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学 位 論 文 題 目	A Numerical Study of Capsule Suspensions under Stokes Flow: Suspension Rheology and Blood Cell Sedimentation
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論文内容要約

A dispersion is a system that colloidal size particles are dispersed in a continuous phase of a different state. These dispersions can be seen in many places in our daily life, such as foams, mists, emulsions, suspensions etc. It is well known that these dispersions have complex physical properties as non-Newtonian behaviours and viscoelastic responses. There have been a number of studies discussing the rheological properties of dispersions in the past centuries. In this thesis, we mainly focus on suspensions of capsules, which belongs to a type between the emulsion and the suspension of solid particles. Examples of the suspensions can been seen in industrial fields and consumer products: paint, ink, cements, muds, toothpaste etc. The presence of particles alters the rheology of suspensions, and the rheology drastically changes by the particle's size, shape, volume fraction, deformability, and density. The suspensions are classified into three categories by the volume fraction of particles. The first category is dilute suspensions for low volume fractions. The second category is semi-diluted suspension, where the interaction between two particles is only considered. When the volume fraction further increases, multiple particle interactions have significant effects, and this last category is called dense suspensions.

A capsule is a liquid drop enclosed by a deformable membrane made of polymers and lipid bilayers. Capsules are found in food-, cosmetics- and chemical-industries. Biological cells, such as red blood cells (erythrocytes) and platelets, may also be categorised into capsules. Predicting the rheology of capsule suspensions is of practical importance in a wide range of medical and engineering applications. Main difficulty to predict capsule motions, deformations and the rheology of the capsule suspension arises from the complexity of the capsules; they have characters of both emulsions and elastic materials. In the case of dense suspensions of capsules, the prediction would be even more difficult because the capsule starts to show complex deformations due to the interactions between each other. For a precise understanding of the capsule suspensions, we need to build physics from a dilute limit to a dense suspension by a bottom up approach. However, there are not much theoretical and computational infrastructure that allows us to precisely

predict the motion of capsule in a wide range of volume fractions. First objective of this thesis is to develop a computational method to simulate the capsule motion precisely and efficiently. Second objective is to clarify the rheology of capsule suspensions under various flow fields, by taking the advantage of our efficient computational method. We mainly focus on the capsule motions, deformations and the viscoelastic properties of the suspensions. Final objective is to clarify the sedimentation of a single red blood cell, as a practical application that would lead to blood diagnosis.

In chapter 2, an acceleration method using GPU is presented. Governing equations for the capsule motions under Stokes flow are presented in section 2.1. For the fluid mechanics, the boundary integral formulation is introduced to solve the flow velocity of the Stokes flow. Equations for the solid mechanics of the capsule membrane are also provided in this section. The numerical methods are presented in section 2.2. Our simulations are based on a numerical method in which the boundary element method (BEM) for fluid mechanics is coupled with the finite element method (FEM) for membrane mechanics. In this section, we mainly discuss the discretization and implementation method of BEM and FEM. We also show the derivation of two additional techniques that support the simulation of BEM: the multipole expansion and the Ewald summation method. The multipole expansion is a method to accelerate the simulation by coarse graining effects from far-fields. The Ewald summation method is introduced to simulate the suspension with a periodic boundary conditions. From section 2.3, we propose a full graphics processing unit (GPU) implementation of a numerical method coupling the BEM of fluid mechanics with the FEM of membrane mechanics. In single GPU computing, the performance achieves 0.12 TFlop/s when computing one capsule (2562 nodes and 5120 elements) and 0.29 TFlop/s for two capsules. The performance increases with the number of capsules, achieving a maximum of 0.59 TFlop/s. We also implement a multi-GPU method with the data communication overlapping the computation. A weak scaling test shows perfect scalability for any number of computational nodes per GPU, indicating that the communication time is completely hidden. For a practical use of the present results, we estimate the computational time required for 10000 time steps. When we simulate one capsule and two capsules on one GPU, only 2.0 and 9.1 minutes are required to complete the simulation, respectively, and a simulation with 256 capsule4s on 16 GPUs takes 3.8 days. The present method allows us to simulate both dilute and dense suspensions within a reasonable amount of time, and it can accelerate the research on the dynamics of particle suspensions in a variety of fields.

In chapter 3, the rheology of a dense suspension of spherical capsules in simple shear flow is presented. The behaviour of neo-Hookean capsules is simulated for a volume fraction up to $\phi = 0.4$ by BEM with multipole expansion. To describe the specific viscosity using a polynomial equation of volume fraction, the

coefficients of the equation is calculated by least squares fitting. The results suggest that the effect of high-order terms is much smaller for capsule suspensions than rigid sphere suspensions, for example, $O(\phi^3)$ terms account for only 8% of the specific viscosity even at $\phi = 0.4$ for the capillary number Ca $\geqq$ 0.1. We also investigate the relationship between the deformation and orientation of capsules with the suspension rheology. When the volume fraction increases, the deformation of the capsules increases while the orientation angle of the capsules with respect to the flow direction decreases. Therefore, both the specific viscosity and the normal stress difference increase with volume fraction by the increased deformation, whereas the decreased orientation angle suppresses the specific viscosity, but amplifies the normal stress difference.

In chapter 4, the deformation of a spherical capsule in oscillating shear flow is presented. We show that a capsule at high frequencies follows the deformation given by a leading-order prediction, which is derived from an assumption of small deformation limit. At low frequencies, on the other hand, a capsule shows an overshoot phenomenon where the maximum deformation is larger than that in steady shear flow. A larger overshoot is observed for larger capillary number or viscosity ratio. Using the maximum deformation in start-up shear flow, we evaluate the upper limit of deformation in oscillating shear flow. We also show that the overshoot phenomenon may appear when the quasi-steady orientation angle under steady shear flow is less than 9.0°. We propose an equation to estimate the threshold frequency between the low frequency range, where the capsule may have an overshoot, and the high frequency range, where the deformation is given by the leading-order prediction. The equation only includes the viscosity ratio and the Taylor parameter under simple shear flow, so it can be extended to other deformable particles, such as bubbles and drops.

In chapter 5, the reorientation phenomenon of a single red blood cell during sedimentation is presented. The cell settles downward due to a density difference between internal and external fluids, and it changes orientation toward vertical orientation regardless of Bond number or viscosity ratio. The reorientation phenomenon is explained by a shape asymmetry caused by the gravitational driving force, and the shape asymmetry increases almost linearly with the Bond number. When velocities are normalised by the driving force, settling/drifting velocities are weak functions of the Bond number and the viscosity ratio, while angular velocity of the reorientation drastically changes: the angular velocity is smaller for lower Bond number or higher viscosity ratio. As a consequence, trajectories of the sedimentation are also affected by the angular velocity, and blood cells with slower reorientation travel longer distance in the drifting direction. We also explain the mechanism of the reorientation using an asymmetric dumbbell. From the analysis, we show

that magnitude of the angular velocity is explained by two main factors: the shape asymmetry and the instantaneous orientation angle.

Though BEM is one of the most accurate method for simulating capsules in Stokes flow, its heavy computational load has been a major issue even only a few capsules are considered. Our efficient method based on GPU implementation released BEM from its drawback, and this method allows us to access simulations from dilute to dense suspensions. By taking advantage of our method, we have analysed the behaviour of the capsule suspensions under various flow fields as simple shear flow, oscillating shear flow and sedimentation phenomenon. From the analysis, new aspects of the capsule suspensions have been clarified in this thesis: including overshoot phenomenon under oscillating shear flow, the viscoelasticity and the reorientation phenomenon under the sedimentation. The findings presented in this thesis are important to understand properties of the capsule suspensions from a fundamental level, and we hope that the findings would be helpful for future applications.