Cluster Size Distribution and Scaling for Spherical Particles and Red Blood Cells in Pressure-Driven Flows at Small Reynolds Number

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The clustering characteristic of purely hydrodynamically interacting particles suspended in pressure-driven flow in a circular cylinder is studied using direct numerical simulation based on the solution of the lattice-Boltzmann equation. We find a universal scaling relation for the cluster size distribution in the subcritical regime for all of the cases considered in this study. This scaling relation is independent of particle shape and concentration.

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Investigation of the characteristics and size distribution of particle clusters in suspension under hydrodynamic interaction is important in understanding various phenomena such as sol-gel transition, crystalline formation, and red blood cell aggregation. It is important to study the scaling relations for the cluster size distribution in order to better predict and describe the flow behavior of the suspension. Although, as far as we are aware, there is no published scaling relation for cluster size distribution of solid particles suspended in pressure-driven flows as presented in this Letter; there are other interesting cases relevant to this study. For example, the rheology of weakly attractive colloidal particles is shown to exhibit a surprising scaling behavior as the particle volume fraction or the strength of the attractive interparticle interaction is varied [1]. There is a critical threshold in volume fraction above which the frequency-dependent linear viscoelastic moduli and stress can be scaled onto universal master curves. In another study, the cluster statistics and scaling behavior of diffusion-controlled deposition of many particles in a line of nucleation sites is studied with Monte Carlo simulations [2]. It is found that the number of clusters with size s, that is $n(s)$ scales as $s^{-\tau}$, where τ is about 1.35.

These scaling behaviors suggest that the process of migration and clustering may drive the system into a state of self-organized criticality [3,4]. It is interesting to see if the cluster size distribution in a suspension of solid particles under shear can be characterized with a ''universal'' scaling relation. Since it is difficult to measure the cluster size distribution experimentally, direct numerical simulation of solid particles suspended in liquid under shear becomes an effective approach.

The focus of the present work is on the suspension and clustering of solid particles in a viscous liquid under purely hydrodynamic interactions in the absence of Brownian motion; that is, the Péclet number is infinitely large. There have been many excellent review articles explaining microscopic and macroscopic behavior of suspensions and cluster formation [5,6]. In this study, we present a general scaling relation for the cluster size distribution of nondeformable solid particles suspended in fully developed pressure-driven flow in a circular cylinder at equilibrium. The system considered in this study represents a broad class of applications in flow of suspensions.

Most of the previous studies of clustering in suspensions either do not consider the hydrodynamic interaction of particles or use a stochastic approach where the clustering is considered as a ''birth-death'' process, described by a master equation or a Fokker-Planck type equation [7,8]. We choose an alternative approach based on direct numerical simulation of the particle motion and interaction, by considering the full hydrodynamic forces on the particle and particle-particle interaction. In this approach, the lattice-Boltzmann equations for the fluid phase are coupled with the Newtonian dynamics equations for the solid particles [9]. The lattice-Boltzmann method used in this study has been thoroughly explained and verified previously [9–11]. This method is enhanced [12] by including the full lubrication forces between solid surfaces at link-to-link level when two particles are near contact. The ''link-to-link'' level calculation of the lubrication force is obtained by summation over each link. This hybrid method, verified by comparing the simulation results with previous theoretical investigation [13], allows correct consideration of the hydrodynamic stresses between two particles near contact when the separation distance is a fraction of the lattice size and therefore much smaller than the particle diameter. With the force and torque on the solid particle correctly calculated, the motion of the suspended particle is determined by solving the Newtonian equation of motion. In this study, we are considering solid particles with infinitely large elastic modulus where particle collision and clustering depend on the normal and tangential lubrication forces and the surrounding flow [6,14]. The mechanism of particle cluster formation is similar to the cases considered by Brady and Bossis [6], Nott and Brady [15], and others for inertialess systems except in some cases here we include the effect of particle and fluid inertia at small but nonzero Reynolds number.

In this study, two shapes of neutrally buoyant solid particles are considered. One is a rigid sphere and the other

is a rigid particle in the shape of a red blood cell (RBC), given below.

The computational domain is a circular cylinder with diameter D and length L. Periodic boundary conditions are applied in the axial direction at $x = 0$ and L such that particles leaving the domain at $x = L$ reenter the domain at $x = 0$. The flow is driven by a constant mean axial pressure gradient, dP/dx. Since the particles are neutrally buoyant and gravity is neglected, the relevant parameter is the particle Reynolds number Re defined as Ud/ν, where d is the diameter of the sphere, ν is the kinematic viscosity of the fluid phase, and U is the characteristic velocity, defined as the maximum velocity if there were no solid particles in the domain, i.e., $U = (D^2/16\nu\rho)dP/dx$, where ρ is the fluid density. Except as indicated otherwise, in these simulations we assume Stokes flow (i.e., $\mathrm{Re} \ll 1$), that is negligible inertia. The cylinder Reynolds number Re_D is defined as UD/ν, where D is the diameter of the cylinder. In the simulations presented here, Re_D is in the range from 20 to 50. Therefore, the flow without the particles is a regular Poiseuille pipe flow. There are a total number of N particles in the domain, where N varies from 100 to 1990, and the volume concentration, c, varies from 7% to 19%.

The initial positions and velocities of the particles are set randomly; however, the initial gap between any pair of particles is larger than 0.5 lattice units. Under pressure-driven flow, the fluid as well as the solid particles in the circular cylinder move, and the relative position between particles change. We assume the particles have a smooth surface and, therefore, the particle-particle interaction is governed by purely hydrodynamic forces [12]. In our simulations, we do not use any artificial forces when particles are near contact. Because of the singularity in the lubrication force [13], there is always a very thin layer of liquid in the gap between the solid particles near contact. The criteria in this study for cluster formation is when the gap between two particle surfaces is less than the minimum gap, a_c. We show further below that as long as a_c is small, the results are independent of this parameter. The collection of particles that are in ''contact'' (i.e., the gap is less than a_c) form a cluster, and the number of particles in one cluster, s, is defined as the size of the cluster. The total number of clusters with size s at time t, denoted as $n(s, t)$, rapidly reaches the equilibrium state after the initial transient period. At equilibrium state, the average number of clusters, given by

$$n(s) = \lim_{T\to\infty} \frac{1}{T} \sum_{t=t_0}^{t_0+T} n(s, t),$$

does not change with time. Denoting N_c as the total number of clusters, the average size of the cluster, defined as $\langle s\rangle = N/N_c = \sum_s sn(s)/\sum_s n(s)$, is then computed based on the equilibrium cluster number. In order to see how the cluster size varies in the initial transient, a time-dependent average size of clusters, $\langle s(t)\rangle$, can similarly be defined as $\langle s(t)\rangle = \sum_s sn(s, t)/\sum_s n(s, t)$. A typical result for $N = 270$ from group 1, see Table I below, is shown in Fig. 1. Since the initial positions of the spheres are at least 0.5 lattice units apart, at $t = 0$ there are only single particle ''clusters,'' that is, $\langle s(t = 0)\rangle = 1$, $n(1, 0) = N$, and $n(s, 0) = 0$ for $s > 1$. During the initial transient period—that is, about the first 3500 time steps (nondimensional time $t/(d/U)$ about 10)—the average cluster size distribution increases until it reaches equilibrium.

TABLE I. Set of parameters considered in each group of simulations (all dimensions are in lattice units).

Group	L	D	d	a_c	c_0
1	128	63	8.12	0.02	20%
2	128	63	7.92	0.05	20%
3	256	127	8.12	0.02	24%

A transition in flow regime occurs at a critical concentration, c_0 which is characterized by a fundamental change in cluster size distribution. The number of single particle ''clusters'' [i.e., $n(1)$] increases with concentration, reaching a maximum value at the critical concentration. Beyond the critical concentration, $n(1)$ decreases with concentration. The post-critical state is characterized by a large size cluster dominating the flow. In this study, we focus on the cluster size distribution in the subcritical regime where $c < c_0$ or the reduced volume concentration, $\alpha = c/c_0 = N/N_0$, is between 0 and 1, where N_0 is the number of particles at the critical concentration.

In order to explore the generality of the scaling relation presented below, we consider three groups of parameters for the spherical particles, as outlined in Table I. The cluster size distribution for sphere volume concentrations from 7% to 19% for all of the groups is shown in Fig. 2. The results show that in general for any given size of the cluster, $n(s)$ increases with volume fraction. The values of $n(s)$ decrease rapidly as s increases, which means that the formation of large clusters is a small probability event. The simulation results converge slowly when $n(s) < 10^{-2}$, re-

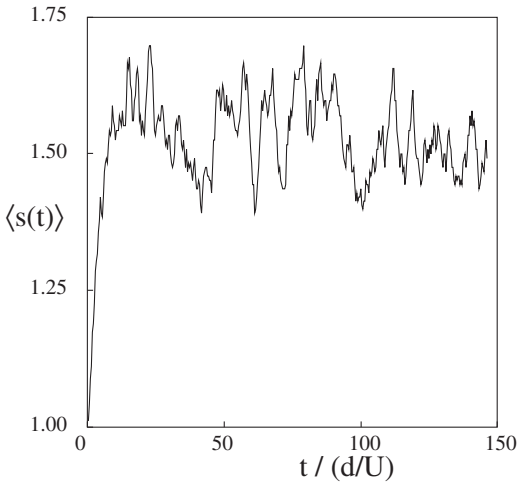

FIG. 1. The average cluster size vs time ($c = 19\%$).

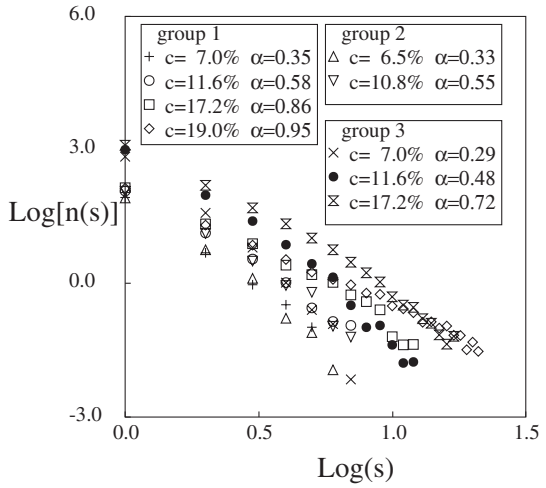

FIG. 2. The cluster size distribution for volume concentration varying from 7% to 19% in logarithm scale. For the definition for the groups, see Table I.

sulting in some scatter when $\log[n(s)] < -2$. However, for $n(s)$ between 10^{-1} to 10^{3}, over a four-decade variation in $n(s)$, the results obtained from our simulations converge rapidly and show almost no scatter.

Although the cluster size distribution depends greatly on the volume fraction, we have found that all the data points presented in Fig. 2 can be scaled onto a universal curve given by,

$$n(s)/n_0 = f(sp), \tag{1}$$

where $p = 1 - \alpha$ and

$$f(x) = x^{-5/2}\exp(-x), \tag{2}$$

as shown in Fig. 3. Here n_0 is the normalization factor. By definition, $N = \sum_s sn(s)$, the normalization factor can be written as

$$n_0 = \frac{Np}{\sum_s (sp)^{-3/2}\exp(-sp)}. \tag{3}$$

In purely shear flow, once a cluster forms, it moves and rotates from compressive to extensional shear axis [6]. In the cases considered here, since the rate of shear varies from a maximum at the wall to zero at the center, a radial concentration gradient exists due to shear [16,17]. In general, the clusters tend to break in the higher shear region and recombine near the center where shear is lower. These clusters evolve permanently with time. Although at any time after the initial transients, particles are captured or released by the clusters, the overall cluster size distribution remains in equilibrium. The competing forces leading to an equilibrium cluster size distribution is a typical phenomenon of self-organized criticality [3,4]. The resulting scaling relation presented above follows the well-known finite-size-scaling method [18], which has been successfully used in stochastic systems [19–21]. When $c > c_0$, however, a large cluster forms and dominates the flow. This super cluster exists most of the time; however, it may break into smaller clusters and then form shortly thereafter. In this post-critical state when the volume concentration increases, the total number of clusters decrease, while the size of the large cluster increases rapidly. The existence of a large cluster at high particle volume concentration in three-dimensional flow inside a circular cylinder (about 28%) is consistent with the results reported by Brady and Bossis [6] and Nott and Brady [15] for a monolayer of particles in shear flow with high particle area concentration of ~40% or volume concentration of ~27%.

To examine the generality of this scaling relation, the cluster size distribution for rigid particles in the shape of RBCs, as shown in Fig. 4, is also considered. The computational domain is a cylinder with 127 lattice units in diame-

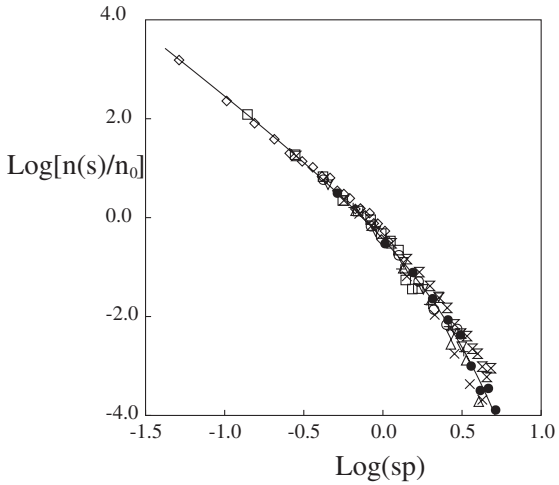

FIG. 3. The computational simulation results for reduced volume concentration, α, ranging from 0.35 to 0.95, are fit by one unique scaling relation (2), shown here as the solid line.

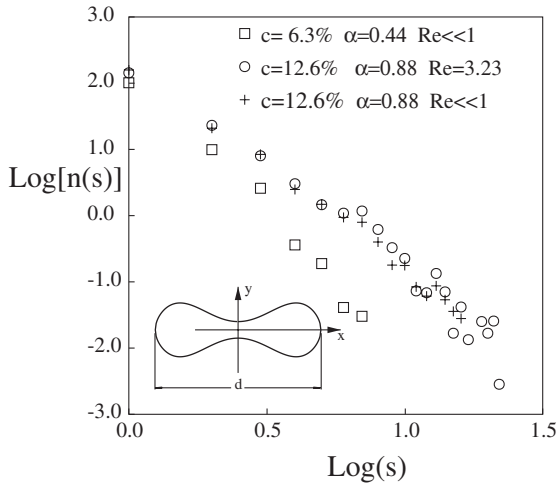

FIG. 4. The computational simulation results for different RBC concentrations and slightly different Reynolds numbers. Inset: RBC is a body of revolution, shaped like a disk.

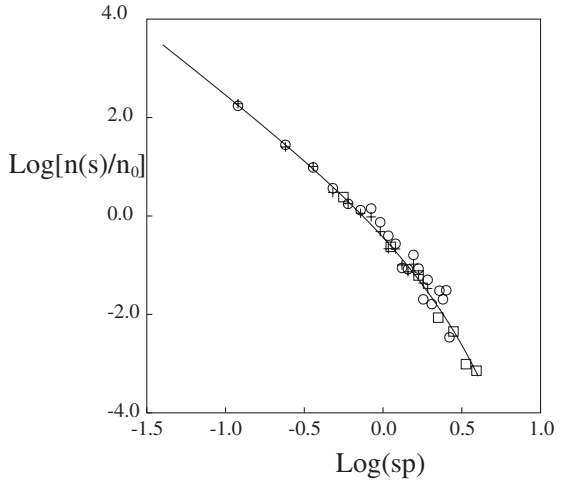

FIG. 5. The computational simulation results of Fig. 4 scaled by Eq. (2), the solid line.

ter and 256 lattice units long. The diameter of the RBC is $d = 2r = 20$ lattice units. The shape of RBC is defined by the revolution of the following contour:

$$y/r = 0.5\sqrt{1 - (x/r)^2}[B_0 + B_1(x/r)^2 + B_2(x/r)^4]$$

for $-r \le x \le r$, about the y axis, where $B_0 = 0.2$, $B_1 = 2.0$, and $B_2 = -1.123$. The critical volume concentration for this system is around $c_0 = 14\%$. Results for volume concentrations of 6.3% and 12.6% with negligible inertia are shown in Fig. 4.

In lattice-Boltzmann method, the simulation can easily be extended to suspension of particles with finite particle inertia. The particle Reynolds number Re is defined the same as for the sphere, except the length scale, d, is the diameter of the RBC (see inset in Fig. 4). The data in Fig. 4, represented by open circles, are results for particle Reynolds number $\mathrm{Re} = 3.23$ and volume concentration $c = 12.6\%$. This case corresponds to a flow Reynolds number, $\mathrm{Re}_D = UD/\nu = 20.5$, based on the fluid viscosity ν, pipe diameter D, and characteristic velocity U defined above. These results show that the particle inertia in the range considered here does not influence the cluster size distribution. Similar to the case of spherical particles, the results for RBC scales onto the same master curve representing the same scaling relation (2), as shown in Fig. 5.

Because the leading term of n_0 is of the order $Np^{5/2}e^p$ in the segment $p \in (0, 1)$, Eq. (3) can be written as $n_0 = Np^{5/2}e^p R_s(p)$, where $[R_s(p)]^{-1} = \sum_s s^{-3/2} \exp[-(s-1)p]$. This function can be approximated by a linear function $R_s(p) \simeq \frac{1}{2}(1 + p)$. Then the normalization factor can be approximated by $n_0 \simeq \frac{1}{2}N(1 + p)p^{5/2}e^p$, which leads to $n(1) \simeq N(1 - \alpha/2) = N_0\alpha(1 - \alpha/2)$. In particular, at small concentration, $\alpha \to 0$, we have $n(1) \simeq N$, which means that almost every particle is separated and no clusters with $s \ge 2$ exist in the system; when $\alpha \to 1$, at the critical concentration, $n(1)$ reaches its maximum value $N_0/2$; that is, in this limit about half of the particles in the system remain dissociated. Furthermore, $R_s(p)$ tends to a constant when $\alpha \to 1$ ($p \to 0$), and the cluster size, $n(s)$, becomes proportional to $s^{-5/2}$. This means that the critical concentration is characterized by the simple power relation of the cluster size distribution, without exponential decay. These results are also confirmed in our numerical simulation.

In summary, we show that in a pressure-driven flow of suspension inside a circular cylinder, the cluster size distribution may follow a universal scaling relation which appears to be independent of particle shape and concentration. The cluster size distribution seems to be insensitive to inertia up to particle Reynolds number $\mathrm{Re} = 3$. There exists a critical concentration, where $n(1)$ reaches its maximum value, and the cluster size distribution becomes a simple power relation. We also show that in this limit about half of the particles remain freely suspended. These results are consistent with the general concept of self-organized criticality [3,4].

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