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Simulation of Dielectrophoretic Motion of Microparticles Using a Molecular Dynamics Approach

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ABSTRACT

We model and simulate dielectrophoresis of micro-scale particles using the finite element method. A soft sphere system molecular dynamics model is presented, which solves a set of equations for the motion of every particle. The model couples most of the significant forces, i.e. the dielectrophoresis (DEP) forces, the particle-particle electrostatic forces, particle-particle interfacial repulsive forces, particle-wall repulsive forces and the hydrodynamic forces in Stokes flow. Since the system of equations is stiff, an implicit scheme is used. To obtain the particle trajectories, a constant time-step is applied. We present some numerical tests computing hydrodynamic force, electrostatic force and DEP force using our model, including simulated trapping of particles in a micro channel by dielectrophoresis. The results are in agreement with the theories and the experimental observations.

1 INTRODUCTION

During the past few decades, the application of dielectrophoresis (DEP) for collecting, positioning and separating particles suspended in liquids has advanced tremendously due to improvements in micro-fabrication techniques. Numerical modeling and simulation of the phenomenon is very helpful for predicting and optimizing design. The motion of the particles and fluids in direct current (DC) fields has been the subject of study for over 100 years, and during the past four decades the behavior of particles in alternating current (AC) fields has also been studied in great detail. DEP is defined as the motion imparted on uncharged particles as a result of polarization induced by non-uniform electric fields. The result can be that the particles move towards regions of a high electric field gradient which is referred as positive dielectrophoresis (pDEP) [1], or the particles move away from the high electric field gra-

dient area, which is referred to as negative dielectrophoresis (nDEP). The behavior depends on the frequency of the AC and the dielectrophoretic properties of the particles and the medium. The pioneer in this area was Herbert Pohl, who wrote a classical text on DEP [1]. Tomas B. Jones contributed a great deal on the theory of electromechanical properties of particles, by developing simple yet general models useful for predicting diverse examples of field-particle interactions [2]. N. G. Green and H. Morgan have made a thorough investigation of the underlying principles and theory of AC electrokinetics paying particular attention to applications for sub-micrometer and nano-particles [3].

In order to simulate the collection or separation process, the direct numerical models for multi-phase flows are widely used because the interactive forces between particle and particle, as well as between particle and fluid, are playing important roles. Generally speaking, among the direct numerical simulation models of two phase flows, the most used ones can be divided into two main classes. The first one is to discretize the Navier-Stokes equations on a fixed, Eulerian grid and move the particles in this grid. Probably the Glowinski's Lagrange Multiplier method [4] is the most generally used one. It has been used in dielectrophoresis simulation by J. Kadaksham [10]. In the case of distributed fluid particles, a similar approach was introduced by Tryggvason and his collaborators [12], in which the shape of particles is often deformable. Therefore, the former is applied in solid-fluid cases, and the latter applied mostly in gas-fluid situations. The second type of method uses moving grids and usually requires re-meshing and re-interpolation. Examples of such techniques developed by Hu [11] and Johanson as well as by Tezduyar [18].

Instead of using multi-phase models, we have chosen to use a molecular dynamics (MD) method [20]. This method provides a way of solving a set of equations of the motion of each particle by replacing them by a set of finite difference equations which are solved on a step-by-step basis. Given particle positions, velocities and other dynam-

ical properties at time t , the updated positions, velocities, etc. at a later time, $t + \Delta t$, can be obtained quite easily and to a sufficient degree of accuracy. In principle, a solution of the equation will automatically satisfy the conservation laws of energy and generated particle trajectories because these equations are strictly reversible in time. The disadvantage of the MD method is that it can be time consuming if the number of particles is large. However in our situation, the number of particles is less than 100, and MD methods could work efficiently.

The MD methods can be divided into two classes. One is hard sphere system models. The motion of hard spheres is characterized by a straight trajectory and a constant velocity, which only changes as a consequence of collision. It has been used to include particle surface roughness as described by O'Dell and Berne [22]. The other one is based on soft sphere systems, which was first reported by Rahman [21]. Unlike the hard sphere MD models, where the generated trajectories are exact but the time intervals are variable, the soft sphere MD models generate approximate trajectories and normally use a constant time interval for all particles. In our system, the velocities of the particles change before collisions happen, therefore, a soft sphere MD model is suitable.

The MD method for soft sphere systems has been extensively used to simulate particle at the atomistic level where Brownian motion plays an important role [7]. However, if the method is modified to suit our problem, it is quite efficient since there will be no need to solve the Navier-Stokes equations. The reason is that according to the specified micro-scale condition, the analytical expression for the hydrodynamic forces between suspended particles in Stokes flows (which is exactly what we have) has been well established. Stimson and Jeffery [6] have shown the hydrodynamic interaction correction functions in great detail between particles. Those functions could be directly adopted to account for hydrodynamic interaction between particles. Besides, since we assume the particles to be spherical, there is no need to consider their deformation. It is reasonable to just add repelling forces to the particles while they are approaching each other's interface. The net DEP force acting on the particle by the field and the interactive electrostatic force from other particles can be also added on the centers of mass of particle. Therefore, we are able to include all the forces into a set of coupled equation of motion (ordinary differential equations) for many-body systems. There is no need to solve the Navier-Stokes equation if we are not interested in the fluid itself. All that is necessary to do is to solve the equations for the motion of particles.

Compared with other soft sphere MD models, our model does not include Brownian force because it is negligible when dealing with the micro size level. Another difference is that, instead of the commonly used motion integration method (the Verlet algorithm), the Implicit Euler method is used to avoid the time step restriction due to the nature of explicit schemes. An earlier version of our model has been used to simulate superpositioned dielectrophoresis

for trapping *E. coli* cells [15].

NOMENCLATURE

r	radius of particle
$\mathbf{E}$	applied electric field
E_0	magnitude of uniform electric field
$\mathbf{F}_E$	total electric force (DEP add inter electrostatic)
$\mathbf{F}_D$	particle-particle electrostatic interaction force
$\mathbf{F}_{DEP}$	dielectrophoretic force
$\mathbf{F}_W$	the force particle collides with the Potential wall
$\mathbf{F}_P$	particle-particle repulsive force
$\mathbf{FG}$	dimensionless hydrodynamic force
$\mathbf{FD}$	dimensionless dielectrophoresis force
$\mathbf{FDIP}$	dimensionless inter electrostatic force
i, j	particle indices
$\mathbf{p}$	effective dipole moment
f_{CM}	Clausius-Mossoti factor
β	Real part of Clausius-Mossoti factor
ω	frequency of AC electric field
$\mathbf{U}$	velocity of fluid
$\mathbf{U}_i$	velocity of particle i
x, y, z	coordinate axes
L	width of the domain for computation
Re_L	Reynolds number based on domain width
t	time
ϵ_m	permittivity of fluid
ϵ_p	permittivity of particle
ϵ_0	permittivity of vacuum
μ	dynamic viscosity of the fluid
ϕ	electric potential
n	time step index
p	pressure
P_1	ratio of hydrodynamic and Stokes drag force
P_2	ratio of DEP force and Stokes drag force
P_3	ratio of inter electro-static and Stokes drag force
P_4	ratio of hydrodynamic and DEP force
P_5	ratio of inter electro-static and DEP force
$R_{i,j}$	distance between particle i and j
$\mathbf{R}_{i,j}$	distance vector of particle i and j
$\hat{\mathbf{R}}_{i,j}$	normalized distance vector of particle i and j
σ_m	conductivity of medium
σ_p	conductivity of particle
N	total number of particles
(x_i, y_i)	the center position of particle i
St	Stokes number

2 THEORY AND MODEL

2.1 DIELECTROPHORESIS

Dielectrophoresis (DEP) is the motion induced by the force from a non-uniform electric field exerted on a polarisable particle [1]. The time-average DEP force $\langle \bar{F}(t) \rangle$ acting on a particle due to an imposed electrical field $\mathbf{E}(\omega)$ can be approximated in terms of dipole effects as:

$$\mathbf{F}_{DEP} = 4\pi r^3 \epsilon_m \beta \mathbf{E} \cdot \nabla \mathbf{E} \quad (1)$$

The real part of the dipolar Clausius-Mossotti factor, β in equation 1 is given by: $\beta = \frac{\epsilon_p^*(\omega) - \epsilon_m^*(\omega)}{\epsilon_p^*(\omega) + \epsilon_m^*(\omega)}$.

Here, $\epsilon^* = \epsilon - j\frac{\sigma}{\omega}$, and $j = \sqrt{-1}$. It is also assumed that the electrostatic force acting on a particle is given by the point-dipole approximation as suggested by J. Klingenberg [8].

It is well known that the polarized particles of a suspension are not only subjected to the applied external electric field, but also give rise to electrostatic forces acting on each other because the polarization also generates an electric field of its own. Therefore, the total electrostatic force $\mathbf{F}_{E,i}$ acting on the i^{th} particle can be written as

$$\mathbf{F}_{E,i} = \mathbf{F}_{DEP,i} + \mathbf{F}_{D,i} \quad (2)$$

where $\mathbf{F}_{DEP,i} = 4\pi r^3 \epsilon_m \beta \mathbf{E}_i \cdot \nabla \mathbf{E}_i$ is the DEP force acting on the i^{th} particle and $\mathbf{F}_{D,i} = \sum_{j=1, j \neq i}^N \mathbf{F}_{D,ij}$ is the net electrostatic interacting force acting the i^{th} particle, which could be approximated as [13]:

$$\begin{aligned} \mathbf{F}_{D,ij} = & \frac{1}{4\pi\epsilon_m} \frac{3}{R^5} (\mathbf{R}_{ij}(\mathbf{p}_i \cdot \mathbf{p}_j) + (\mathbf{R}_{ij} \cdot \mathbf{p}_i)\mathbf{p}_j \\ & + (\mathbf{R}_{ij} \cdot \mathbf{p}_j)\mathbf{p}_i - \frac{5}{R^2} \mathbf{R}_{ij}(\mathbf{p}_i \cdot \mathbf{R}_{ij})(\mathbf{p}_j \cdot \mathbf{R}_{ij})) \end{aligned}$$

where the effective dipole moment $\mathbf{p} = 4\pi\epsilon_m r^3 \beta \mathbf{E}$. Actually, this expression neglects higher order (multipole) terms. Hence, the use of the point-dipole approximation should strictly speaking be limited to situations where the radius of the particle is less than the characteristic length (for instance the length of the electrodes).

2.2 HYDRODYNAMIC FORCE IN STOKES FLOW

One of the aims in this paper was to take the hydrodynamic force into account. The governing equations of the motion of an incompressible fluid, the Navier-Stokes equations, could be non-dimensionalized as [19]:

$$Re \left(\frac{\partial \mathbf{U}}{\partial t} + \mathbf{U} \cdot \nabla \mathbf{U} \right) = -\nabla p + \nabla^2 \mathbf{U} \quad (3)$$

$$\nabla \cdot \mathbf{U} = 0 \quad (4)$$

where Re is Reynolds number defined as $Re = \frac{UL}{\nu}$, which determines the relative importance of the fluid inertia and viscous forces. However, in micro flows, the nonlinear terms can be neglected, and in such cases the governing equations are the Stokes equations can be written as:

$$Re \left(\frac{\partial \mathbf{U}}{\partial t} \right) = -\nabla p + \nabla^2 \mathbf{U} \quad (5)$$

$$\nabla \cdot \mathbf{U} = 0 \quad (6)$$

Based on the Stokes equations, a suspension of colloidal particles is considered. The motion of a given particle induces a flow field in the solvent, which will be felt by

every other particle. As a result, these particles experience a force which can be said to result from hydrodynamic interaction with the original particle. By solving the Stokes equation for a two-particle case, the expression for the hydrodynamic force is obtained [14]:

$$\mathbf{F}_{drag,1} = -6\pi\mu r \mathbf{U}_1 + 6\pi\mu r \frac{3r}{4R_{21}} (1 + \hat{R}_{21} \hat{R}_{21}) \cdot \mathbf{U}_2$$

where $\mathbf{1}$ is the unit tensor, and $\hat{R}_{12} = \frac{\mathbf{x}_2 - \mathbf{x}_1}{|\mathbf{x}_1 - \mathbf{x}_2|}$, which is a vector, and $R_{i,j}$ is the distance between particle i and j , which is a scalar.

Correction resulting from n -body interactions ($n \geq 3$) are of the order $(\frac{r}{R_{ij}})^2$ or higher and need not to be taken into account. As an example, a particle A may affect a particle C directly, or indirectly by affecting a particle B that is affecting particle C. The indirect influences are expressed by correction functions, and since they are of order $(r/R_{ij})^2$ or higher ([14]), only direct particle-particle influences need to be considered.

Therefore, the above expression can be generalized to:

$$\mathbf{F}_{drag,i} = - \sum_{j=1}^N \zeta_{ij} \cdot \mathbf{U}_j \quad (7)$$

where $\zeta_{ii} = 6\pi\mu r \mathbf{1}$, $\zeta_{ij} = 6\pi\mu r \frac{3r}{4R_{ij}} (1 + \hat{R}_{ij} \hat{R}_{ij}) \cdot \mathbf{U}_j$, and $\mathbf{F}_{drag,i}$ is the total force that the i^{th} particle experiences from the fluid. Actually, Equation 7 is described as the mobilities matrix by Stokesian dynamics [14].

To maintain stability and to avoid the time step restrictions of explicit methods, the velocity $\mathbf{U}_i$ in Equation 7 is discretized using an implicit scheme. Therefore, a nonlinear matrix solver must be utilized.

2.3 NUMERICAL MODELLING AND METHODS

Ignoring Brownian motion (Brownian motion is negligible in micro scale [5]), the buoyancy force (assuming the particle has the same density as the fluid), and the motion of the buffer solution, the equation of the motion of the i^{th} suspended particle could be written as

$$m_p \frac{d\mathbf{U}}{dt} = \mathbf{F}_{E,i} - \mathbf{F}_{drag,i} \quad (8)$$

Typically, when the particle radius is smaller than 10 μm in a buffer solution with a viscosity close to that of water, the inertial effects on particle motion can be neglected [3]. The repulsive forces from the interfaces of the other particles ($\mathbf{F}_{P,i} = \sum_{j=1, j \neq i}^N \mathbf{F}_{P,ij}$) are also included as well as the repulsive force from the wall ($\mathbf{F}_{W,i}$). Hence, a total force equation for the i^{th} particle is:

$$\mathbf{F}_{E,i} - \mathbf{F}_{drag,i} + \mathbf{F}_{W,i} + \mathbf{F}_{P,i} = 0 \quad (9)$$

The short-range repulsive forces acting between particles, arising from steric interaction, will act over a distance ranging from Ångströms to nanometers. The particles themselves are considerably larger (several μm [8]).

Thus, particles are perceived as hard spheres, with a short-range pair interaction potential:

$$V(R_{ij}) = \begin{cases} 0, & R_{ij} \geq \delta, \\ \infty, & R_{ij} < \delta. \end{cases} \quad (10)$$

However, because discontinuous forces severely complicate dynamic simulations which do not include lubrication forces, a continuous short-range expression for $\mathbf{F}_{P,ij}$ which is an exponential repulsion is selected:

$$\mathbf{F}_{P,ij} = -F_0 \exp[-\kappa(\frac{R_{ij}}{\delta} - 1)] \mathbf{e}_r \quad (11)$$

where κ^{-1} characterizes the range of the repulsive force, and the pre-factor F_0 is chosen as the DEP force scale. Actually, for the repulsive force from the wall, $F_{W,i}$, the same function is employed, but with a different F_0 .

Now, after all force expressions have been specified, they can be coupled, and the following equation for motion of particles i ($i = 1 \dots N$) is obtained:

$$6\pi\mu r \mathbf{U}_i = \sum_{j=1, j \neq i}^N 6\pi\mu r \frac{3r}{4R_{ij}} (1 + \hat{R}_{ij} \hat{R}_{ij}) \cdot \mathbf{U}_j + \mathbf{F}_{E,i} + \mathbf{F}_{W,i} + \mathbf{F}_{P,i} \quad (12)$$

Since $\mathbf{U}_i = \frac{d\mathbf{x}_i}{dt}$, all unknown functions in Equation 13 depend on the position of the particles ($\mathbf{x}_i$ and $\mathbf{x}_j$) and the electric field $\mathbf{E}$. While the potential is given, the electric field $\mathbf{E}$ is also a function of the position of $\mathbf{x}_i$. Hence, in nature, it is equivalent to a system of positions of N particles. Whether it is a linear or nonlinear system depends on how the velocity of the particle is discretized. It can be discretized with an explicit scheme, for example, the Forward-Euler scheme or the Verlet scheme (also known as the Leap-frog scheme). If it is discretized with fully implicit schemes, the system of equations becomes nonlinear. After non-dimensionalization, it can be expressed as:

$$\frac{d\mathbf{x}_i}{dt} = P_1 \mathbf{F}\mathbf{G}_{i,j} \cdot \frac{d\mathbf{x}_j}{dt} + P_2 \mathbf{F}\mathbf{D}_i + P_3 \mathbf{F}\mathbf{DIP}_{ij} + \mathbf{F}_{W,i} + \mathbf{F}_{P,i} \quad (13)$$

with the following definitions:

- Characteristic variables:

L : Length
 V_0 : Potential
 T : Time

- Dimensionless variables:

$$\begin{aligned} P_1 &= \frac{3r}{4L} \\ P_2 &= \frac{2\beta r^2 \epsilon_m V_0^2 T}{3L^4 \mu} \\ P_3 &= \frac{2\epsilon_m \beta^2 r^5 V_0^2 T}{\mu L^7} \\ &= 3\beta \left(\frac{r}{L}\right)^3 P_2 \end{aligned}$$

- Dimensionless functions

$$\begin{aligned} \mathbf{F}\mathbf{D}_i &= \nabla |\mathbf{E}^*|^2 \\ \mathbf{F}\mathbf{G}_{ij} &= \frac{1}{R_{ij}^*} (1 + \hat{\mathbf{R}}_{ij}^* \hat{\mathbf{R}}_{ij}^*) \\ \mathbf{F}\mathbf{DIP}_{ij} &= \frac{1}{(R_{ij}^*)^5} (\mathbf{R}_{ij}^* (\mathbf{p}_i^* \cdot \mathbf{p}_j^*) + (\mathbf{R}_{ij}^* \cdot \mathbf{p}_i^*) \mathbf{p}_j^* + (\mathbf{R}_{ij}^* \cdot \mathbf{p}_j^*) \mathbf{p}_i^* \\ &\quad - \frac{5}{(R_{ij}^*)^2} \mathbf{R}_{ij}^* (\mathbf{p}_i^* \cdot \mathbf{R}_{ij}^*) (\mathbf{p}_j^* \cdot \mathbf{R}_{ij}^*)) \end{aligned}$$

where $\mathbf{F}\mathbf{G}$ is the dimensionless hydrodynamic force, $\mathbf{F}\mathbf{D}$ is the dimensionless DEP force and $\mathbf{F}\mathbf{DIP}$ is the dimensionless electrostatic force. From the definition of P_1, P_2 and P_3 , and Equation 13, the scaling relationship between DEP forces and hydrodynamic force can be determined.

Another dimensionless parameter is defined as:

$$P_4 = \frac{P_2}{P_1} = \frac{8\beta r \epsilon_m V_0^2 T}{9L^3 \mu} \quad (14)$$

From Equation 14 it can be seen that when other parameters are fixed (β, r, L, ϵ_m , etc.), the relationship of the magnitudes of the two forces is:

$$\frac{FD}{FG} \sim V_0^2$$

Hence, when the applied external electric potential increases, the hydrodynamic force would play a less important role compared to the DEP force.

In order to investigate the relative importance of the electrostatic particle-particle force and DEP force, another parameter is defined:

$$P_5 = \frac{P_3}{P_2} = 3\beta \left(\frac{r}{L}\right)^3 \quad (15)$$

Equation 15 implies that if β is fixed and $L \gg r$, the DEP force will dominate. This is the case in most applications of dielectrophoresis. However, if the size of the particle is comparable with the length scale L , the particle-particle electrostatic force would become important. It is noteworthy that the DEP force depends on the gradient of electric field, while the particle-particle electrostatic forces depend on the intensity of the electric field. This means that the more uniform the electric field is, the more important the particle-particle electrostatic force will be. In the extreme case, where there the electric field gradient is very small, the DEP force is zero, while the particle-particle electrostatic force is still present and increases with the intensity of the electric field. At the other extreme, when the electric field gradient is very large, the particles would move by DEP force without forming chains even when they are very close to each other. Both phenomena can be predicted from our simulation results.

One of the advantages of the explicit schemes is that it does not require a solver, just an update of the positions based on the previous time-step. The disadvantage

is the strict time-step restriction for a stiff system (since both the DEP force and the repulsive forces are short-range forces, the system is quite stiff). Explicit schemes can cause numerical instability if the strict time-step restriction is not satisfied. Thus, the implicit scheme (Backward-Euler method) is chosen. Netlib's free nonlinear system library Minpack [25] has been modified to be used in our computation, which employs a modified Newton method and has many attractive features to improve the speed of computing a Jacobian matrix. Besides, another important strategy is used in this paper to cut down the nonlinear system computation work: Only the hydrodynamic forces and the interactive electrostatic forces in a certain distance range are calculated. This is a reasonable simplification since all forces are short-range. Thus, the non-linear matrix becomes a rather sparse one. The simplification significantly decreases the computation work.

As the system is solved on a step-by-step basis, our model generates approximate trajectories and uses a constant time interval for all particles. Generally speaking, the choice of time step should anyway satisfy the criterion that it should be considerably smaller than the typical time it takes for a particle to travel a distance equal to its own radius. Hence, $\Delta t u \approx 0.1r$ is chosen.

Different constant time steps were used in the different simulations. Since the particles are subjected to different forces, and the velocities of the particles are proportional to the force, the time step may be expressed as

$$\Delta t \sim \frac{r}{F_{max}}$$

Note that the time step needs to be small enough to catch all the physical phenomena properly. The Finite Element method (FEM) is used to calculate the DEP force in the whole domain. Based on the solution of finite element, a second-order interpolation is used to obtain the DEP forces at any position of the domain. The calculation is done with the help of FemLego [17], a toolbox for symbolic computation based on Maple and Fortran. Unstructured and nonuniform triangle and tetrahedron elements are used as well as adaptive meshes. The basic functions are of second order. The mesh files are created by Femlab [24].

Up until now, simulations have been made in 2D cases. In a simpler version of the model in which the interactive forces are neglected, behavior in 3D cases has been predicted [15].

3 RESULTS AND DISCUSSION

In this section, we discuss the results obtained with our numerical simulations both for hydrodynamic and dielectrophoretic suspensions (both in a uniform and in a non-uniform electric field).

3.1 HYDRODYNAMIC SIMULATIONS

First, the results for the hydrodynamic forces in Stokes flow are presented. Assuming that there is no bulk flow

speed, two particles are put close to each other. The aim is to see how the motion of one particle affects the other. The initial positions of the two particles are shown in the Figure 1(a).

Figure 1: Hydrodynamic simulation of a case with two particles

The domain has a characteristic length $L = 100 \mu\text{m}$, with a particle radius $r = 5 \mu\text{m}$. The fluid is assumed to have the same dynamic viscosity as water. Two simulations are performed, referred to as Case A, and Case B. The two particles are particle A and particle B. In Case A, the constant force only acts on particle A (which is the lower one in Figure 1. In Case B, a constant downwards force is exerted on both particle A and particle B.). The configuration is shown in the table below.

Force	Case A	Case B
particle A	$F_{down} = 1$	$F_{down} = 1$
particle B	$F_{down} = 0$	$F_{down} = 1$

In the simulations, $P_1 = \frac{3r}{4L} = 0.015$, and $Re \approx 0.01$. The Stokes number, defined as $St = \frac{\tau U_0}{L}$, is zero since the relaxation time τ is zero (because the inertial effect is ignored). When $St = 0$, the particles will follow the fluid streamline perfectly.

In Case A, particle A has the lower initial position and is subjected to a certain downward force and to the hydrodynamic force induced by particle B. Particle B has an upper initial position and is subjected to the hydrodynamic force only. The history of the particle positions is shown in Figure 2:

It is easy to see that particle B is dragged by particle A. Particle B moves downwards at a lower velocity. The velocity of particle A is also enhanced. As the distance increases, the hydrodynamic force is decreasing. It is more clear to see from the history of the velocities shown in Figure 3 how the distance change.

Figure 3 shows that in the beginning, when the two particles are very close to each other, the velocities of both particles have maximum values. Then the velocities of both particles decrease as the distance increases. In the end, when the two particles are rather far apart, the velocity of

Figure 2: The history of the particle positions of Case A

Figure 3: The history of the particle velocity of Case A

particle A is approaching a constant velocity. Meanwhile, the velocity of particle B is approaching zero.

Figure 4: The history of the particle position in Case B

In Case B, both particles are subjected to a constant downwards external force and hydrodynamic forces. The

history of the positions of the two particles is shown in Figure 4. The two particles keep the distance until the end, and the velocities have not been changed. It is well known that in very low Reynolds number flow, if two particles have the same velocity, then their distance will not be changed until some other force influences them. However, the effect of the hydrodynamic force behaves as to enhance the final velocities of the two particles, as seen in Figure 5.

Figure 5: The history of velocity comparison of two particles

3.2 SIMULATIONS OF THE ELECTROSTATIC FORCE BETWEEN PARTICLES

In this section, the behavior of particles in a domain with an external uniform electric field is simulated. The DEP force is also calculated (although it is zero in this geometry because the gradient of electric field is zero) but there are electrostatic forces between particles because of dipole-dipole interaction which are not zero if the intensity of electric field is not zero. In the initial time, 20 particles are distributed uniformly in the domain (Figure 6(a)). The domain length scale is also $L = 100 \mu\text{m}$, the particle radius is $r = 0.02 \times L = 5 \mu\text{m}$, the potential is $\phi = 1 \text{ V}$, $\beta = 0.5$, and it is assumed that there is no bulk flow. The time scale is set to $T = \frac{3L^3\mu}{2\beta r^2\epsilon_m V_0^2}$, hence the dimensionless parameters are:

$$P_2 = 1 \text{ and } P_3 = 0.24 \times 10^{-4}$$

Results with the electrostatic forces and without hydrodynamics force in three time moments are shown in Figure 6(b) (with the distribution of the particles when dimensionless time $t = 0.075$), Figure 6(c) (when $t = 0.25$) and Figure 6(d) (when $t = 0.75$).

From these figures, the process of how "pearl-chains" are formed can be seen. The dipole-dipole interaction causes the particles to attract each other in the direction of the electric field, and repel each other in the direction perpendicular to the electric field. Most particles form pairs when $t = 0.075$. The particles on the middle line do not pair because they are subjected to equal attractive force in both directions and arrive in a force quasi-equilibrium (it

Figure 6: Particle distribution without hydrodynamic force

is not a real equilibrium) state. At $t = 0.25$, the distribution is almost the same, and this state is maintained for a rather long time. In the end, when $t = 0.75$, they form five chains. The reason why it takes longer to form chains than to form pairs is that in the beginning the pairs are a bit further apart than their diameter and the force magnitude decreases rapidly with distance. With the same parameter

Figure 7: Particle distribution with hydrodynamic force

setting, it can be predicted how the coupled hydrodynamic force behaves in the 'micro scale together with electrostatic interactive force. The dimensionless parameter involved is $P1 = 0.015$, which is the same as the hydrodynamic simulation part. The particle distributions at $t = 0.075$ (Figure 7(b)), $t = 0.25$ (Figure 7(c)), $t = 0.75$ (Figure 7(d)) are also shown to be comparable to the results shown in Figure 6.

The differences are obvious in the beginning. At $t = 0.075$, the particles have already formed four chains because the hydrodynamic force enhance their velocities.

They repel each other further in horizontal direction, and attract each other more in vertical direction. In middle horizontal line, the four particles are contact with their neighbors, which is different from what we see in Figure 7(b). The chains are not straight lines, because the particles are subjected to different hydrodynamic forces.

When $t = 0.25$ (Figure 7(c)), the chains are straightened. This is because the hydrodynamic force decreases as the velocities of the particles decrease. Therefore, the hydrodynamic force becomes smaller and smaller while the magnitudes of the electrostatic forces almost remain the same, so the chains becomes straight due to fact that that the electrostatic force dominates the motion of the particles. At $t = 0.75$ (Figure 7(d)) the electrostatic forces completely dominate the process because the hydrodynamic force continues to decrease (due to the velocity decrease of the particles). Therefore, the distribution becomes similar to the one in Figure 6(d).

3.3 SIMULATION OF DEP WITHOUT BULK FLUID FLOW

In this section, simulation results of pDEP and nDEP in a channel without bulk flow speed but with interactive forces from hydrodynamic and electrostatic field are presented. When changing of frequency of the AC, the particles are subjected to either pDEP or nDEP.

Figure 8: Meshes (as used for calculations in femLego) around the pointed electrodes

The structure of the geometry is narrow to catch the micro sized particles, because the DEP force is very large near the tips of the electrodes. In the area close to the tips, very fine meshes are used for calculations with the finite element method (Figure 8). The electric potential is $\phi = 0$. at the top and $\phi = 1$. at the bottom. Initially, there are 27 particles distributed in the centre area of the domain (Figure 9).

The complex permittivity of polarisable particles is frequency-dependent. That means, in some frequency range, it experiences an attracting pDEP force, whereas it in another range is subjected to a repelling nDEP force. The results are the distribution of the particles at different time moments due to the pDEP and nDEP force.

Figure 9: Initial distribution of particles

In the pDEP simulation, the parameters are:

$$\begin{aligned} r &= 0.02L \\ P1 &= \frac{r}{L} = 0.015 \\ P2 &= 100 \\ P3 &= 0.24 \times 10^{-2} \end{aligned}$$

The simulation results are shown in Figure 10. The left picture is when $t = 0.075$, and the right picture is when $t = 0.15$. The results are in agreement with the theory. Particles concentrate on the two tips of electrodes, where the electric field gradient is strongest, and they align parallel with the electric field lines. In the direction perpendicular to the electric field lines, the particles repel each other somewhat because of their interactive electrostatic forces. This is not so obvious, because the external pDEP is very strong. The calculated results also verified by experimental observations as shown in Figure 11.

Figure 10: Particle distribution under pDEP conditions

Figure 11: Alignment of *E. coli* bacteria under pDEP conditions

In a certain frequency range, the real part of Clausius-Mossotti factor would become negative ($\beta < 0$). This re-

sults in an nDEP force. In the computation, the parameters used are the same as in the pDEP case, except that $P_2 = -100$. The results are shown in Figure 12. The distribution of particles when are shown for $t = 0.075$ (the left picture shows) and $t = 0.15$ (the right picture).

Figure 12: Particle distribution of nDEP

From Figure 12, it can be seen that in the area close to the sharp tips of the electrodes, there are no particles since the nDEP forces are strongest there. The particles are accumulated in the areas of left and right vertical boundaries of the domain, where the nDEP forces are weakest. The particles are still showing the direction of alignment, which is parallel to the direction of the electric field.

3.4 SIMULATION OF PARTICLE TRAPPING

In this section, the simulation results of trapping latex beads in a micro channel are presented. An array of interdigitated electrodes are supposed to be at the bottom of the channel. If the length of the electrodes is longer than the length scale of the particles, a 2D model can be used. A bulk fluid flow is carrying the particles through the channel. Since the Reynolds number is very small, the flow could be assumed to be a Poiseuille flow (Figure 13). In a fully developed Poiseuille flow, the speed profile is

$$U(y) = U_{max} \left(1 - \frac{|y - \frac{L}{2}|}{\frac{L}{2}}\right)^2$$

After non-dimensionalization, the force the particles obtain from the flow could simply be coupled into our MD model in the same way as the other forces. The details have been discussed in one of our previous papers [15], in which a simpler model than the one we used here was presented and applied.

The isolines for the electric potential $Re \approx 0.01$ are shown in Figure 14.

The length scale of the structure is $2L = 100 \times 2 = 200 \mu\text{m}$, the width is $L = 100 \mu\text{m}$, the applied voltage is 10 V, $\beta = 0.5$, $\epsilon_m \approx 80\epsilon_0$, radius of particle is $r = 5 \mu\text{m} = 0.02L$, and the maximum flow speed is $U_{max} \approx 50 \mu\text{ms}^{-1}$.

Initially, 12 particles are supposed to be at rest in the middle of the channel. The subsequent trajectories of the particles are shown in Figure 15. The pDEP forces are small in the area far from the tips of electrodes, and reach maximum values at the tips of the electrodes.

The final positions of the particles are shown in Figure 16. The particles are aggregated in the area of the tips of

Figure 13: Geometry of the electrodes and the flow profile in the channel

Figure 14: Electric potential isolines

Figure 15: Trajectories of the particles in the trapping system

the electrodes, where the pDEP forces are strongest. The particles could hardly form chains, because the gradient of electric field is very large at the edges of the electrodes, so the DEP force dominates the motion of the particles. Therefore, it is reasonable to use dielectrophoresis to separate particles with different size and properties since they would be subjected to different DEP forces and would not form chains.

This model could be used in simulation for trap-and-release filters and particle sorters, and in optimization of channel design. We have performed simulations to enhance

Figure 16: Final positions of the trapped particles

the trapping efficiency of *E. coli* cells [15] and separation of particles [16] based on a simplified version of this model without taking the hydrodynamic and particle-particle electrostatic forces into account. The model presented in this paper could provide even more accurate results. Therefore, this model can be easily used to separate a mixture of particles with different dielectrophoretic properties or sizes.

4 CONCLUSIONS

In this paper, we have derived a set of equations to describe the motion for the interacting particles subjected to a DEP force. The interactive hydrodynamic force is included by introducing correction functions for particle interaction in a Stokes flow. The interactive electrostatic force due to the DEP polarization of particles is also included. The particles often have been regarded as rigid bodies. A "soft-sphere model" MD method has been used to simulate the particles motion. In the procedure, configurations are generated by solving a set of Newton's equations of motion for each of the interacting particles. In practice, these equations of motion are replaced by a set of finite difference equations and are solved in a step-by-step manner. An implicit scheme is used to discretize the finite difference equations in order to eliminate the time restriction which comes from the nature of explicit schemes. The time step restriction then only comes from the physical procedure. In principle, the time interval should be small enough to allow the particle to pass a distance less than the radius of particles in one time interval.

Simulation results based on our model have been presented and discussed. For micro sized particles we simulated interactive hydrodynamic forces, electrostatic forces (separately and together), and the DEP force together with particle-particle electrostatic forces. For the last case, we simulated the behavior under pDEP and nDEP conditions for micro sized particles. We showed that a hydrodynamic force would enhance particles motion in a micro fluid system. We also showed that the dimensionless parameter $P5$ determines the relative importance between the DEP force and the particle-particle electrostatic force. While the electric field is determined, the larger the ratio between the non-dimensionalized particle radius and the characteristic length scale is, the larger the ratio between the particle-

particle electrostatic forces and the DEP force would be. This means that the larger the particles are, the easier they will form pearl-chains. However, if the electric field gradient is very large, the particles would hardly form chains even if they are very close to each other. The theoretic prediction is well in agreement with experimental results.

Based on the procedure of the derivation of the model and the simulation results, we conclude that the model provides good efficiency and accuracy. More extensive numerical studies and applications could be carried out based on this model, for instance in aggregation and separation of biological cells with different DEP properties. The model could also be modified to suit simulation for DEP of nanoparticles, especially rigid bodies. The present model is only for 2D discs, but could be extended to the 3D cases where the particles are spheres or ellipsoids.

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REFERENCES

- [1] H. A. Pohl "Dielectrophoresis" *Cambridge University Press, UK*, pp. 6-15, 1978.
- [2] T. B. Jones "Electromechanics of Particles" *Cambridge University Press, UK*, pp. 34-49, 1995.
- [3] H. Morgan "AC Electrokinetics: Colloids and Nanoparticles" *Research Studies Press, UK*, pp. 50-54, 2001.
- [4] R. Glowinski *et al.* "A Fictitious Domain Approach to the Direct Numerical Simulation of Incompressible Application to Particulate Flow" *Journal of Computational Physics*, 169, 363-426, 2001.
- [5] A. Castellanos *et al.* "Electrohydrodynamic and dielectrophoresis in microsystems: scaling laws" *Journal of Physics D: Applied Physics*, 36, 2584-2598, 2003.
- [6] M. Stimson *et al.* "The motion of two spheres in a viscous fluid." *Proc.R.Soc.A.*, 222, 110-116, 1974.
- [7] B. J. Alder *et al.* "Studies in molecular dynamics 1, General method" *Journal of Chemistry Physics*, 31, 459-466, 1959.
- [8] M. Parthasarathy, & D. J. Klingenberg *et al.* "Electrorheology: mechanics and models" *Materials Science and Engineering*, R17, 57-103, 1996.
- [9] A. T. Kadaksham *et al.* "Dielectrophoresis of Nanoparticles" *Electrophoresis*, 25, 3625-3632, 2004.
- [10] J. Kadaksham *et al.* "Manipulation of Particles Using Dielectrophoresis" *Mechanics Research Communications*, 33, 108-122, 2005.
- [11] H. H. Hu *et al.* "Direct Simulation of Flows of Solid-Liquid Mixtures" *Int J. Multiphase Flow*, 22, 355-52, 1996.
- [12] G. Tryggvason *et al.* "Direct Numerical Simulations of Flows with Phase Change" *Computers and Structures*, 83, 445-453, 2005.
- [13] J. Kadaksham *et al.* "Dynamics of Electrorheological Suspensions Subjected to Spatially Nonuniform Electric Fields" *J. of Fluids Engineering*, 126, 170-179, 2004.
- [14] <http://www.tn.utwente.nl/cdr/PolymeerDictaat/node37.html>
- [15] F. Aldaeus *et al.* "Superpositioned Dielectrophoresis for Enhanced Trapping Efficiency" *Electrophoresis*, 26, 4252-4259, 2005.
- [16] F. Aldaeus *et al.* "Multi-Step Dielectrophoresis for Separation of Particles" *submitted*
- [17] G. Amberg *et al.* "Math. Comp. Simulation" *Math. Comp. Simulation*, 49, 257-274, 1999.
- [18] A. Johnson *et al.* "3D Simulation of Fluid-Particle Interactions with the Number of Particles Reaching 100" *Comp. Mech. Appl. Mech. Engng.*, 145-301, 1997.
- [19] K. K. Pijush *et al.* "Fluid Mechanics" *Academic Press, USA*, 97-99, 2002.
- [20] M. Elimelech *et al.* "Particle Deposition and Aggregation: Measurement, Modelling and Simulation" *Journal of Chemistry and Physics*, 63, 2376-2394, 1975.
- [21] A. Rahmane "Correlations in the Motion of Atoms in Liquid Argon" *Physics Review*, 136A, 1773-1798, 1964.
- [22] J. O'Dell *et al.* "Molecular Dynamics of the Rough Sphere Fluid" , Butterworth-Heinemann press, USA, 222-224, 1995.
- [23] <http://www.fluent.com>
- [24] <http://www.mathworks.com>
- [25] <http://www.netlib.org>