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Direct numerical simulation of AC dielectrophoretic particle–particle interactive motions

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ABSTRACT

Under an AC electric field, individual particles in close proximity induce spatially non-uniform electric field around each other, accordingly resulting in mutual dielectrophoretic (DEP) forces on these particles. The resulting attractive DEP particle–particle interaction could assemble individual colloidal particles or biological cells into regular patterns, which has become a promising bottom-up fabrication technique for bio-composite materials and microscopic functional structures. In this study, we developed a transient multiphysics model under the thin electric double layer (EDL) assumption, in which the fluid flow field, AC electric field and motion of finite-size particles are simultaneously solved using an Arbitrary Lagrangian–Eulerian (ALE) numerical approach. Numerical simulations show that negative DEP particle–particle interaction always tends to attract particles and form a chain parallel to the applied electric field. Particles usually accelerate at the first stage of the attractive motion due to an increase in the DEP interactive force, however, decelerate until stationary at the second stage due to a faster increase in the repulsive hydrodynamic force. Identical particles move at the same speed during the interactive motion. In contrast, smaller particles move faster than bigger particles during the attractive motion. The developed model explains the basic mechanism of AC DEP-based particle assembly technique and provides a versatile tool to design microfluidic devices for AC DEP-based particle or cell manipulation.

1. Introduction

Dielectrophoresis refers to the motion of polarized particles under a spatially non-uniform electric field. Due to the simplicity in miniaturized integration of electric fields into microfluidics, dielectrophoresis has become one of the most popular techniques for particle manipulation in microfluidics [1]. One of the most interesting applications is directed assembly of individual colloidal particles or biological cells into microscopic functional structures. For example, electrically functional microwires can be fabricated from the assembly of metallic nanoparticles suspended in an aqueous medium [2]. Two-dimensional (2D) crystals have also been constructed from individual particles using a similar dielectrophoretic (DEP) assembly technique [3–5]. In addition, this technique has been exploited to assemble hematopoietic stem cells into a multilayered structure, mimicking the hematon for blood cell production [6]. Assembly of live biological cells and functionalized microparticles could open a new door for the development of novel tools for tissue engineering and biosensing [7,8].

Attractive chaining phenomenon of individual particles is the basis of DEP assembly technique. When an electric field is imposed in a particle suspension, the presence of particles locally distorts the electric field. If individual particles are close to each other, the non-uniform electric field around each particle becomes asymmetric with respect to its center, and accordingly induces a mutual DEP force acting on each other. If the mutual DEP force arising from the particle–particle interaction is attractive, particles tend to approach each other and eventually form a chain. Hwang et al. [9] performed an experimental study on the DEP particle–particle interaction, in which a pair of spherical particles, initially presenting an angle with respect to the applied electric field, were attracted to form a chain parallel to the electric field. Additionally, the alignment and assembly of two rod-shaped particles, as a result of the DEP particle–particle interaction, were also experimentally observed [10].

Besides growing experimental studies on the DEP assembly technique, further efforts have also been made on numerical simulations to gain an insightful understanding of the DEP particle–particle interaction. Aubry and her co-workers [11–14] developed a Lagrange multiplier-based numerical model to study the particle motion resulting from the DEP particle–particle interaction. The DEP force was calculated using a simplified point dipole (PD)

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method in their model, which is sufficiently accurate when the gap between two particles is larger than the particle size [15]. Later, Kang and Li [16] investigated the DEP particle–particle interaction by balancing the DEP force and Stokes drag force. However, the approximation solution for the DEP particle–particle interactive force adopted in their study is also valid exclusively when the gap between particles is larger than the particle size. Maxwell stress tensor (MST) method has been demonstrated as the most rigorous approach for DEP force calculation [17–19]. Ai and Qian [20] adopted the MST method to account for the distortion of the electric field due to the presence of particles, and investigated particle–particle interactive motions under DC electric fields based on an arbitrary Lagrangian–Eulerian (ALE) method. It was found that the negative DEP particle–particle interaction always tends to chain particles parallel to the applied DC electric field. Recently, Ai and Qian's model was further implemented by other numerical methods, such as smoothed profile method [21], boundary element method [22], and immersed boundary method [23], which predicted similar attractive motions of initially separated particles. In particular, House et al. [22] found that non-spherical particles could self-align with the applied electric field during the attractive chaining. It was also demonstrated that positive DEP particle–particle interaction tends to chain particles perpendicular to the applied electric field [23]. Note that all these studies considering finite-size particles with the MST method are under DC electric fields. However, AC electric fields are typically preferred in the application of DEP-based particle assembly, because electrophoresis of inherently charged particles can be eliminated in AC electric fields. In addition, it is feasible to switch the DEP motion from positive to negative, and vice versa, by tuning the frequency of AC electric fields. AC electric fields can also inhabit the electrolysis of water, a very common disadvantage for the DEP technique under DC electric fields.

In this study, we developed a transient numerical model to investigate DEP particle–particle interactive motions under AC electric fields. The MST method is adopted to calculate the time-averaged AC DEP force acting on each particle. The fluid flow field, AC electric field and particles' motions are simultaneously solved using the ALE moving mesh algorithm. Transient positive and negative DEP motions of a single particle undergoing spatially non-uniform AC electric fields are first simulated to demonstrate the capability of the developed numerical model. AC DEP interactive motions of a pair of particles of identical and dissimilar sizes are subsequently studied to reveal the mechanism of AC DEP-based particle assembly technique.

2. Mathematical model

We consider two circular particles suspended in an incompressible Newtonian fluid confined in a square with a side length of L, as illustrated in Fig. 1. The center of the square fluid coincides with the midpoint of the connecting line of the two particles, which is selected as the origin of the 2D Cartesian coordinate system (x, y). The radii of the particles initially located in the third quadrant and the first quadrant are b and c, respectively. The two particles are initially separated with a center-to-center distance of R, presenting an angle of θ with respect to the x-axis. An AC electric field is applied along the x-axis to induce the DEP particle–particle interaction, and meanwhile excluding electrophoretic and electroosmotic effects in this study. It has been theoretically demonstrated that the effect of Brownian motion is usually negligible in short-range DEP particle–particle interactions [20]. In addition, our numerical method requires a finite separation distance between the two particles, which is larger than a typical thickness of electric double layer (EDL). For example, the EDL thickness of

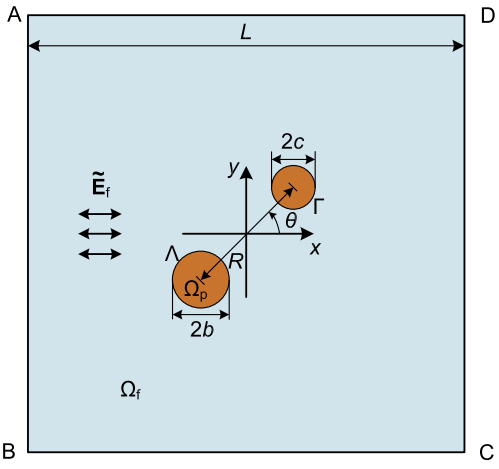

Fig. 1. Two particles are suspended in a fluid medium under an externally applied AC electric field $\tilde{\mathbf{E}}_f$. The origin of the Cartesian coordinate systems (x, y) is located at the midpoint of the connecting line of the two particles and also the center of the square fluid domain ABCD. The distance between the two particles and the angle between the connecting line of the two particles and the external electric field are, respectively, R and θ. The fluid domain and particle domain are denoted by Ω_f and Ω_p, respectively. The surfaces of the particles in the first quadrant and the third quadrant are denoted by Γ and Λ, respectively.

a charged surface in a 0.1 M KCl solution at 25 °C is approximately 1 nm. Therefore, the EDL interactive force and van der Waals force are ignored in the present study.

The net charge density in the entire computational domain is zero because of the thin EDL assumption. Therefore, the distribution of the quasi-static electric potential is governed the Gauss's law, given by

$$\nabla \cdot (\tilde{\varepsilon}_f \nabla \tilde{\phi}_f) = 0 \quad \text{in } \Omega_f, \tag{1}$$

and

$$\nabla \cdot (\tilde{\varepsilon}_p \nabla \tilde{\phi}_p) = 0 \quad \text{in } \Omega_p, \tag{2}$$

where $\tilde{\varepsilon}_f = \varepsilon_f - j\sigma_f/\omega$ and $\tilde{\varepsilon}_p = \varepsilon_p - j\sigma_p/\omega$ are, respectively, the complex permittivity of the fluid and particle, $\tilde{\phi}_f$ and $\tilde{\phi}_p$ are, respectively, the complex potential in the fluid and particle. In the above, ε_f and σ_f are the permittivity and conductivity of the fluid, respectively. Similarly, ε_p and σ_p are the permittivity and conductivity of the particle, respectively. ω is the angular frequency of the AC electric field. $j = \sqrt{-1}$ is the imaginary unit. The superscript "$\sim$" represents complex variables.

Electric potential applied to generate the AC electric field is given by

$$\tilde{\phi}_f = \frac{\phi_0}{2} \quad \text{on AB}, \tag{3}$$

and

$$\tilde{\phi}_f = -\frac{\phi_0}{2} \quad \text{on CD}. \tag{4}$$

Electric insulation is applied on all the other boundaries

$$\mathbf{n} \cdot \tilde{\varepsilon}_f \nabla \tilde{\phi}_f = 0 \quad \text{on AD and BC}, \tag{5}$$

where $\mathbf{n}$ is the unit normal vector on the corresponding boundary. The electric potential and the normal component of the electric displacement are both continuous at the interface between the fluid and particle, given by

$$\tilde{\phi}_f = \tilde{\phi}_p \quad \text{on } \Lambda \text{ and } \Gamma, \tag{6}$$

$$\mathbf{n} \cdot \tilde{\varepsilon}_f \nabla \tilde{\phi}_f = \mathbf{n} \cdot \tilde{\varepsilon}_p \nabla \tilde{\phi}_p \quad \text{on } \Lambda \text{ and } \Gamma. \tag{7}$$