전기유변유체의 대변역 전단 유동에 대한 3차원 모의실험

심훈구, 안경현, 이승종
서울대학교 공과대학 응용화학부

Three-dimensional dynamics simulation of ER fluids under LAOS

Hoon Goo Sim, Kyung Hyun Ahn, Seung Jong Lee
School of Chemical Engineering, Seoul National University

Introduction

Electrorheological (ER) fluids show dramatic changes in their rheological properties upon the application of electric field. This behavior is related with the microstructural change of ER fluids. As ER devices usually operate in a dynamic mode with large deformation, the behavior under large amplitude oscillatory shear (LAOS) is of particular importance among the rheological properties (Hyun *et al.*, 2002). So far, however, there are only a few explanations of LAOS behavior with respect to the microstructural changes of ER fluids. The purpose of this paper is to understand the LAOS behavior of ER fluids and to investigate the mechanism of strain overshoot phenomenon in terms of microstructural change. The characteristics of higher harmonic contributions to the stress signal as well as microstructural analysis will also be presented.

Model and simulations

Using the point dipole approximation (Klingenberg, 1993), the equation of motion of particle i can be written in dimensionless units:

$$\frac{d\mathbf{r}_i}{dt} = \sum_{j \neq i} \mathbf{F}_{ij}^{el} + \sum_{j} \mathbf{F}_{ij}^{\prime el} + \sum_{j \neq i} \mathbf{F}_{ij}^{rep} + \mathbf{u}^{\infty}(\mathbf{r}_i) \quad (1)$$

where $\mathbf{F}_{ij}^{el}$ is the electrostatic force between particles, $\mathbf{F}_{ij}^{\prime el}$ is the electrostatic force between the particle and its image, $\mathbf{F}_{ij}^{rep}$ is the short-range repulsive force, and $\mathbf{u}^{\infty}(\mathbf{r}_i)$ is the hydrodynamic force due to the ambient flow at $\mathbf{r}_i$. The shear stress $\sigma_{xz}(t)$, acting in the shear direction x on a plane normal to the electric field direction z, can be expressed as follows,

$$\sigma_{xz}(t) = -\frac{1}{V} \sum_{i} r_{zi} F_{xi}^{total}, \quad (2)$$

where V is the fluid volume, r_{zi} is the position of z-component of particle i, and F_{xi}^{total} is the total electrostatic and repulsive forces acting on particle i in x-direction. When the strain amplitude exceed certain value, the stress response became non-sinusoid because of higher harmonics contributions and can be expressed as follow,

$$\sigma(t)=\sum_{n=1}^{\infty}\sigma_n\sin(\omega_n t+\delta_n)=\gamma_0\sum_{n=1}^{\infty}G_n'\sin(\omega_n t)+G_n''\cos(\omega_n t) \quad (3)$$

where the amplitude $\sigma_n(\omega_0,\gamma_0)$ and the phase angle $\delta_n(\omega_0,\gamma_0)$ of the harmonics depend on both strain amplitude γ_0 and frequency ω_0. G_n' and G_n'' in Eq. (3) are defined as the nth components of storage and loss modulus, respectively. Such higher harmonics contributions can be transformed into frequency domain by Fourier transformation (FT) method. Time dependent cluster size $S(t)$ is defined as:

$$S(t)=\frac{1}{N}\sum_{k=1}n_k(t)^2 \quad (4)$$

where N is the number of clusters and $n_k(t)$ is the number of particles in the kth cluster including the percolated chains.

Results and discussion

Fig. 1 is the initial configuration that is used in the numerical simulations in this study. The simulation box consists of 1000 particles at a volume fraction of 5%. The particles form clusters of particle-width strings, which align to the electric field direction between the upper and lower electrodes. Fig. 2 shows the fundamental storage modulus G_1' and loss modulus G_1'' obtained from FT analysis. The fundamental storage modulus G_1' remains constant up to certain strain amplitude, above which G_1' decreases with γ_0^{-2} irrespective of the imposed frequency. As for the fundamental loss modulus G_1'', it begins to increase above its linear viscoelastic value and reaches a maximum before decreasing with $\gamma_0^{-1.5}$ as the strain amplitude increases at low frequency. The maximum of the fundamental loss modulus decreases with increasing frequency. Parthasarathy and Klingenberg (1999) pointed out that nonlinearity first arises from slight rearrangement of unstable structures. Further increase in the fundamental loss modulus is attributable to the cluster re-formation process. As for the types of LAOS behavior of ER suspension, there exists a frequency dependence: type III (weak strain overshoot) at low frequency and type I (strain thinning) at high frequency.

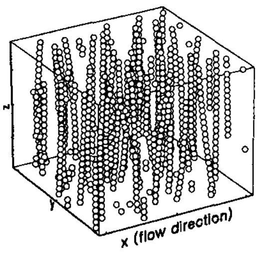

Fig. 1. Initial configuration. Electric field is applied to z direction

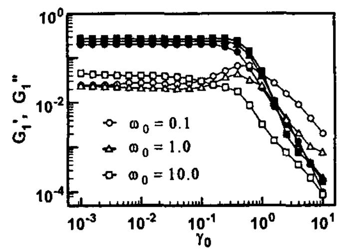

Fig. 2. Fundamental modulus (G_1', G_1'') as a function of strain amplitude.

Fig. 3 shows the intensities of odd harmonics as a function of strain amplitude for single cluster. The intensity of each harmonic increases as a power of strain amplitude with different slope depending on the order of harmonics till the fundamental modulus maintains its linear viscoelasticity (Fig.2). This behavior differs from the scaling law of Carreau model (Wilhelm *et al.*, 2000), where the slope of higher harmonics is two regardless of harmonic order. Further increase in strain amplitude causes the variation of higher harmonics intensity, which implies the global destruction of clusters. Fig. 4 shows the characteristic feature of cluster dynamics. Under large oscillatory shear flow, the clusters are destructed and can be recombined into clusters periodically. During this process, the broken clusters form stable configurations while dissipating their electrostatic energy at low frequency. The more energy dissipation, the larger G_1'' will be caused. When the shear rate becomes greater, because the broken clusters have no enough time to form a stable configuration, further increase in G_1'' cannot be taken place.

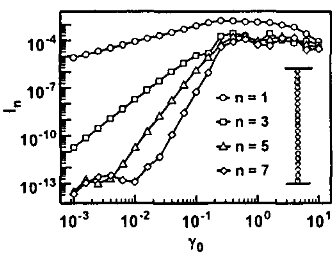

Fig. 3. Intensity of odd harmonics for single cluster as a function of strain amplitude

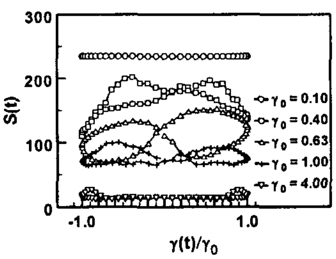

Fig. 4. Time dependent cluster size $S(t)$ as a function of normalized strain at $\omega_0 = 0.1$

Fig. 5 shows the microstructural change of clusters during a half cycle at low and high frequency at $\gamma_0 = 0.4$. The cluster re-formation process is made up of destruction and formation of clusters and accompanies the relaxation during the oscillation. As shown in Fig. 5 (left), the broken clusters tend to align with the electric field during the re-formation process. The alignment or the rearrangement of fractured cluster to the electric field dissipates electrostatic energy into the viscous continuous phase. This re-formation process results in a further increase of fundamental loss modulus (Fig. 2).

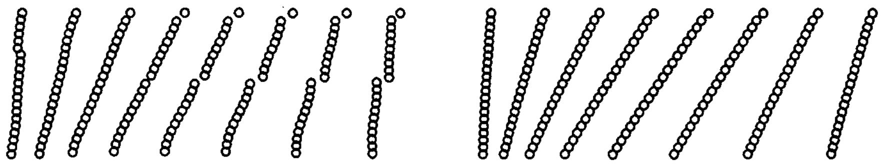

Fig. 5. Snapshots of a single cluster during a half cycle: (left) $\omega_0 = 0.1$, (right) $\omega_0 = 10.0$ at $\gamma_0 = 0.4$:

References

Hyun, K., Kim, S. H., Ahn, K. H. and Lee, S. J., 2002, Large amplitude oscillatory shear as a way to classify the complex fluids, *J. Non-Newtonian Fluid Mech.*, **107**, 51-65.

Klingenberg, D. J., 1993, Simulation of the dynamics oscillatory response of electrorheological suspensions: Demonstration of relaxation mechanism, *J. Rheol.*, **37**, 199-214.

Parthasarathy, M. and Klingenberg, D. J., 1999, Large amplitude oscillatory shear of ER suspensions, *J. Non-Newtonian Fluid Mech.*, **81**, 83-104.

Wilhelm, M., Reinheimer, P., Ortseifer, M., Neidhoer, T. and Spiess, H. W., 2000, The crossover between linear and non-linear mechanical behavior in polymer solutions as detected by Fourier-transformed rheology, *Rheol. Acta,* **39**, 241-246.