

Direct Numerical Simulations of Colloidal Dispersions under External Force

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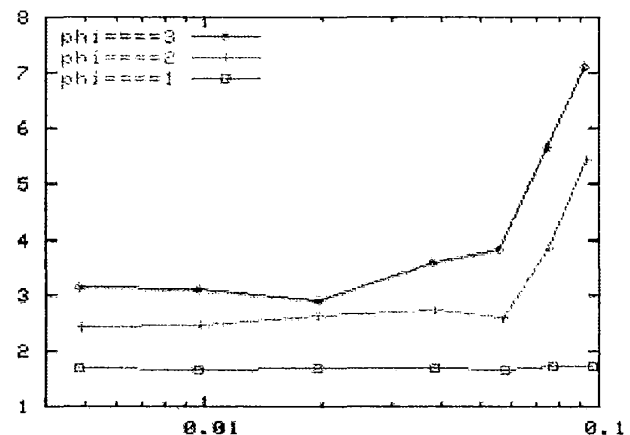
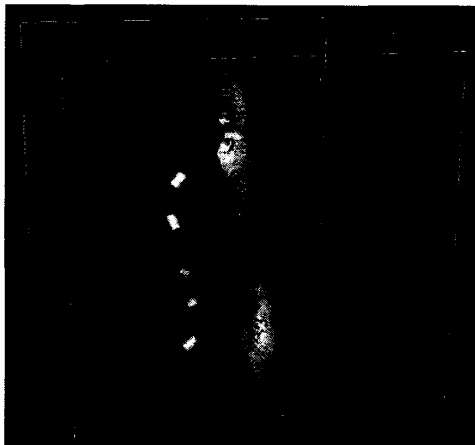
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コロイド分散系では、流体を介して粒子間に働く流体力学相互作用と流体の熱揺らぎを反映した粒子のブラウン運動との競合が重要な役割を果たすことが多い。最近我々が開発したコロイド分散系のためのシミュレーションコード [KAPSEL:<http://www-tph.cheme.kyoto-u.ac.jp/kapsel/>] では、コロイド粒子の周りの流体の運動を直接数値計算で取り扱うための効率の良い方法を実装している。今回は、これまでの手法にさらに熱揺らぎを導入するための手法について解説する。この拡張により、各種コロイド分散系について流体力学相互作用と熱揺らぎの両者を正確に考慮した直接数値シミュレーションが実現可能となる。さらに本講演では、シア流や電場などの外力・外場の下にあるコロイド分散系について行った直接数値シミュレーションの結果を示す。

There have been proposed several numerical methods applicable to colloidal dispersions. Recently, it has been shown that the use of diffuse colloid/fluid interfaces with non-zero thickness ξ much improves the efficiencies of the simulations [1, 2]. Along with this line, we developed a method for direct numerical simulations (DNS) of electro-hydrodynamic phenomena in charged colloidal dispersions [KAPSEL:<http://www-tph.cheme.kyoto-u.ac.jp/kapsel/>] [3]. This method enables us to compute the time evolutions of colloidal particles, ions, and host fluids simultaneously by solving Newton, advection-diffusion, and Navier-Stokes equations so that the electro-hydrodynamic couplings can be fully taken into account [4]. The electrophoretic mobilities of charged spherical particles are calculated in several situations. The comparisons with approximation theories show quantitative agreements for dilute dispersions without any empirical parameters; however, our simulation predicts notable deviations in the case of dense dispersions [5].

We recently modified our DNS code for particle dispersions to take into account the effect of Brownian motions of the particles. The new code has been applied to several cases where coupling between hydrodynamic interaction and the thermal fluctuation becomes important (left figure) [6]. DNS simulations have been performed for several systems under external fields. Striking examples include chain formations of likely charged particles due to the application of



Left: A snapshot of a fluctuating polymer chain of $N=10$. Right: Shear viscosity vs. shear rate for a Brownian particle dispersion. The colloid volume fractions are 0.51, 0.41, and 0.2 for $\phi = 3, 2$, and 1, respectively. Clear shear thickening behavior is observed for high volume fraction cases when shear rate is increased.

external electric fields. The mechanism behind this phenomena has been analyzed. Also a clear tendency of the shear thickening behavior of colloidal dispersions has been obtained when we apply shear flow to the system (right figure) [7]. The origin of the thickening will be discussed.

References

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