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Research articles

Regime of aggregate structures and magneto-rheological characteristics of a magnetic rod-like particle suspension: Monte Carlo and Brownian dynamics simulations

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ABSTRACT

In the present study, we address a suspension composed ferromagnetic rod-like particles to elucidate a regime change in the aggregate structures and the magneto-rheological characteristics. Monte Carlo simulations have been employed for investigating the aggregate structures in thermodynamic equilibrium, and Brownian dynamics simulations for magneto-rheological features in a simple shear flow. The main results obtained here are summarized as follows. For the case of thermodynamic equilibrium, the rod-like particles aggregate to form thick chain-like clusters and the neighboring clusters incline in opposite directions. If the external magnetic field is increased, the thick chain-like clusters in the magnetic field direction grow thicker by adsorbing the neighboring clusters that incline in the opposite direction. Hence, a significant phase change in the particle aggregates is not induced by an increase in the magnetic field strength. For the case of a simple shear flow, even a weak shear flow induces a significant regime change from the thick chain-like clusters of thermodynamic equilibrium into wall-like aggregates composed of short raft-like clusters. A strong external magnetic field drastically changes these aggregates into wall-like aggregates composed of thick chain-like clusters rather than the short raft-like clusters. The internal structure of these aggregates is not strongly influenced by a shear flow, and the formation of the short raft-like clusters is maintained inside the aggregates. The main contribution to the net viscosity is the viscosity component due to magnetic particle-particle interaction forces in relation to the present volumetric fraction. Hence, a larger magnetic interaction strength and also a stronger external magnetic field give rise to a larger magneto-rheological effect. However, the dependence of the viscosity on these factors is governed in a complex manner by whether or not the wall-like aggregates are composed mainly of short raft-like clusters. An increase in the shear rate functions to simply decrease the effect of the magnetic particle-particle and the particle-field interactions.

1. Introduction

A suspension composed of magnetic fine particles smaller than micron-size has a recognised potential for application in a variety of engineering fields[1–5]. The specific application field for a magnetic particle suspension is usually dependent on an appropriate combination of both the geometrical and the magnetic characteristics of the particles. In the aspect of the geometrical shape, magnetic particles used for the synthesis of a magnetic suspension may typically exhibit spherical, rod-like, plate-like, disk-like and cube-like geometries. In the aspect of the magnetic properties, the characteristics of the particle magnetization are generally complex and consequently, for the purpose of analysis of the physical phenomena that are strongly dependent on the magnetic characteristics, several particle models have been developed.

These conventional modelling methods may be classified as a dipole model with a fixed magnetic moment [6–8] or with a changeable magnetic moment [9,10], a magnetic charge model [11–14] and a multi-dipole model [4,15,16]. The multi-dipole model is often suitable as a magnetization model for magnetic particles with a complex geometrical shape. The physical behaviour of a magnetic suspension in a flow field and an external magnetic field is generally more complex for the case of dispersed particles with a complex shape or magnetic characteristics. In order to accomplish a successful application of these suspensions in the commercial field, the analysis and development of an accurate

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control of the physical characteristics is considered to be indispensable.

Typical application areas of magnetic particle suspensions are the fields of magnetic recording material engineering [4], fluid engineering [1–3], biomedical engineering [5] and environmental resource engineering [17–19]. In the field of magnetic recording material engineering, magnetic particle suspensions are treated as an intermediary medium to obtain the final goal of recording materials. An example of a control technique for obtaining a successful application may be to control the growth of the crystal structure of the magnetic material by means of an external magnetic field. The primary applications in the field of fluid engineering are mechanical dampers and actuators [2,3]. These applications require magnetic suspensions with a large magneto-rheological characteristic whilst their fluid characteristics have to be controlled in a desirable manner to exhibit suitable properties by means of an applied magnetic field and a flow field. Magnetic colloidal dispersions, known as ferrofluids, may be used for controlling the process of heat transfer [20,21] where a sophisticated cooling technique is indispensable in the engineering fields of microelectronic devices and nuclear reactors. The kind of studies relating to the development of controlling the heat transfer in the engineering applications have recently been expanded to the application of new functional nanofluids [22–25]. In the field of biomedical engineering, it is hopeful that the application of magnetic suspensions may facilitate a magnetically targeted drug delivery system [5,26,27] and magnetic particle hyperthermia [28–31]. There are also challenging technological applications to be found in environmental resource engineering for the recovery of specific substances such as hazardous heavy metal molecules found in environmental waste and pollutants and the extraction of valuable noble metal molecules from water, i.e. from seas, lake, etc., [23–25].

In the present study we focus on the application field of fluid engineering. Mechanical dampers and actuators require suspensions with a large magneto-rheological effect that is controlled using an external magnetic field together with a sophisticated mechanical design incorporating a fluid reservoir and orifice. In the pioneering days of magnetic fluids or ferrofluids, a variety of studies had been conducted from the viewpoint of their application to mechanical dampers and actuators [1]. However, ferrofluids composed of nano-sized spherical magnetic particles in a base liquid cannot exhibit a sufficiently strong magneto-rheological effect and so a successful application regarding mechanical dampers and actuators is unlikely, although the design of a mechanical seal using a ferrofluid is an example of a successful commercial application [32–34]. The current trends regarding ferrofluids are described in the Ref. [35], which includes studies in regard to phase behaviour and polydispersity. Hence, in order to develop devices making use of magneto-rheological characteristics, we are required to synthesize suspensions that exhibit a sufficiently large magneto-rheological characteristic that is able to provide a practical function in a commercial product. Since it is known that non-spherical magnetic particles under certain conditions will offer a large resistance to the ambient flow[36–38], rod-like, disk-like and cube-like particles may be hopeful magnetic particle geometries for synthesizing magneto-rheological suspensions.

Modern synthesis technologies enable one to generate magnetic particles with a variety of shapes and magnetic properties such as rod-like [39–43], disk-like [44,45] and cube-like particles [46–51]. Different from the conventional synthesis technologies, where a new magnetic characteristic is generated by altering the composition of the constituting materials (molecules), the new generation of fine particles is made by design in order to obtain the most desirable properties as functional particles [52,53]. The concept of this development approach corresponds to particular kinds of design engineering with regard to mechanical machines and such non-spherical particle suspensions have actively been studied from various points of view. Dynamic behaviours such as particle orientation and tumbling motion in magnetic rod-like particle suspensions have been investigated by particle-based simulations [6,7,12,54,55]. Features such as yield stress in these suspensions may be strongly dependent on aggregation factors such as the formation and orientation of linear chain-like clusters [56,57]. Moreover, the internal structure of aggregates may undergo a regime change in the particle aggregation due to a dependency on the magnetic field strength and magnetic particle-particle interaction strength [58]. The geometrical shape of non-spherical particles has a significant influence on the magneto-rheological characteristics [59–61] since, for example, rod-like particles offer a much larger resistance to the ambient flow than spherical particles, resulting from the magnetic particle-particle interactions and a restriction of their orientation to the magnetic field direction. If a dilute suspension of magnetic rod-like particles is addressed, certain assumptions may be made for which theoretical approaches are feasible for investigating the rheological characteristics [36,38,62,63].

In contrast to ferromagnetic particles, spindle-like haematite particles are magnetized in a direction normal to the particle axis direction, exhibit much weaker magnetization than the magnetite [41–43,64,65] and give rise to quite different properties. For instance, suspensions composed of spindle-like haematite particles were theoretically predicted to exhibit a negative viscosity under certain conditions of an applied magnetic field [66–69], and this has been experimentally verified using a cone-plate-type rheometer [70]. The aggregate structures of rod-like haematite particles have been investigated by molecular simulations for the case of a non-equilibrium thermodynamic state [71].

There are a variety of studies regarding suspensions of disk-like and cube-like particles by means of both theoretical and experimental approaches. For the case of magnetic disk-like particles, orientational characteristics and aggregate structures have been investigated [72,73] and also the dependence of the magneto-rheological characteristics on a variety factors, including the aggregate structures, has been elucidated [59,74–76]. The sedimentation characteristics of magnetic plate-like particles in the gravitational field are found to be strongly dependent on their orientational properties [77]. Cube-like particles are not an axisymmetric particle but are the next simpler model for theoretical analyses or simulations. Recently, therefore, the microstructure of mono-layers and multi-layers of cube-like particles on a material surface has actively been elucidated experimentally and theoretically [78–82] although currently the rheological characteristics of both cube-like and disk-like particles have not been sufficiently investigated [76,83].

As already pointed out, we here concentrate on suspensions composed of magnetic particles from a fluid engineering point of view and address suspensions composed of ferromagnetic rod-like particles. These particles are typically magnetized in the particle axis direction and exhibit a large magneto-rheological effect [36,38,63], which is in contrast to rod-like haematite particle suspensions where a negative magnetic rheological effect may arise for particular conditions of an external magnetic field [66–70]. As already mentioned, specialised magnetic particles are generated by design in order to obtain the most desirable characteristics as functional particles [52,53], therefore it may be valuable to elucidate the rheological features of a suspension of rod-like particles exhibiting various kinds of magnetic characteristics. From this background, in a previous study [58], we treated a suspension composed of magnetic rod-like particles that are modelled as a spherocylinder with a magnetic dipole moment at the particle centre orientated in the particle axis direction. In that study, we