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Numerical study of interactive motion of dielectrophoretic particles☆

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ABSTRACT

Dielectrophoresis is one of the popular ways to manipulate bio-particles. In this work, numerical simulations of two-dimensional interactive motion of multiple dielectrophoretic particles in an electrolyte subjected to a uniform DC electric field are performed. The dielectrophoretic forces on particles are calculated by an integral of the Maxwell Stress Tensor (MST) on both sides of the particle surfaces. It is shown that behaviors of interactive motion of dielectrophoretic particles are strongly affected by the difference in permittivity between the particles and the electrolyte. Similar particles (all positive or negative electrophoresis) will finally form a chain parallel to the electric field, whereas dissimilar particles (mixed positive and negative electrophoresis) will form a chain that is perpendicular to the electric field. The particle velocity and time behavior of interactive motion are investigated. The key findings are as follows: as the ratio $(\varepsilon_p{:}\varepsilon_f)$ increases, the chain-formation time decreases for a P–P particle chain, but increases for an N–N particle chain. The chain-formation time will decrease with increase of the particle size ratio $a_{\max}{:}a_{\min}$ for a three-particle chain with different particle sizes.

1. Introduction

Dielectrophoresis (DEP) is a phenomenon where a force is exerted on a dielectric particle in a nonuniform electric field [1–3], the DEP force drives the particles toward higher or lower electric field regions depending on the properties of the particle and the electrolyte. Recently, the DEP manipulation of colloids and biological particles has become more popular in microfluidics. Electrical polarization of finite-size particles can distort the local electric field, resulting in a further nonuniform field around particles. Consequently, an interactive DEP force between particles can be induced even in a uniform electric field. The interactive DEP force can lead to a particle chain observed in particle assembly experiments. DEP assembly of particles has become one of the most important techniques to assemble micro–nano materials in microfluidic applications. For instance, DEP can be used to assemble hematopoietic stem cells into a multilayered structure for studying the process of blood cell production [4], and fabricate biosensors using DNA/protein molecules [5]. The existing DEP force calculation was first developed by Pohl [6] using an equivalent dipole moment (EDM). The EDM has been widely used owing to its simplicity, but it is not accurate in some situations like a high number density or large size of particles [7,8], where the gap between particles is comparable to or smaller than the particle size, and the particles are likely to interact with each other. EDM becomes inapplicable when there is interaction between dielectrophoretic particles. In addition, the Clausius–Mossotti (CM) factor in EDM may not be exactly applicable to non-spherical particles. DEP force calculation based on the Maxwell stress tensor (MST) [8] gives accurate results in all situations in theory, but is cumbersome in implementation. The particles experience hydrodynamic and DEP forces during electrophoresis, while particle motion may distort both the electric and flow fields, which will in turn affect the forces acting on the particles. Fluid–particle–electric field interactions as well as DEP should be fully taken into account in order to accurately predict the electrokinetic particle transport in a microfluidic system. Kang and Li [9] investigated relative motions of a pair of spherical particles in DEP by applying a semi-analytical approximation to the solution of dielectric forces acting on particles and their trajectories. However, their approximate solution is valid only when the initial gap between particles is larger than the particle size. Furthermore, the assumption of a constant Stokes drag is not applicable for DEP particle–particle interaction. House

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et al. [10] studied the DEP particle–particle interactions for ellipsoidal particles using the boundary element method. The boundary element method, however, can only be used in a linear problem in which a thin electric double layer (EDL) is assumed for the DEP interaction force. Using an arbitrary Lagrangian–Eulerian (ALE) method, Ai and Qian [11–14] performed direct numerical simulations of two-dimensional liquid–solid DEP interaction of a pair of cylindrical particles in an externally applied uniform DC electric field. In their works, the flow, electric field and particle motions are solved simultaneously. Later, Kang and Maniyeri [15] performed direct numerical simulations to investigate the DEP interaction of multiple particles. They employed a finite difference method and a smoothed representation technique for solving the electric field. However, all above authors considered the particles as completely insulating medium, and therefore the field inside the particles could be ignored. In general, particle polarization in a field is mainly due to a difference in permittivity between the particle and the surrounding electrolyte. The particle permittivity should therefore be taken into account for a complete DEP study. Recently, Hossan and Dillon [16] investigated the DEP motions of multiple particles using a hybrid immersed interface–immersed boundary method with an aim to examine DEP particle interaction including effect of permittivity difference between the particles and the electrolyte, but DEP particle interaction of multi-particles with different sizes has not been studied. Ai and Qian [17] used arbitrary Lagrangian–Eulerian (ALE) method to perform the direct numerical simulations of two-dimensional DEP particle–particle interactions in an AC electric field. The main objective of this work is to explore dynamic behavior of interactive motion of multiple particles with different sizes in an applied uniform DC electric field via numerical solutions based on the full Navier–Stokes equation and an Arbitrary Lagrangian–Eulerian (ALE) algorithm in which the flow field, electric field and the particle motion are solved simultaneously in the Eulerian framework and the Lagrangian framework. The stress tensor of flow field and electrical field are, respectively, integrated on the particle surfaces to obtain the hydrodynamic force and dielectrophoretic force on the particles. The ALE method has been successfully applied to the particle transportation in a cylindrical channel [18].

2. Validation of numerical accuracy of dielectrophoretic force by Maxwell stress tensor (MST)

To verify the numerical accuracy of MST in calculating electrophoretic force, a comparison is made between the dipole approximation method and the MST method when they are applied to a numerical example as detailed in Refs. [19,20]. A cylindrical particle with permittivity ε_p is immersed in an electrolyte with permittivity ε_f. Based on the equivalent dipole method, the DEP force acting on the particle can be written as follows [19]:

$$f_x = 2C\left[\frac{\partial\varphi}{\partial x}\frac{\partial^2\varphi}{\partial x^2} + \frac{\partial\varphi}{\partial y}\frac{\partial^2\varphi}{\partial x\partial y}\right] \tag{1}$$

$$f_y = 2C\left[\frac{\partial\varphi}{\partial x}\frac{\partial^2\varphi}{\partial x\partial y} + \frac{\partial\varphi}{\partial y}\frac{\partial^2\varphi}{\partial y^2}\right] \tag{2}$$

where φ is the applied electric potential without particles, and the constant C is given by

$$C = \pi\varepsilon_f\frac{\varepsilon_p - \varepsilon_f}{\varepsilon_p + \varepsilon_f}a^2. \tag{3}$$

The subscripts f and p denote the fluid and the particle, respectively, and a is the particle radius. Because the permittivity and electrical field are discontinuous across the particle–fluid interface,

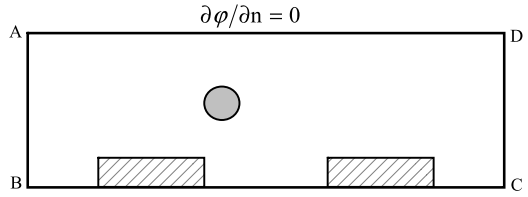

Fig. 1. Computational domain and boundary conditions of the numerical example for validation.

one needs to calculate MST on both sides of the particle surface [19,20]. The Maxwell stress tensors read as follows:

$$\boldsymbol{T}_p^E = \varepsilon_p\left[\boldsymbol{E}_p\boldsymbol{E}_p - \frac{1}{2}\left(\boldsymbol{E}_p\cdot\boldsymbol{E}_p\right)\boldsymbol{I}\right] \tag{4}$$

for particle side of surface

$$\boldsymbol{T}_f^E = \varepsilon_f\left[\boldsymbol{E}_f\boldsymbol{E}_f - \frac{1}{2}\left(\boldsymbol{E}_f\cdot\boldsymbol{E}_f\right)\boldsymbol{I}\right] \tag{5}$$

for fluid side of surface

where I denotes the second-order unit tensor, and $\boldsymbol{E}_f$ and $\boldsymbol{E}_p$ are the electric field in the fluid and in the particle, respectively. The electrophoretic force of particle is obtained by an integral of MST over the particle surface:

$$\mathbf{F}_{\text{dep}} = \oint\left(\boldsymbol{T}_p^E - \boldsymbol{T}_f^E\right)\cdot\mathbf{n}ds \tag{6}$$

where $\mathbf{n}$ is the unit normal vector on the particle surface pointing to the fluid. The numerical example used for validation and the related parameters are given in Ref. [20]. A particle is located in an electric field, as shown in Fig. 1. Two electrodes with different voltages are located at the domain bottom. The voltages on electrode surfaces are applied to generate a nonuniform electric field. The boundaries AB and CD are treated as periodical condition and the others are electrically insulated boundaries $\partial\varphi/\partial n = 0$, and $\varepsilon_p\frac{\partial\varphi_p}{\partial n} = \varepsilon_f\frac{\partial\varphi_f}{\partial n}$ on particle surface. The permittivity of the particle and the electrolyte are $\varepsilon_p = 2.5\varepsilon_0$ and $\varepsilon_f = 80\varepsilon_0$, where ε_0 is the permittivity of vacuum. The computational domain is a rectangle ($160\,\mu\text{m}\times 60\,\mu\text{m}$), the electrode dimensions are ($40\,\mu\text{m}\times 4\,\mu\text{m}$), the gap between the electrodes is $40\,\mu$m. The voltages on electrode surfaces are 10 V and 0 V, respectively. The grids in vicinity of particle surface have been sufficiently refined. A relative error criterion of 10^{-3} of dielectrophoretic forces of particle is used to obtain grid-independent numerical solutions in the present example. COMSOL Multi-physics is employed to compute the dielectrophoretic forces of the particle. The numerical details can be found in Refs. [11–14].

A comparison of the electrophoretic force on a cylindrical particle calculated by the MST and the EDM is shown in Fig. 2.

It can be seen that EDM and MST method give almost the same DEP force for a small particle, $a \le 2\,\mu$m in the present example. Deviation of EDM and MST increases with the increase of the particle radius. It has been known that EDM is based on the point–dipole assumption, which is accurate only for a single small particle, the MST is theoretically exact in general. All following numerical results of this work are obtained by MST method.

3. Governing equations and boundary conditions for particle interaction in an electric field

A particle with permittivity ratio $(\varepsilon_p{:}\varepsilon_f) > 1$ is defined as a positive dielectrophoretic particle, abbreviated as a P particle in this paper. A particle with $(\varepsilon_p{:}\varepsilon_f) < 1$ is defined as a negative dielectrophoretic particle, or an N particle. Particles are called similar when they are either all P particles (P–P), or all N particles