Concentration Tuned Interactions and Structures in Suspensions under One Gradient AC Electric Field

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ABSTRACT

Effects of concentration of suspensions were studied on long range collective anisotropic interactions among polarized particles in a gradient ac electric field by experiment and simulation. In the 0.01% (v/v) suspension, the particles were just packed in the high electric field regions because the dielectrophoretic (DEP) force on particles dominated over the dipole-dipole interactions; secondly, in the 1% (v/v) suspension, the particles formed structures as grass grows from the bank edge close to the water. These structures are caused by the competition between the DEP force and the dipole-dipole interactions, and also by the memory of the polarization interactions. Density difference between spheres and corn oil degraded the memory of polarization interactions and influenced particle motion, especially in the 0.01% (v/v) suspension although its effect was reduced. The particle motion and structuring are both sensitive to the concentration of suspensions and the concentration method is well promising.

Key Words: concentration method, long range collective anisotropic interactions, concentration tuned interactions, concentration tuned structures, memory of polarization interaction,

1 INTRODUCTION

Recent studies of electrohydrodynamics (EHD) of suspensions under high electric fields are motivated by its technological potentials for the separation, filtration, orientation, and sorting of particles and cells, the manipulation of multiphase flows, and chemical and biochemical reactions. The electric manipulation of fluid flow and particle motion as well as biological sample is the most active field in micro- and nano-fluidics. Applications of an ac electric field in technologies overcome challenges like electrolyzing liquids and uncontrollable net charges on particles under a dc electric field. Besides its amplitude, the frequency of the ac electric field or frequency spectra of the sample system can be used as control variable also.

And so it becomes very urgent to understand electro-hydrodynamics of a suspension under one high gradient ac electric field. Its core topics are electric-field-induced and hydrodynamic interactions among the polarized particles. For decades, this type of interactions has been posing challenges for theoretical and experimental exploration.

We are using a simple approach to attack these EHD problems. Our method includes two parts. The first part is to vary the concentration of suspensions and so vary the distance between two particles in the suspensions. We probe effects of the concentration of suspensions on interactions among the particles, particle motion and structure formation of the particles. The other part is the molecular dynamics (MD) simulation of particle motion and particle structuring in the high gradient electric field. In the MD simulations, the DEP force, the Stokes' drag force, the effective gravitational force and the dipole-dipole interaction forces among the polarized particles are considered.

This report is organized as follows. In Section 2, we summarize the basic experimental results with different particle volume factions of the suspensions. In Section 3, we will briefly describe the MD simulation and present the simulation results. In Section 4, we will discuss data from the experiments and simulations. A plain physics picture will be presented about relations among the particle volume fraction, long-range collective interactions, particle motion and the structure formation. In the last Section, we will address some challenges in MD simulations of suspensions of high particle volume fractions.

2 SUMMARIES OF EXPERIMENTS

As shown in Figure 1 is the electric chamber of 12cm x 6cm x 3mm with a well grounded transparent conducting cover for here experimental research of the suspensions. Grounding of the chamber top provides well-defined boundary conditions. The chamber houses a periodic electrode array with a gap of 2mm between the two

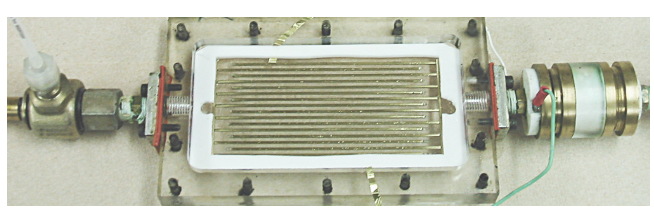


Figure 1: Photo of the electric chamber.

Δ Both the authors equally contributed to this work.

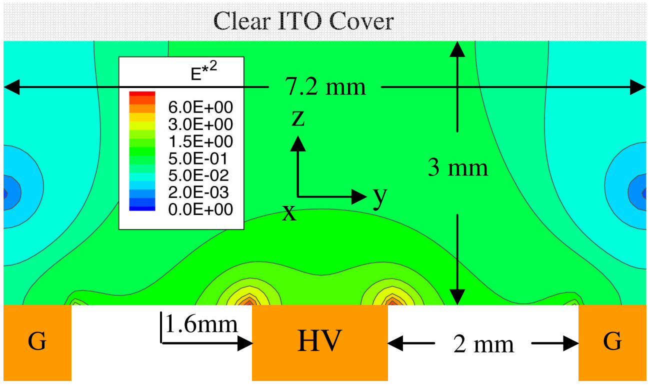
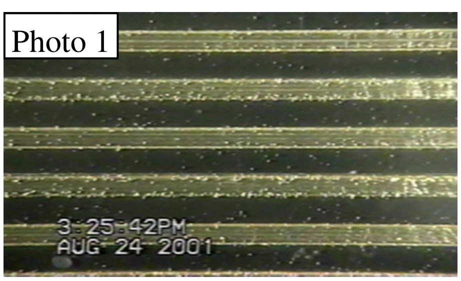
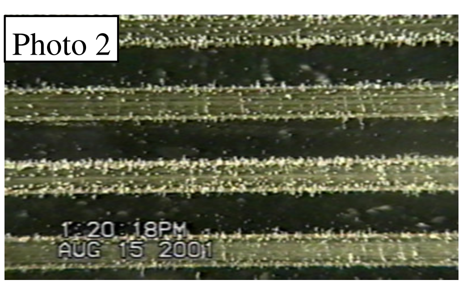


Figure 2: Calculated electric field in the minimum domain of 3.6 x 7.2 x 3.0 mm in the chamber that will be used for the MD simulation. G is the grounded electrode and HV is the energized electrode. It is shown that there is one high electric field region around each edge of the energized or grounded electrode.

electrodes on the chamber bottom. The electric field in the chamber space was distributed in the cross section plane of the chamber perpendicular to the electrode direction. The electric field was obtained by solving the Laplace equation with the boundary conditions that were described by Refs. [1-3]. The calculated electric field was plotted in Figure 2.

Experiments were conducted in the chamber shown in Figure 1. Used uspensions consist of 89.6µm Al_2O_3 spheres and corn oil. The density of the spheres (3.75 g/cm^3) is about four times that of the corn oil (0.92g/cm^3). To diminish the effects of the gravitational force, the electric chamber with a suspension was slowly rotated around its horizontal axis to prevent the particles from settling down to the 'bottom' of the chamber. All reported experimental results were obtained with the chamber rotating at 4 rpm. Pictures of the particle distribution and the structures were taken for the suspensions of three different concentrations and shown in Figure 3.





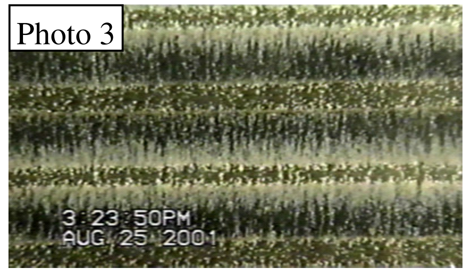


Figure 3: Photos of aggregation and structures of aluminum oxide spheres in the three suspensions with different particle volume fractions in the high electric field regions around both the energized and grounded electrodes in the corn oil under the high gradient electric field generated by the periodic electric electrode array as shown by the photo of Figure 1. At 100 Hz, Re (β) of the mismatch between the dielectric constants of the spheres and corn oil is 0.34. Al_2O_3 sphere diameter is 89.6um and its density is 3.75 g/cm^3. The density of corn oil is 0.92g/cm^3 and its viscosity is 0.06 Pas at 23°C. When the suspensions were exposed to electric fields, the suspension in the chamber was rotated around a horizontal axis at 4 RPM. **Photo 1**: the particle volume fraction is 0.01% (v/v), the externally applied voltage is 3kV/100Hz and exposure of the suspension time to the electric field is 942 seconds. **Photo 2**: the particle volume fraction is 0.1% (v/v), the externally applied voltage is 1kV/100Hz and exposure time of the suspension to the electric field is 312 seconds. **Photo 3**: the particle volume fraction is 1% (v/v), the externally applied voltage is 3kV/100 and the exposure time of the suspension to the electric field was 83 seconds.

3 MD SIMULATIONS

The numerical simulation focuses on motion and structuring of Al_2O_3 spheres in corn oil when the suspension was exposed to a high gradient electric field that was generated by a spatially periodic electrode array built in the chamber bottom, shown in Figure 1 and described in detail by Refs [2][3]. Parameters of the suspensions and the chamber for the simulation are exactly same as those in the experiments described above and in Ref [2][3]. When the suspension is exposed to an ac electric field, they are positively polarized. The fluid chamber measures 60 (width) x 120 (length) x 3.0 (height) mm and is driven to rotate around an axis at 4 rpm to prevent particles from settling down onto the 'bottom' of the chamber. In this process, one particle in the suspension is subjected to below combined forces. The first one is the DEP force from the gradient of the electric field, the second one is the dipole-dipole interaction force among polarized particles, the third one is the Stokes' drag force and the last one is the effective gravitational force. And the governing equation to describe Newtonian dynamics of the suspension of dielectric particles in corn oil under these combined forces can be expressed as

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$$m\frac{d^2\boldsymbol{r}_i}{dt^2} = \boldsymbol{F}_i - 3\pi\eta d\frac{d\boldsymbol{r}_i}{dt} + \boldsymbol{R}_i(t) + \frac{4}{3}\pi(\rho_p - \rho_f)\left(\frac{d}{2}\right)^3\boldsymbol{g}$$

In Equation (1), m is the particle mass. In the right hand side of Equation (1), $\boldsymbol{F}_i$ denotes all electric forces on a particle; the second term is the Stokes' drag force; $\boldsymbol{R}_i$ is a Brownian force that can be neglected and the last term is a rotation-and-time-dependent effective gravitational force on the i-th particle.

$$\boldsymbol{F}_i = \sum_{i\neq j} f_{ij} + g_i \text{ where } f_{ij} = -\frac{\partial\Phi_{ij}}{\partial r}\boldsymbol{e}_r - \frac{1}{r}\frac{\partial\Phi_{ij}}{\partial\theta}\boldsymbol{e}_\theta \text{ where}$$

$$\Phi_{ij} = \frac{1}{4\pi\varepsilon_0\varepsilon_f}\left(\frac{\boldsymbol{p}_i\cdot\boldsymbol{p}_j}{r_{ij}^3} - \frac{3(\boldsymbol{p}_i\cdot\boldsymbol{r}_{ij})(\boldsymbol{p}_j\cdot\boldsymbol{r}_{ij})}{r_{ij}^5}\right), \quad \boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j,$$

$\boldsymbol{p}_i = 4\pi\varepsilon_0\varepsilon_f\left(\frac{d}{2}\right)^3 \mathrm{Re}(\beta)\boldsymbol{E}_{rms}$. f_{ij} is a non-zero time-average dipole-dipole interaction force on the i-th particle from the j-th particle, and

$g_i = 2\pi\varepsilon_0\varepsilon_f (d/2)^3 Re(\beta)\nabla E_{rms}$, a non-zero time-average dielectrophoretic force from a gradient ac electric field. Parameters and variables in above equations and formulas were specified and explained in Ref. [3].

For the boundary conditions of the calculation domain, we assume that the electric field in the chamber is two-dimensional and normal to the electrode direction; and also periodic boundary conditions are applied when simulations are performed. A 'natural minimum unit' of 7.2x3.6x3.0 mm is chosen for the numerical simulations. Trajectories of articles are determined by solving the governing equation with a converged electric field obtained at the calculation beginning. Detailed descriptions of the simulation method and operation are in Reference of [3].

The simulations have partially reproduced experimental data about motion and structuring of particles under the gradient ac electric field when the corn oil was 'not' flowed, and also provide more details about involved interactions of electrostatics and hydrodynamics, and their effects on motion and clustering of the particles. Shown in Figure 4 is a transient snap shot of the particle distribution for the 0.1% (v/v) suspension.

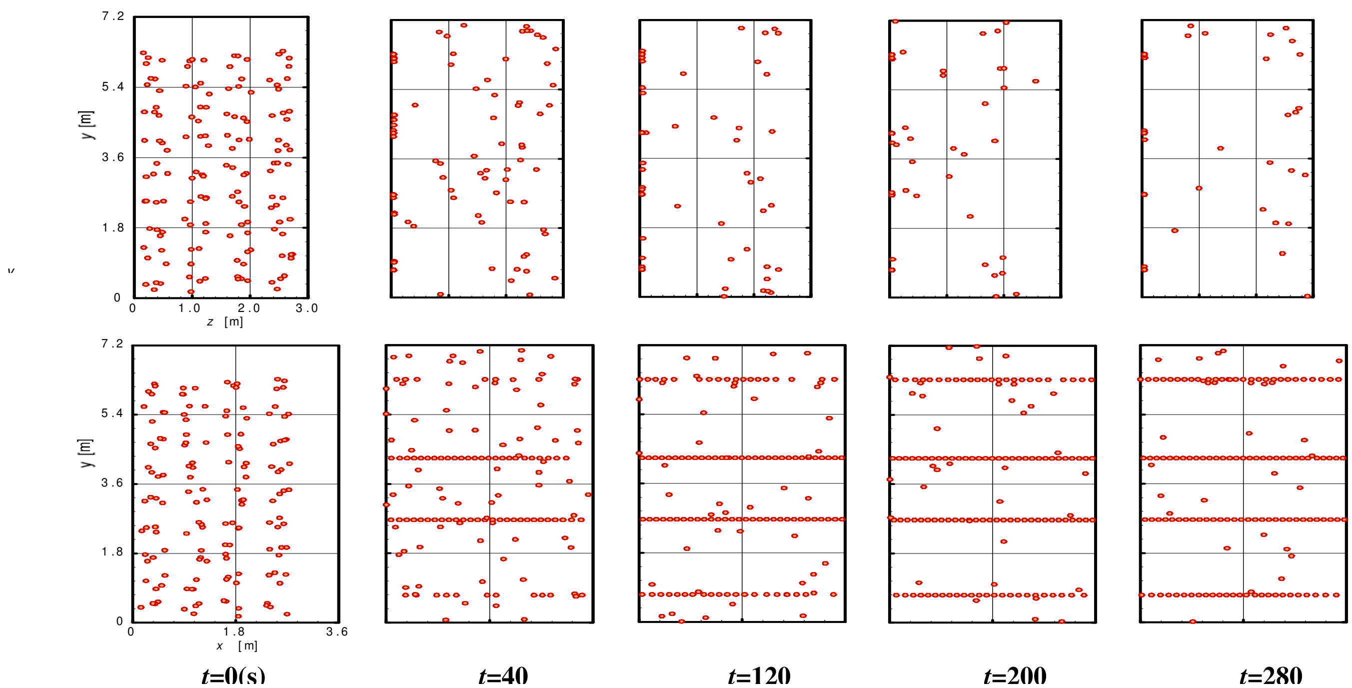

Figure 4: All the suspension parameters for this simulation are the same as the experiments used above. The particle volume fraction of the suspension is 0.1% (v/v) and the external applied voltage is 3kV/100Hz. ***t*** is the exposure time of the suspension to the gradient electric field.

4 DISCUSSIONS

According to available data from the simulations and experiments, first, anisotropic interactions among the polarized particles have memory for all the suspensions of three particle concentrations of 0.01, 0.1 and 1% (v/v), and the memory is kept when particles are transported to the high electric field regions by the positive DEP force. Secondly, in the 0.01% (v/v) suspension, the DEP force dominates over the dipole-dipole interactions and the particles were just packed in the high electric field areas around each edge of the energized or grounded electrode. In the 1% (v/v) suspension, the DEP force competed with the dipole-dipole interactions and so some structures formed around the high field area as grass grows from the river bank edge close to water. In the 0.1% (v/v) suspension, the dipole-dipole interaction increases with increase in the particle volume fraction and the particles are no longer packed at random completely, instead, in the high field area, some short chain-like structures form. Finally, the effective gravitational effects still degraded the memory of the anisotropic polarization interactions, especially in the extremely dilute suspension although we reduced effects of the effective gravitational force by rotating the chamber with the suspension.

These relations between the particle volume fractions and the final structures or particle distribution can be understood as follow. The force between two polarized particles has two important features. First, it is long-range, decaying as a power law r^{-4} where r is a distance between two particles [5]; and so, this type of interactions is collective in a multi-body system. In the second place, it is strongly anisotropic. There is one attractive or repulsive interaction between the two particles based on their relative orientation. In the 0.1% (v/v) suspension, because of large distances among the particles, the dipole-dipole interaction is relatively weak and the particles are just packed at random or 'uniformly' under action of the DEP force. And therefore, the particle configuration has not been 'modulated' or 'correlated' by the strongly anisotropic property of dipole-dipole interactions among the polarized particles. However, when the particle volume fraction is increased, distances among the particles are reduced and so the anisotropic dipole-dipole interactions become strong to modulate or correlate the particle configuration, as we experimentally observed.

5 CONCLUSION AND FURTHER WORK

The simulations and experiments demonstrate that the particle configuration and structures are very sensitive to the particle volume fraction. The concentration method is well promising we developed here to long-range collective anisotropic interactions among the particles in combined electric and flow fields.

In the experiment, we will improve control of material properties and choose a better suspension model system.

In the simulation, currently the simulations are still being performed on the 124-CPU (64-bit Opteron) cluster of the Levich Institute of the City College of the City University of New York. For one 0.1% (v/v) suspension, if its 12 CPUs are used for this job, it takes about 20 days of 12 CPUs to get the particle configuration at 500th second since the electric field is applied. In the future work, on the one hand, we will use more powerful computing resource; the other hand, we will have to develop a hybrid method to cut short the simulation time. The hybrid method should keep the feature of anisotropic properties of interactions and deliver a computing speed of the continuous model.

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