



## How colloid–colloid interactions and hydrodynamic effects influence the percolation threshold: A simulation study in alumina suspensions



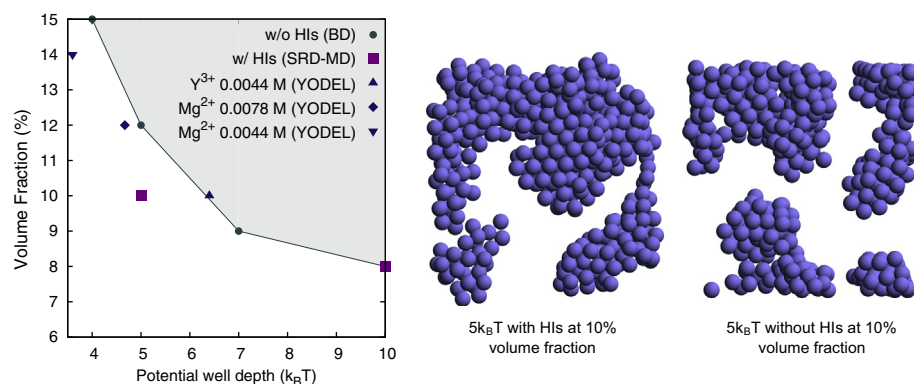
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### GRAPHICAL ABSTRACT



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### ABSTRACT

The percolation behavior of alumina suspensions is studied by computer simulations. The percolation threshold  $\phi_c$  is calculated, determining the key factors that affect its magnitude: the strength of colloid–colloid attraction and the presence of hydrodynamic interactions (HIs). To isolate the effects of HIs, we compare the results of Brownian Dynamics, which do not include hydrodynamics, with those of Stochastic Rotation Dynamics–Molecular Dynamics, which include hydrodynamics. Our results show that  $\phi_c$  decreases with the increase of the attraction between the colloids. The inclusion of HIs always leads to more elongated structures during the aggregation process, producing a sizable decrease of  $\phi_c$  when the colloid–colloid attraction is not too strong. On the other hand, the effects of HIs on  $\phi_c$  tend to become negligible with increasing attraction strength. Our  $\phi_c$  values are in good agreement with those estimated by the yield stress model by Flatt and Bowen.

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## 1. Introduction

The rheology of colloidal suspensions covers a vast number of technological applications, from food products and pharmaceuticals, to ceramic processes and cement industry [1]. A fundamental rheological property of interest is yield stress, which is the amount of stress needed to deform and induce flow to an otherwise mechanically rigid colloidal network [2]. Since the knowledge of yield stress is highly beneficial [3–5], several models have attempted to provide a quantitative definition of yield stress as a function of key factors such as interparticle forces and microstructural information [6,7,2]. However, the limitation in these models is that they are often idealized i.e. they lack a clear representation of other important variables that also contribute to yield stress. This work focuses on one important parameter that is often overlooked in these models i.e. percolation threshold  $\phi_c$ . Zhou et al. [2] have found that yield stress is dominated by inter-particle forces when  $\phi > \phi_c$ , and by structural effects of weak links when  $\phi < \phi_c$ . While this observation is only qualitative, it explains the deviation of previous theoretical models from experimental data [2]. Their results also illustrate the significance of including  $\phi_c$  in the prediction of yield stress. Quite recently, a more complete yield stress model (YODEL), incorporating  $\phi_c$  quantitatively, was proposed by Flatt and Bowen [8,9]. While YODEL shows a good agreement with experiments, it still uses  $\phi_c$  as a fitting parameter. This drawback mainly stems from the absence of a straightforward experimental approach that can accurately determine  $\phi_c$  [9]. Moreover, the phenomenon itself, despite its common occurrence, is still poorly understood.

To this end, numerical simulations can serve as a convenient tool for understanding the variables that influence  $\phi_c$ . Simulations can provide an effective means for predicting the rheology and kinetics of colloids and have greatly contributed to our knowledge of complex systems [10,11]. Among the simulation methods available in literature, the most widely used approach is Brownian Dynamics (BD) [12]. BD treats the fluid as a continuum medium providing friction and thermal noise. The positions of the colloids are evolved using stochastic equations of motion. In its simplest formulation, thermal fluctuations are properly accounted for but hydrodynamic interactions (HIs) are neglected. This results in a substantial increase in computational efficiency. Since the systems in question are often large, this feature of BD makes it highly suitable for the study of percolation.

Nevertheless, HIs are omnipresent in nature and their role in the aggregation kinetics of colloids has been observed [13–15]. Tanaka and Araki [14] have presented strong indications that HIs influence the transient gel formation of colloidal particles. Other works have shown that HIs lead to the formation of less compact clusters, suggesting that this effect might significantly alter the value of  $\phi_c$  [16,17]. However, the studies in Refs. [14,16,17] concerned 2D systems, small systems and simple potentials, respectively, so that the supposed HIs effects on  $\phi_c$  were not verified. Therefore, to gain a better understanding of  $\phi_c$ , an accurate representation of HIs in percolating systems is necessary. At present, the challenge in attacking the problem numerically comes from the computational cost associated with it. For example, the extension of BD with the Yamakawa–Rotne–Prager tensors [18,19] is valid for relatively dilute suspensions. Alternatively, HIs can be taken into account using particle-based or lattice-based methods. Dissipative Particle Dynamics (DPD) [20] is a particle-based approach in which the system is completely defined by specifying all the positions and momenta of solvent particles. In this sense, DPD is similar to Molecular Dynamics. The difference is that instead of using an explicit force term, it uses a weight function to define the collision rules. On the other hand, the Lattice

Boltzmann (LB) technique [21,22] is a lattice-based model where a linearized and preaveraged Boltzmann equation is discretized and solved on a lattice.

In this work, we employ the hybrid Stochastic Rotation Dynamics–Molecular Dynamics (SRD–MD) method that was first introduced by Malevanets and Kapral [23–25]. In SRD–MD, coarse-graining is achieved by grouping the fluid particles into manageable cells. While there is no technique including HIs that is as fast as BD, SRD–MD is relatively simple and fast compared to the particle based and lattice based models described above. In fact, SRD is sometimes referred to as the “Ising model” of hydrodynamics [10] and the simplicity of the approach has allowed the analytical derivation of transport coefficients [26,27].

The main objective of this paper is to determine how attraction strength and HIs influence the percolation behavior, with focus on the determination of  $\phi_c$ . We note that developing numerical methods to determine  $\phi_c$  is very important, especially for systems in which experimental determination is difficult. In Section 2.1, we present the system under study and the simulation techniques employed. In Section 2.2, we describe how we characterized the aggregation kinetics, reorganization and percolation threshold for our system. In Section 3, we present our BD results for  $\phi_c$  as a function of the strength of interparticle forces and we compare these results with the ones obtained from SRD–MD simulations and those estimated by the yield stress model in Refs. [9,28].

## 2. Methodology

### 2.1. Models and simulation techniques

In developing our model, we had a twofold aim: (a) the model should be sufficiently simple to study effectively the influence of attraction strength and HIs on the aggregation and percolation behavior; (b) the model should be sufficiently realistic to allow the comparison with the results concerning the experimental system presented in Refs. [9,28], where Stuer and Bowen applied YODEL for doped alumina suspensions.

In our model we use spherical colloids suspended in water (with density  $\rho_f = 1000 \text{ kg m}^{-3}$ , and viscosity  $\eta = 10^{-3} \text{ Pa s}$ ) at room temperature (293 K). The colloids have a radius of  $a = 255 \text{ nm}$  and a mass of  $M = 2.76 \times 10^{-16} \text{ kg}$ . At variance with the experimental system, in most simulations we do not consider the size dispersion of the colloids, in order to have a simpler picture about the influence of attraction and HIs. However, some simulations including size dispersion have been made. The influence of this factor on the percolation behavior is discussed in the last part of the paper.

The suspension is placed in a simulation box of side length  $L$  and periodic boundary conditions are imposed to model a large percolating system. The value of  $L$  is adjusted depending on the volume fraction  $\phi$  and number of colloids  $N$  being studied:  $L = \sqrt[3]{4N\pi a^3 / (3\phi)}$ .

To describe the interaction between the colloids, we use Derjaguin–Landau–Verwey–Overbeek (DLVO) theory. In this formulation, the total interaction is the sum of two contributions: the attraction due to van der Waals forces  $U_{ij}^{\text{vdW}}$ ; and electrostatic repulsion  $U_{ij}^{\text{el}}$  due to the double layers formed by surface charges. Hence we have

$$U_{ij}^{\text{DLVO}} = U_{ij}^{\text{vdW}} + U_{ij}^{\text{el}}, \quad (1)$$

where the van der Waals term is given by

$$U_{ij}^{\text{vdW}} = -\frac{A}{6} \left\{ \frac{2a^2}{r_{ij}^2 - (2a)^2} + \frac{2a^2}{r_{ij}^2} + \ln \left[ \frac{r_{ij}^2 - (2a)^2}{r_{ij}^2} \right] \right\}. \quad (2)$$

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