=-\frac{2C_1^2bce^{cx}}{\left(a+be^{cx}\right)^3}\mathbf{a}_x$$

Finally, exact value of the force acting on particle calculated by equivalent dipole method is given by formula [9]:

(11) $$\mathbf{F}_{\mathrm{a}}=\varepsilon_1\pi r_0^2L_{\mathrm{d}}k_{\mathrm{CM}}\left(\varepsilon_2,\varepsilon_1\right)\nabla\left(E_{\mathrm{a}}^2\right)$$

And introduction of equation (10) yields final form of analytical force, which depends on parameters of nonlinear dependence of dielectric permittivity from spatial coordinates. Minus sign means that force is acting from right to left side.

(12) $$\mathbf{F}_{\mathrm{a}}=-2\varepsilon_1\pi r_0^2L_{\mathrm{d}}k_{\mathrm{CM}}\left(\varepsilon_2,\varepsilon_1\right)\frac{C_1^2bce^{cx}}{\left(a+be^{cx}\right)^3}\mathbf{a}_x$$

where k_{CM} is a Clausis-Mosotti coefficient. Numerical solution of the Laplace's equation (2) allow us using adaptive finite element method calculate distribution of potential $V(x)$. Value of the force $F(x)$ acting on the particle is given by (12). For approximation of the unknown potential $V(x)$ Lagrange's polynomial of the third rank was used and calculation process was interrupt, when relative error in every element was less than 10^{-3}. On the following figures relative error resulting from numerical solution of the Laplace's equation was defined as [10]

$$error = \frac{V(x) - V_a(x)}{V_a(x)} 100\% \tag{13}$$

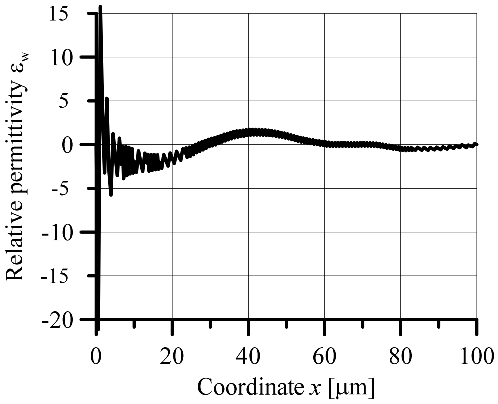

Fig.3. Relative error of potential $V(x)$ for parameter $c = -0{,}1$

Because for $c = -0{,}1$ dependence of permittivity from coordinate x is almost linear (Fig.2), then potential in great extend is homogeneous. Relative error calculation of potential is less than $20{\cdot}10^{-6}\%$ (Fig.3). Relative error of electric field strength is also small and is the same order (Fig.4). Force acting on particle is proportional to derivative of electric field and its error is less than $30.10^{-3}\%$.

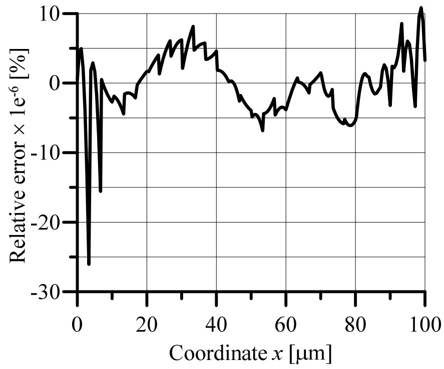

Fig.4. Relative error of potential $E(x)$ for parameter $c = -0{,}1$

For $c = -10$ the shape of the permittivity relative x is in great extend nonlinear, what causes substantially greater error in computations of $E(x)$

The second difference on (Fig.5) potential results in substantially greater error in computations force $F(x)$ (Fig. 7) to value about 3%.

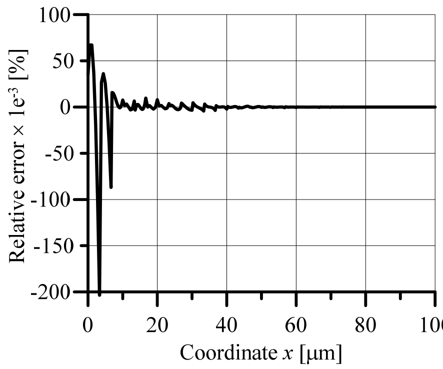

Fig.5. Relative error of potential $E(x)$ for parameter $c = -10$

This is caused mainly by two factors. First through increasing of field inhomogeneity and what is as a result, increasing electric field gradient, and secondly, by using Lagrange's polynomial to approximate unknown potential in every finite element. As it is well known these potentials do not assure potential continuation on elements boundaries. Because force is proportional to second derivative of potential, error in computation of these derivatives causes arising great errors in calculation of force F. Application of Hermite's lub Argyris's polynomials, which guaranty continuity of derivatives on element boundaries can help to solve this problem.

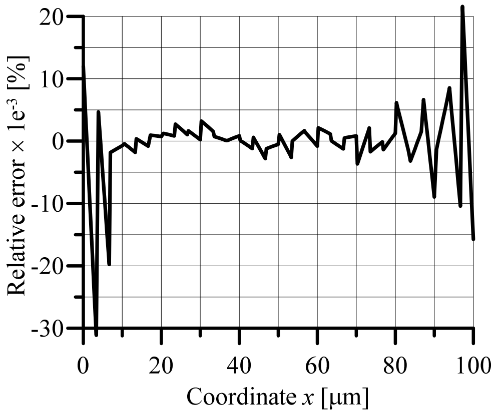

Fig.6. Relative error of potential $F(x)$ for parameter $c = -0{,}1$

Comparisons of relative error computation for two values of parameter **c** show (Fig. 6 and Fig.7) that for highly inhomogeneous electric field computational error is substantial.

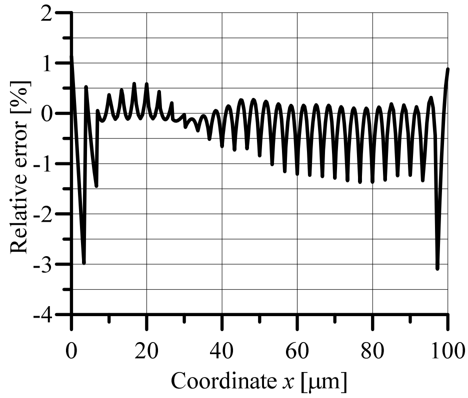

Fig.7. Relative error of potential $F(x)$ for parameter $c = -10$

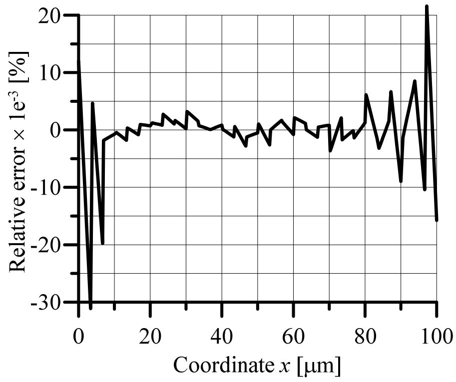

Fig.8. Force $F(x)$ for two values of parameter c

On figure 8 dependence of the force $F(x)$ from coordinate x is shown. For highly inhomogeneous case this dependence is highly nonlinear especially at beginning of the coordinate's origin.

Let us now examine which influence on computational accuracy has placement of particle with the same permittivity as surrounding dielectric (see figure 9).

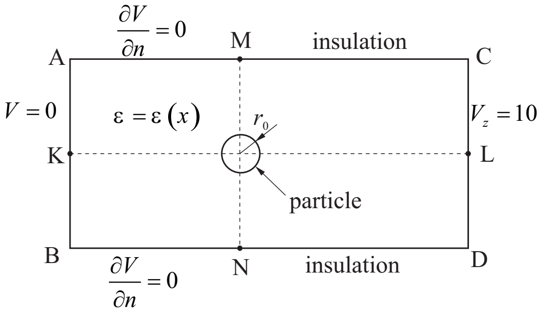

Fig.9. Particle placed in symmetry axis in inhomogeneous medium

From mathematical point of view both cases as in Fig 1 and 9 are completely equivalent, so analytical solution is in both cases identical. But in the case of numerical solutions with boundary element method, additional errors arise due to fulfillment of continuity conditions of electric field on particle-dielectric boundary.

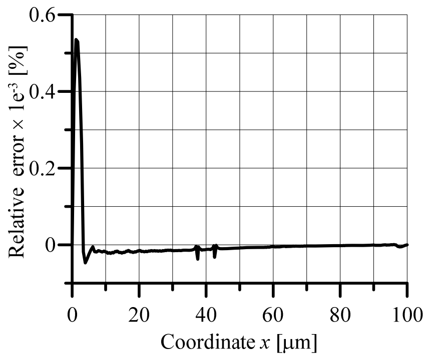

Fig.10. Potential $V(x)$ for parameter value $c = -1$

Particle is placed at coordinate $x_p = 40\mu m$. On figure 10 elative error of potential in function coordinate x is depicted. One can see hat on both sides of the coordinate $x_p = 40\mu m$ we have increasing error. Also at beginning of x-axis the error is substantial.

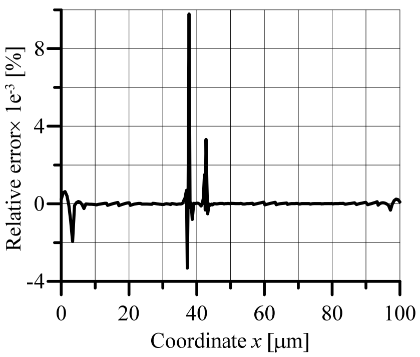

Fig.11. Dependence of electric field $E(x)$ from coordinate x for parameter value $c = -1$

Differentiation of potential causes yet greater error in electric field (see Fig. 11) and subsequently yet greater error in computation of force $F(x)$. The value of the error attains level 7%. This should be taken into account in computation forces by numerical methods.

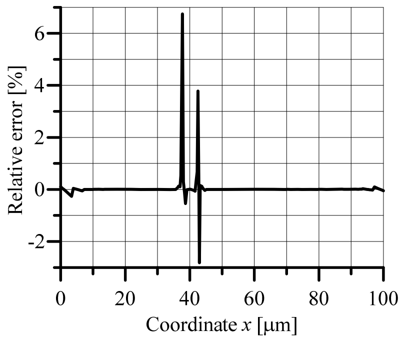

Fig.12. Dependence of force $F(x)$ from coordinate x for parameter value $c = -1$

Conclusions

In this article, cylindrical particle in uniform electric field perpendicular to the particle was considered. Error calculation of numerical method of force computation is presented. I was shown which errors and where are cause by finite element method used in solution Laplace'a equation.

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