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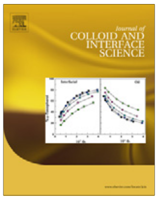

Modeling and simulation of dielectrophoretic particle–particle interactions and assembly

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ABSTRACT

Electric field induced particle–particle interactions and assembly are of great interest due to their useful applications in micro devices. The behavior of particles becomes more complex if multiple particles interact with each other at the same time. In this paper, we present a numerical study of two dimensional DC dielectrophoresis based particle–particle interactions and assembly for multiple particles using a hybrid immersed interface-immersed boundary method. The immersed interface method is employed to capture the physics of electrostatics in a fluid media with suspended particles. Particle interaction based dielectrophoretic forces are obtained using Maxwell's stress tensor without any boundary or volume integration. This electrostatic force distribution mimics the actual physics of the immersed particles in a fluid media. The corresponding particle response and hydrodynamic interactions are captured through the immersed boundary method by solving the transient Navier–Stokes equations. The interaction and assembly of multiple electrically similar and dissimilar particles are studied for various initial positions and orientations. Numerical results show that in a fluid media, similar particles form a chain parallel to the applied electric field, whereas dissimilar particles form a chain perpendicular to the applied electric field. Irrespective of initial position and orientation, particles first align themselves parallel or perpendicular to the electric field depending on the similarity or dissimilarity of particles. The acceleration and deceleration of particles are also observed and analyzed at different phases of the assembly process. This comprehensive study can be used to explain the multiple particle interaction and assembly phenomena observed in experiments.

1. Introduction

Due to a high degree of selectivity and sensitivity, dielectrophoresis (DEP) has become one of the most promising and popular tools for characterization, manipulation, and actuation of biomaterials and biological entities in micro/nanofluidic devices. In dielectrophoresis, an applied electric field polarizes dielectric particles or materials and hence causes a net force due to unequal electric fields on the accumulated charges. This net force drives the particles toward higher or lower electric field regions depending on the properties of the medium and the particles. Dielectrophoresis works both on charged and neutral particles. Since the inception of microfabrication techniques, a growing number of researchers have been using this phenomenon, and many valuable applications such as cell separation [1], sorting [2], trapping [3] as well as isolation [4], concentration [5], and characterization of biological particles [6] have already been demonstrated. In recent years, dielectrophoretic force has also been used for the assembly of colloidal particles into a structure [7], the formation of tissues using biological cells [8], and fabrication of biosensors using DNA/protein molecules [9] .

Dielectrophoretic assembly has better control and faster response rates compared to the other micro/nano assembly processes such as capillary [10], sedimentation [11], chemical [12], and electro-optical [13]. In dielectrophoresis, two major contributing factors are particle polarization and electric field nonuniformity. Particles in a close proximity alter the electric field and create local nonuniformity in the electric field between particles. Due to this asymmetric electric field, dielectrophoresis based particle–particle interaction forces act on each other. This interaction force can be manipulated to assemble micro/nano particles and biological cells. Chung et al. [14] demonstrated the large scale assembly and integration of carbon nanotubes by dielectrophoresis. Velev and Kaler developed an electrically activated biosensor using dielectrophoretic interaction forces with on-chip electronic

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circuits [9]. Using in vitro dielectrophoretic assembly, Gerard et al. [15] created an artificial microenvironment by multilayered cell aggregation for hematon, a blood producing stem cell. Assembly of live cells and functionalized microparticles were reported by Gupta et al. [16].

Despite many engineering and biomedical applications of dielectrophoretic assembly, the underlying fundamental mechanisms behind this self-assembly process have not yet been fully understood due to the complexity of the transient micro/nanoscale physics. The phenomenon becomes more complex with an increase in the number of interacting particles [17]. Along with experimental investigations, many researchers have used numerical techniques to simulate these complex dynamic phenomena since numerical simulations are fast, efficient, and the relevant parameters can be readily changed in a controlled manner. Kang and Li [18] analyzed particle trajectories by balancing Stokes drag and dielectrophoretic forces using similar particles. However, their approximate solution is valid only if the initial gap between particles is larger than the particle size. Moreover, constant Stokes drag is not appropriate for dielectrophoretic particle–particle interaction. Aubry and co-workers [19,20] quantified the inherent dielectrophoretic force and particle–particle interaction force based on two characteristic length scales – spatial nonuniformity of the electric field and the distance between two particles – using Lagrange multiplier methods. They concluded that the particle–particle interaction force can be nullified by selecting an appropriate liquid media so that the Clausius–Mossotti factor becomes small. However, Aubry and co-workers calculated dielectrophoretic forces using a simplified point dipole method which is not valid when particles are close to each other [20]. Recently Ai and Qian [21] studied dielectrophoretic particle–particle interaction with their relative motion in the suspending media using the commercial finite element package COMSOL by adopting the arbitrary Lagrangian–Eulerian (ALE) method. The ALE approach is computationally expensive as it requires continuous remeshing, and it becomes extremely challenging if one has to consider more particles. House et al. [22] studied the dielectrophoretic particle–particle interactions for ellipsoidal particles using the boundary element method. The boundary element method can only be used in a linear problem such as a dielectrophoretic interaction force using a thin electric double layer (EDL) assumption. All these aforementioned numerical studies considered particle–particle interaction and assembly for similar particles only, but these phenomena are quite different for dissimilar particles [23].

In this study, we present a systematic investigation into the fundamental physics behind particle assembly with multiple similar and dissimilar particles using a hybrid immersed boundary and immersed interface method. The immersed boundary method has been demonstrated to be a stable, efficient, and accurate method for fluid flow with solid–fluid interaction, especially in biological applications with moving inner boundaries [24–26]. On the other hand, the immersed interface method, with a fast algorithm, is particularly well suited for the solution of electric field calculations using the Laplace or Poisson equations with large coefficient jumps across the interface [27]. This hybrid method is simpler, computationally less expensive, and more efficient compared to boundary-fitted methods such as ALE methods. This coupled immersed boundary-immersed interface method is capable of capturing the underlying physics of dielectrophoresis for multiple particles, handling the complex shape and geometry of particles as well as various electrode configurations. Multi-particle interaction forces were calculated based on the Maxwell and hydrodynamic stress tensor, and thus, this study has relaxed many simplified and limiting approximations such as the effective dipole moment and Stokes drag assumptions used in earlier studies.

2. Theory

In this study, we assume that the electric field induced particle interaction and particle assembly are attributed only to DC dielectrophoresis, and we neglect other electrokinetic effects such as electrophoresis and electro-osmosis. Electrophoresis can be neglected if the particles are not charged. On the other hand, the electro-osmotic contribution is very minor due to the ultra small electric double layer [21]. The effect of van der Waals force was not considered here as our numerical algorithm requires a finite separation distance (typically a grid spacing) between particle–particle and particle–wall. For the typical grid spacing considered in this study, the van der Waals force as well as the Brownian force is much smaller than the electrostatic and hydrodynamic force [21]. To reduce the computational complexities, we have only considered two dimensional geometries. However, the mathematical models presented in this study can easily be extended to three dimensional objects.

The physics of dielectrophoretic particle assembly can be explained in terms of the charge distribution at the interface between a particle and its suspending media under an external electric field. Because of the different dielectric properties between particles and surrounding liquid, the charge accumulations are uneven and hence produce an induced electric dipole – a net positive charge on one side and a net negative charge on the other side of the particle. Thus, in the presence of a nonuniform electric field, unequal opposing forces are created at the opposite sides of the particle, and the particle experiences a net force. The nonuniformity in the electric field can be imposed externally by geometric or electrode configurations. Alternatively, it can be induced locally due to the presence of another particle in close proximity. The direction of this net force depends on the polarizability of the surrounding media and suspended particle. When a particle is more polarizable compared to the media, the net force is directed toward the higher electric field region and vice versa [23]. Under this dielectrophoretic force, the particle travels within a suspending media, induces a flow in a stationary media, and alters the adjacent flow field in a moving media. Hence, in dielectrophoresis, there are complex interactions among the electric field, the particle positions and orientations, and the hydrodynamic flow field.

2.1. Governing equations and boundary conditions

To develop a mathematical model, we consider two particles suspended in a rectangular domain (Fig. 1a) filled with an incompressible and Newtonian viscous fluid. The particle domains are represented by Ω_p with the particle surfaces represented by Γ_p, $p = 1, \ldots, N_p$, where N_p is the number of suspended particles. Considering the typical applied electric field frequency and the characteristic time scale in microfluidic devices, dielectrophoresis can be described as a combination of a quasi-electrostatic and a flow problem. The governing equation for electric potential distribution for a quasi-electrostatic problem can be described by the Gauss' electrostatic law:

$$\nabla \cdot (\tilde{\varepsilon} \nabla \tilde{\varphi}) = 0. \tag{1}$$

The complex permittivity $\tilde{\varepsilon}$ and the complex potential $\tilde{\varphi}$ are given as

$$\tilde{\varepsilon} = \varepsilon - j\sigma/\omega \tag{2}$$

$$\tilde{\varphi} = \varphi(\vec{x})e^{j\omega t} \tag{3}$$

where ε is permittivity, σ is electrical conductivity, and t is time. The angular frequency ω is related to frequency f as $\omega = 2\pi f$. In a low frequency range, the electrical conductivity of the system