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Simulation of Traveling Wave Dielectrophoresis Using a Meshless Method

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Abstract

Manipulation and separation of micron-sized particles, particularly biological particles, using the dielectrophoretic effect is an emerging application in BioMEMS technology. This paper presents a numerical simulation for the four-phase traveling dielectrophoresis (DEP) using a novel meshless method - weighted least square finite difference (LSFD) scheme. The exact boundary condition and nonuniform point distribution were used in the calculation. Numerical results including the electrical potential, electrical field, traveling wave DEP forces and particle behavior are presented. Although the LSFD scheme was originally proposed in solving incompressible viscous flow, it is further demonstrated in this paper that the method is also well suited for solving various DEP problems in which extremely high gradient of electric field exists in the computational domain, e.g. edges of the electrodes. The LSFD method enables the computational ease of free point/mesh distribution in these areas, and hence it is feasible in the modelling of DEP systems.

1 Introduction

With the benefit from the development of micro-electromechanical systems (MEMS), micromachining, and miniaturization technology, it is now possible to conduct biomedical assay and analysis in very small sample volumes (e.g. microliter or nanoliter). Those emerging microfluidic systems such as lab-on-a-chip and micro total analysis system (µTAS) highly impact the field of biomedical science. Generally, the first step in the operation of a biomedical process consists of concentrating and separating the analytes (bioparticles) of interest from the background matrix and positioning them into selected locations for subsequent analysis. Dielectrophoresis (DEP) has a great potential for such applications. Dielectrophoretic force, which arises from the interaction of non-uniform AC electric field with the induced dipole in the particle [1], is particularly suited for manipulation of biological particles, such as cells [2], viruses [3] and DNA [4]. Two types of DEP are widely used, i.e. the two-phase DEP and multiphase DEP. An AC electric signal of two phases is used in the former application, while in the latter a multiphase signal is used as the case for the traveling wave DEP (twDEP).

This paper presents a numerical simulation of electric fields and DEP forces in the four-phase traveling wave interdigitated electrode array using the weighted least-square finite difference (LSFD) scheme, which was proposed by Shu’s group to solve incompressible viscous flow [5]. To the knowledge of the authors, the meshless method is well suited for solving DEP problems in which extremely high gradient of electric field exists, e.g. edges of the electrodes [6]. Using the LSFD scheme, numerical solutions of electric fields and traveling wave DEP forces are obtained for the parallel electrode array. Particle behaviour in the travelling field including levitation and traveling movement is studied.

2 Theory and Methodology

2.1 The four-phase traveling wave DEP

Fig. 1 shows the diagram of the interdigitated microelectrode array system. The electrode array is formed on the top of a glass substrate using microfabrication techniques. The width of electrode stripe is \(d_1\) and the spacing between adjacent electrodes is \(d_2\). A 90° phase-shifted electric signal is applied to the electrode system.

Fig. 1 The four-phase traveling wave array (twDEP).

The time-averaged force acting on a spherical particle comprises two components, the in-phase and out-of-
phase components, which are referred to as DEP and "SDS", or imaginary part supporting points. Matrix geometric information about the distribution of the
where 0
as [5]
components of the phasor, respectively. \( \text{Re} \text{f}_{0m} \mathbb{R}((\mathbf{V} \mathbf{\phi}_{0 \mathbf{r}}) + |\mathbf{V} \mathbf{\phi}_{0 \mathbf{r}}^\dagger|) \) (1a)
\( \text{Im} \text{f}_{0m} \mathbb{I}m((\mathbf{V} \mathbf{\phi}_{0 \mathbf{r}}) + |\mathbf{V} \mathbf{\phi}_{0 \mathbf{r}}^\dagger|) \) (1b)
where \( \varepsilon_0 \) is the permittivity of free space, \( \varepsilon_\infty \) is the relative permittivity of the surrounding medium, \( a \) is the particle radius, \( f_{0m} \) is the Clausius-Mossotti factor (CM factor). \( \text{Re} \) and \( \text{Im} \) denote the real and imaginary components, respectively. \( \phi_x \) and \( \phi_y \) are the real part and imaginary part of the potential phasor \( \phi = \phi_x + i\phi_y \), respectively. The potential phasor or can be solved from the quasi-electrostatic form of Maxwell’s equations[7]
\( \nabla \phi \phi = 0 \) (2)
For the electric field discussed in this work, this reduces to Laplace’s equation for the real and imaginary components of the phasor, respectively
\( \nabla^2 \phi_x = 0 \) and \( \nabla^2 \phi_y = 0 \) (3)

2.2 The least-square finite difference scheme
The least-square finite difference (LSFD) scheme was first proposed by H. Ding et al with application for solving natural convection in a cavity [5]. The method is based on the use of a weighted least-square approximation procedure together with a twodimensional Taylor series expansion. The functional value (e.g. electrical potential) near a reference node can be approximated by the functional value and its derivatives at the reference point by using up to 3rdorder derivatives to the second-order derivatives to the second-order (Eqn. (3)) correspond to the third and the fourth items in the derivative vector \( \mathbf{dF} \), respectively [6]. These two items for each reference point can be represented as
\[
\mathbf{dF} = \mathbf{D} \left( \mathbf{S}^T \mathbf{W} \mathbf{S} \right)^{-1} \mathbf{S}^T \mathbf{W} \mathbf{A} \mathbf{F} = \mathbf{C} \mathbf{A} \mathbf{F}
\] (4)
where \( \mathbf{dF} \) is the derivative vector comprising the derivatives of the functional value up to 3rd order. Matrix \( \mathbf{S} = \mathbf{SD} \), where the matrix \( \mathbf{S} \) contains all the geometric information about the distribution of the supporting points. Matrix \( \mathbf{C} \) is here defined as a coefficient matrix.
As discussed in [5], the above scheme allows us to approximate the second-order derivatives to the second-order accuracy and the first-order derivatives to the third-order accuracy. In this paper, the electric potential and electric field from DEP electrode array are solved using the above LSFD scheme.

2.3 Numerical Discretization
The two items in the left hand of the Laplace’s equation (Eqn. (3)) correspond to the third and the fourth items in the derivative vector \( \mathbf{dF} \), respectively [6]. These two items for each reference point can be represented as
\[
\begin{align*}
\left( \frac{\partial^2 \phi_x}{\partial x^2} \right) &= \sum_{j=1}^{n_0} A_{1j} \phi_j - \phi_x \\
\left( \frac{\partial^2 \phi_y}{\partial y^2} \right) &= \sum_{j=1}^{n_0} A_{2j} \phi_j - \phi_y
\end{align*}
\] (5)
\[
\begin{align*}
\left( \frac{\partial^2 \phi_x}{\partial y \partial x} \right) &= \sum_{j=1}^{n_0} A_{3j} \phi_j - \phi_x \\
\left( \frac{\partial^2 \phi_y}{\partial x \partial y} \right) &= \sum_{j=1}^{n_0} A_{4j} \phi_j - \phi_y
\end{align*}
\] (6)
where \( C_{3j} \) represents the entry of Matrix \( \mathbf{C} \) at 3rd row and \( j \)-th column, and \( C_{4j} \) likewise. \( \phi \) presents for the real part \( \phi_x \) or imaginary part \( \phi_y \) of the potential phasor.
Substituting Eqns. (5) and (6) into Eqn (3) gives the following relationship
\[
\begin{align*}
- \sum_{j=1}^{n_0} \left( C_{3j} \phi_x + C_{4j} \phi_y \right) \phi_j + \sum_{j=1}^{n_0} \left( C_{3j} \phi_x + C_{4j} \phi_y \right) \phi_j &= 0
\end{align*}
\] (7)
Repeating the same process to each point in the domain, a general matrix equation is achieved by adjusting coefficients in a relative row of the coefficient matrix \( \mathbf{A} \)
\[
\mathbf{A} \mathbf{F} = \begin{bmatrix}
\phi_1 \\
\phi_2 \\
\vdots \\
\phi_n
\end{bmatrix} = 0
\] (8)
where \( n \) is the number of points in the domain.
By applying the boundary conditions (see 3.1) into Eqn. (8), the electric potential distribution in the domain can be solved.

3 Results and discussion
3.1 Boundary condition
The problem can be simplified to two-dimensional since the electrodes are quite long compared to their width. The boundary conditions for real part and imaginary part of the potential phasor are shown in Fig. 2, respectively. The problem space covers two halves of selected electrodes and the gap between them. The electric potential was solved using an exact boundary condition, where the potential on the bottom \( y = 0 \) is such that the derivative of the potential is zero (Neumann boundary condition) at the gaps while the potential is definite on the electrode. This type of mixed boundary condition leads to the difficulty of obtaining analytical solutions.

Fig. 2 The problem space for the traveling wave array showing the complete boundary conditions.
3.2 Results

Nonuniform grid point distribution smoothly generated with a grid spacing of 0.5-2 µm in the problem domain was used to solve the problem, as shown in Fig. 3. The problem was solved for a representative design with \(d_1=d_2=d=10\ \mu\text{m}\).

![Fig. 3 Grid point distribution for solving the problem.](image)

The real and imaginary parts of the electric potential phasor are shown in Fig. 4a and b, respectively. The real part is the mirror image of the imaginary part about vertical line through the center of the gap and vice versa.

![Fig. 4 (a) The nondimensional real part \(\phi_x\), and (b) imaginary part \(\phi_y\) of the traveling wave potential phasor.](image)

The logarithmic magnitude and direction of the vector \(\nabla(|\nabla \phi_x|^2+|\nabla \phi_y|^2)\) regarding the conventional DEP (cDEP) force component (Eqn (1a)) are plotted in Fig. 5. As shown in (a), the magnitude of the vector is constant with \(x'\) across the array at sufficient height \((y\sim1.5d)\) above the electrode. The maximum value exists at the electrode edges. As shown in (b), above \(y'\sim1.5\), the vectors point straightly downwards. In the area near the electrode, they direct more and more towards the side edges (at \(x'=0.5, 1.5\)).

![Fig. 5 (a) log_{10} (magnitude), and (b) vector direction of the vector for the cDEP force component: \(\nabla(|\nabla \phi_x|^2+|\nabla \phi_y|^2)\).](image)
Similarly, the vector $\nabla \times (\nabla \phi_x \times \nabla \phi_y)$ for the twDEP force component (Eqn (1b)) is shown in Fig. 6. The magnitude of the vector is constant against $x'$ at sufficient height above the electrode, and maximum value exists at the electrode edges. However, the vectors point laterally towards the negative $x$ direction above the height of $1.5d$. Closer to the electrodes, the vectors show a more complicated pattern around the edges.

The above discussion implies that the actual particle movement comes from the combined contributions of both cDEP and twDEP force components. The former is responsible for the levitation of the particle provided that negative DEP takes place ($\text{Re}(f_{cm}) < 0$) while the latter gives rise to the traveling wave movement of the particle in positive $x$ or negative $x$ direction along the channel.

The particle velocity of the traveling movement caused by the traveling wave DEP force at the levitation height can be calculated from Stokes' formula

$$v_t = \frac{I_{twDEP}}{6\eta \pi a}$$

Here $\eta$ is the viscosity of the fluid.

For particles of different dielectric properties, it means that they will behave differently and therefore they can be separated in the electric field. For example, for the latex bead of 6 $\mu$m in diameter with the following parameters: $V_{rms}=5$ V, $\text{Re}(f_{cm})=-0.45$ and $\text{Im}(f_{cm})=-0.50$, then the levitation height is 43.3 $\mu$m. At this height, the traveling velocity of particle is 87.9 $\mu$m/s in the DI water of viscosity $\eta=1.002 \times 10^{-3}$ Pa.s. While for the another particle has the values of $\text{Re}(f_{cm})=-0.25$ and $\text{Im}(f_{cm})=-0.40$, it will be levitated to the height of 39.6 $\mu$m and its traveling velocity is 125.2 $\mu$m/s at this height. The particles will be separated on the basis of the levitation height and the traveling movement.

4 Conclusion

Numerical solutions for the four-phase traveling wave electrode array have been presented based on a novel meshless numerical method. The problem was solved using the exact boundary condition which has the advantage over the first-order approximate boundary condition. The method provides a fast and simple way of determining DEP and TWD components for electrode arrays. The numerical results demonstrate that bioparticles can be manipulated and separated by the electrode arrays.

References


