Simulations of a binary-sized mixture of inelastic grains in rapid shear flow

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In an effort to explore the rapid flow behavior associated with a binary-sized mixture of grains and to assess the predictive ability of the existing theory for such systems, molecular-dynamic simulations have been carried out. The system under consideration is composed of inelastic, smooth, hard disks engaged in rapid shear flow. The simulations indicate that nondimensional stresses decrease with an increase in d_L/d_S (ratio of large particle diameter to small particle diameter) or a decrease in ν_L/ν_S (area fraction ratio), as is also predicted by the kinetic theory of Willits and Arnarson [Phys. Fluids **11**, 3116 (1999)]. Furthermore, the level of quantitative agreement between the theoretical stress predictions and simulation data is good over the entire range of parameters investigated. Nonetheless, the molecular-dynamic simulations also show that the assumption of an equipartition of energy rapidly deteriorates as the coefficient of restitution is decreased. The magnitude of this energy difference is found to increase with the difference in particle sizes.

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I. INTRODUCTION

Flowing granular materials are prevalent in both nature and industry. Examples include avalanche flows, landslides, pharmaceuticals processing, mineral transport, and grain conveying. In many practical systems, the particles are characterized by a distribution of sizes. Such polydispersity is expected to affect the bulk behavior of the flowing material (e.g., stresses), and is known to lead to segregation among particles of different sizes. Although kinetic-theory models for monodisperse systems display reasonable agreement with rapid flows (i.e., flows in which collisions between particles can be considered instantaneous), extension of such theories to even two particle sizes remains a challenging task. A complementary approach involves the use of molecular-dynamic (MD) simulations, which can easily be adapted to simulate systems characterized by a nonuniform size distribution. These simulations not only provide an effective means of probing the hydrodynamic behavior of binary mixtures, but are also useful in assessing the validity of existing kinetic theories and their inherent assumptions.

Over the past two decades, several constitutive theories for binary mixtures of smooth, inelastic particles have been developed. Among the earliest efforts were those of Shen [1] and Farrell, Lun, and Savage [2], who examined the simple shear flow of binary-sized spherical particles. Shen used a simple averaging procedure to describe the stresses of the mixture, whereas Farrell and coworkers followed the more rigorous methods of the dense-gas kinetic theory. As part of the latter effort, the single particle velocity distribution function was represented as a Maxwellian distribution. In both of these works, only *collisional* modes of transfer were considered, and thus the resulting constitutive relations are most appropriate for relatively dense flows. The dense-gas kinetic-theory approach was also employed by Jenkins and Mancini [3] for binary mixtures of both circular disks and spheres and by Huilin *et al.* [4] for binary mixtures of spheres. Similar to the work of Farrell, Lun, and Savage [2], the single particle velocity distribution was assumed to be Maxwellian in both works. Unlike the previous effort, however, these constitutive theories include both kinetic and collisional contributions to transport, and they are applicable to a general flow field. Furthermore, these theories account for differences in particle size and/or density. A more precise theory for spheres was put forth by Jenkins and Mancini [5]. In their work, the single particle velocity distribution function was *not* assumed to be Maxwellian. (Strictly speaking, the velocity distribution is Maxwellian only for elastic spheres in a uniform steady state [6]). Instead, it was assumed to take the form of a perturbed Maxwellian, and was determined as an approximate solution to the relevant Boltzmann equations (i.e., Chapman-Enskog expansion method). Furthermore, the equilibrium radial distribution function at contact was treated according to the revised Enskog theory for mixtures [7], whereas earlier studies used the standard approach of evaluating the radial distribution function at a specific point between the two particles. The resulting constitutive theory was later corrected and extended to a higher-order approximation, namely, the second Enskog approximation, by Arnarson and Willits [8] for spheres and Willits and Arnarson [9] for disks. (For a more detailed discussion on the differences between these theories, the reader is referred to Ref. [10].) This level of approximation is expected to be valid for mixtures of particles with similar radii and mass [9]. For example, the latter effort includes a comparison of viscosities between the Willits and Arnarson theory, the earlier theory of Jenkins and Mancini [3], and simulations of a binary mixture of *perfectly* elastic disks with a diameter ratio of 1.25. Over a range of overall solids fractions, the Willits and Arnarson theory displays an excellent match with the simulation data, whereas predictions from the Jenkins and Mancini theory are considerably lower in value.

With the exception of the earlier kinetic theory of Jenkins and Mancini [3] and the theory of Huilin *et al.* [4], a common feature of each of the aforementioned theories for binary mixtures is the assumption of equipartition of granular

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energy, which refers to the kinetic energy associated with the fluctuating motion of individual particles. (Similar to the Maxwellian velocity distribution, this assumption is strictly true only for a mixture of elastic spheres in a uniform steady state [6].) Because the equipartition assumption provides an explicit relation between the granular temperature (or granular energy) of the large and small particles, the resulting constitutive relations can be expressed as a function of a *single* temperature. Correspondingly, only one granular energy balance (associated with this temperature) is necessary in order for the system to be fully specified. If the assumption of equipartition of energy is lifted, a granular energy balance for each of the two particle types is required, resulting in a *multitemperature* theory. (Note that although the Jenkins and Mancini theory [3] was developed for multitemperature systems, applications of this theory which appear in the literature incorporate the assumption of equipartition of energy, thereby reducing the predictions to a single-temperature form.)

In addition to the theoretical contributions described above, several studies involving MD simulations of rapidly flowing, binary mixtures have been performed to investigate the stresses exhibited by these mixtures. Ladd and Walton [11] used a hard-sphere approach to simulate the shear flow of a binary-sized mixture of smooth, inelastic spheres. They reported the shear stress as a function of the particle size ratio for a relatively dense (overall solids area fraction $\nu = 0.5$) and fairly elastic (coefficient of restitution $e = 0.95$) system. As shown in Ref. [5], a comparison of their (previously unreported) simulations for $e = 0.8$ with the predictions of Jenkins and Mancini [5] exhibits reasonable agreement, whereas lesser agreement is observed in a similar comparison with the theory proposed by Farrell, Lun, and Savage [2]. A hard-sphere approach was also employed by Nakagawa and Imaizumi [12], who simulated a plane Couette flow of rough, inelastic disks. For systems with a fixed solids fraction in the range $\nu = 0.38-0.5$, the simulation results indicated that collisional stresses tend to decrease with an increased difference in the particle size. More recently, Karion and Hunt [13] carried out soft-sphere simulations of binary-sized, spherical particles in a two-dimensional Couette flow. Their simulations were performed in the dense limit ($\nu = 0.75$) for inelastic, rough particles ($e = 0.8$ and friction coefficient $= 0.5$). A comparison of the simulation data for stresses with the predictions of the earlier Jenkins and Mancini [3] effort indicates that the theoretical model drastically underpredicts the simulation results, which the authors attribute to inherent differences between disks (theory) and spheres (simulations). Their simulation results also demonstrate that an equipartition of energy is not exhibited for the systems that were examined. Namely, the disparity between the granular energy of the two particle types becomes greater with the size difference between the two particle types.

Although the previous simulation studies have shed light on the bulk behavior of binary flows, the focus of these studies has been largely on relatively dense flows with enduring, frictional contacts. In an effort to expand on this knowledge, the goal of the current study on binary-sized, rapid granular flows is twofold. First, the detailed hydrodynamics associated with a binary size distribution is systematically probed over a wide range of system parameters (i.e., overall solids fraction, solids fraction ratios, diameter ratios, and coefficients of restitution). To accomplish this task, two-dimensional simulations of smooth, inelastic disks are performed for the case of simple shear flow. (Due to the presence of a constant velocity gradient, simple shear flow does not lead to size segregation, and thus allows for a straightforward calculation of the stress field.) Second, because the assumptions associated with the simulations are identical to those inherent in the kinetic-theory models (i.e., smooth, inelastic particles engaging in instantaneous collisions), the simulation results are used to assess the validity of existing theory for binary flows. The results indicate that the kinetic-theory predictions for stresses are in good agreement with the simulation data over the range of parameters investigated. The assumption of equipartition of energy, however, is found to rapidly deteriorate away from the elastic limit. This effect is most dramatic at large size differences and small restitution coefficients.

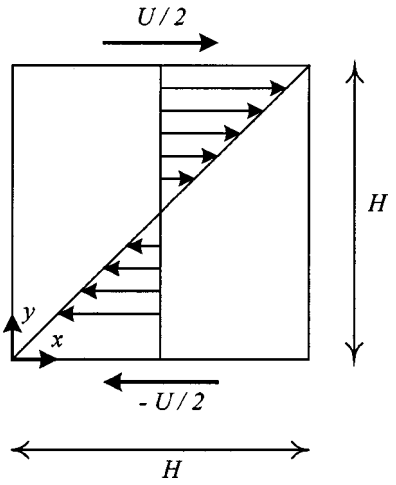

FIG. 1. Simple shear flow system.

II. SIMULATION DESCRIPTION

The two-dimensional system under consideration consists of N circular particles that undergo continual shearing in the x direction. Particles of two sizes are present; the larger particles have diameter d_L and the smaller particles have diameter d_S. All particles are perfectly smooth (frictionless), inelastic disks with constant restitution coefficient e and density ρ. As no external forces or interparticle forces are present, the particles move in straight-line trajectories between collisions. These collisions are assumed to be binary and instantaneous. As depicted in Fig. 1, the flow field is an $H \times H$ square, and is characterized by a constant velocity gradient. In particular, the particles at the top boundary move with mean velocity $U/2$ and those at the bottom boundary move with mean velocity $-U/2$, thereby giving rise to the shear rate $\gamma = U/H$.

To simulate the aforementioned system, an event-driven, hard-sphere approach is utilized. This approach involves three steps, namely, the determination of the next collision,

the advancement of particles in time until that collision, and the implementation of collision dynamics for the two colliding particles. The search for future collision partners is made by solving a quadratic equation for collision time. In order to make this search more efficient, a link-cell algorithm is utilized [14]. Once the minimum collision time is determined, the position of each particle is advanced in time based on its current velocity. The postcollision velocities of the colliding pair are then found according to the relations

$$\mathbf{V}_L^* = \mathbf{V}_L - \frac{m_S}{m_L + m_S}(1+e)[\mathbf{k}\cdot(\mathbf{V}_L - \mathbf{V}_S)]\mathbf{k}, \tag{1}$$

$$\mathbf{V}_S^* = \mathbf{V}_S + \frac{m_L}{m_L + m_S}(1+e)[\mathbf{k}\cdot(\mathbf{V}_L - \mathbf{V}_S)]\mathbf{k}, \tag{2}$$

where the subscripts L and S refer to the large and small particles, respectively, $\mathbf{V}^*$ is the postcollision particle velocity, $\mathbf{V}$ is the precollision velocity, m is the particle mass, e is the coefficient of restitution, and $\mathbf{k}$ is unit vector pointing from the center of particle 1 to the center of particle 2. [Equations (1) and (2) are derived from the conservation of linear momentum and the definition for e, namely, $\mathbf{k}\cdot(\mathbf{V}_L^* - \mathbf{V}_S^*) = -e\mathbf{k}\cdot(\mathbf{V}_L - \mathbf{V}_S)$, which quantifies the level of inelasticity experienced in a collision.] In order to attain a state of simple shear, the Lees-Edwards boundary condition [15] is implemented on the top and bottom boundaries, whereas periodic conditions are enforced at the left and right boundaries.

To fully define the simulated system, the following inputs are required: d_L, d_S, ν, ν_L, m_L, e, γ, and H, where the subscripts L and S refer to quantities associated with the large and small particles, respectively. Note that the additional quantities U, ν_S, and m_S are determined via the shear rate ($\gamma = U/H$), overall solids area fraction ($\nu = \nu_L + \nu_S$), and assumption of constant density

$$m_s = \rho(\pi d_s^2/4) = \left(\frac{m_L}{\pi d_L^2/4}\right)(\pi d_s^2/4), \tag{3}$$

respectively. Furthermore, the number of large and small particles in a given simulation is found according to the definition of area fraction

$$\nu_L = \frac{N_L(\pi d_L^2/4)}{H^2} \quad \text{and} \quad \nu_S = \frac{N_S(\pi d_S^2/4)}{H^2}, \tag{4}$$

where N_L and N_S refer to the number of large and small particles, respectively. Thus, a set of dimensionless parameters that characterize the system include H/d_L, d_L/d_S, ν, ν_L/ν_S, and e. For the current study, H/d_L is kept constant at 19.817 (the implications of which will be discussed in the following section), and the remaining four dimensionless parameters are used as independent control parameters. In particular, these quantities are systematically varied over the ranges $d_L/d_S = 1-5$, $\nu = 0.1-0.5$, $\nu_L/\nu_S = 0.5-4$, and $e = 0.8-0.99$. The remaining needed dimensional quantities, namely, m_L, γ, and H, are each set equal to unity.

To initialize the system, the particles are approximately evenly spaced in both directions (i.e., small random displacements to particle positions are made in the x and y directions). Furthermore, the initial velocity field is set equal to the sum of a mean component (based on particle position in the shear field) plus a small random component ($\sim$0.1% of U). Once this initialization is complete, the simulation then proceeds from collision to collision as described above. Eventually, a statistical steady state is reached, after which data on the mean stresses is gathered. More specifically, in order to ascertain whether a steady state has been reached, the granular energy (i.e., kinetic energy of the velocity fluctuations) of the system is tracked as the simulation proceeds

$$E = E_L + E_S = \tfrac{1}{2}m_L\langle V'^2\rangle_L + \tfrac{1}{2}m_S\langle V'^2\rangle_S, \tag{5}$$

where E refers to the ''mixture'' granular energy, the subscripts L and S refer to quantities associated with the large and small particles, respectively, V'^2 refers to the square of the fluctuating velocity component, and $\langle\ \rangle$ refer to a quantity averaged over all of the relevant (i.e., large or small) particles in the domain. For the range of parameters considered in this study, the granular energy typically reaches a statistically steady value in 500–1000 collisions per particle. At this point, the simulation is allowed to run for at least an additional 4000 collisions per particle, over which period the stress data is collected. In particular, the kinetic contribution to the stress tensor $\mathbf{P}^{\mathbf{k}}$ is based on the relation

$$\mathbf{P}^{\mathbf{k}} = \mathbf{P}_L^{\mathbf{k}} + \mathbf{P}_S^{\mathbf{k}} = \rho\nu_L\langle\mathbf{V}'\mathbf{V}'\rangle_L + \rho\nu_S\langle\mathbf{V}'\mathbf{V}'\rangle_S, \tag{6}$$

where $\mathbf{V}'$ refers to the fluctuating component of the velocity vector. Because $\mathbf{P}^{\mathbf{k}}$ does exhibit minor fluctuations during the steady-state period, the final reported value of $\mathbf{P}^{\mathbf{k}}$ represents the average taken over 10 000 steady-state snapshots. The collisional contribution to the stress tensor $\mathbf{P}^{\mathbf{c}}$ is found according to

$$\mathbf{P}^{\mathbf{c}} = \mathbf{P}_{LL}^{\mathbf{c}} + \mathbf{P}_{LS}^{\mathbf{c}} + \mathbf{P}_{SS}^{\mathbf{c}} = \frac{1}{H^2\Delta t}\left(\sum_{\substack{\text{all } LL\\ \text{collisions}}} d_L\mathbf{J}\mathbf{k} + \sum_{\substack{\text{all } LS\\ \text{collisions}}} \frac{d_L + d_S}{2}\mathbf{J}\mathbf{k} + \sum_{\substack{\text{all } SS\\ \text{collisions}}} d_S\mathbf{J}\mathbf{k}\right), \tag{7}$$

where the subscripts LL, LS, and SS refer to stress contributions arising from collisions between two large particles, a large and small particle, and two small particles, respectively; Δt is the period of simulation time over which steady-state data is gathered; and the impulse $\mathbf{J} = m_L\mathbf{V}_L - m_L\mathbf{V}_L^*$ represents the momentum exchanged between particles 1 and 2 during a collision. Prior to reporting, the dimensional forms of the stresses given in Eqs. (6) and (7) are first made dimensionless via division by $\rho d_L^2\gamma^2$.

III. RESULTS AND DISCUSSION

For purposes of both validation and benchmarking, the molecular-dynamic simulations were first performed using

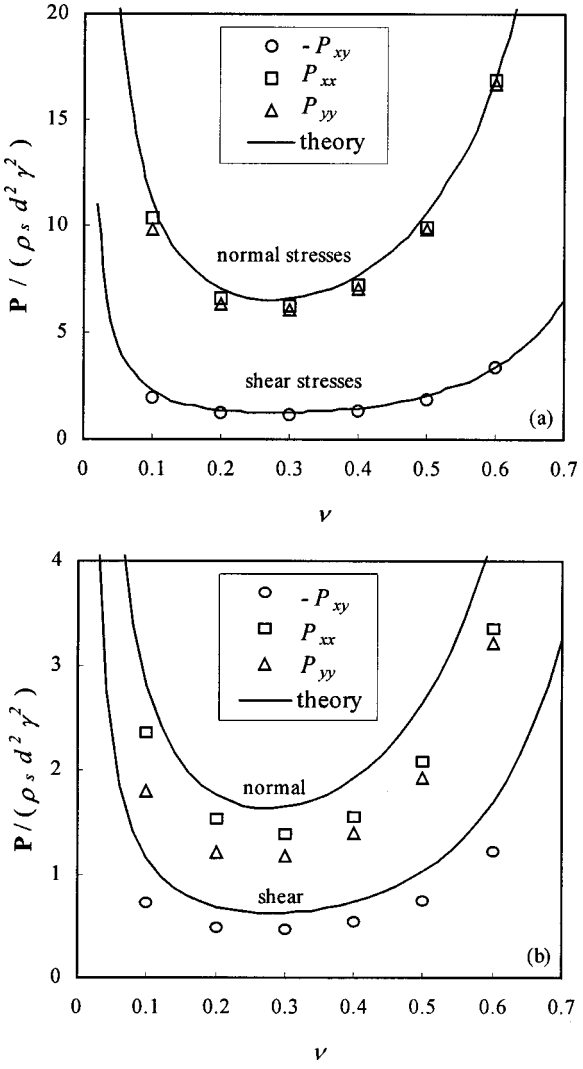

FIG. 2. Stresses in monodisperse systems with kinetic-theory predictions of Jenkins and Richman [16] for (a) $e=0.95$ and (b) $e=0.8$.

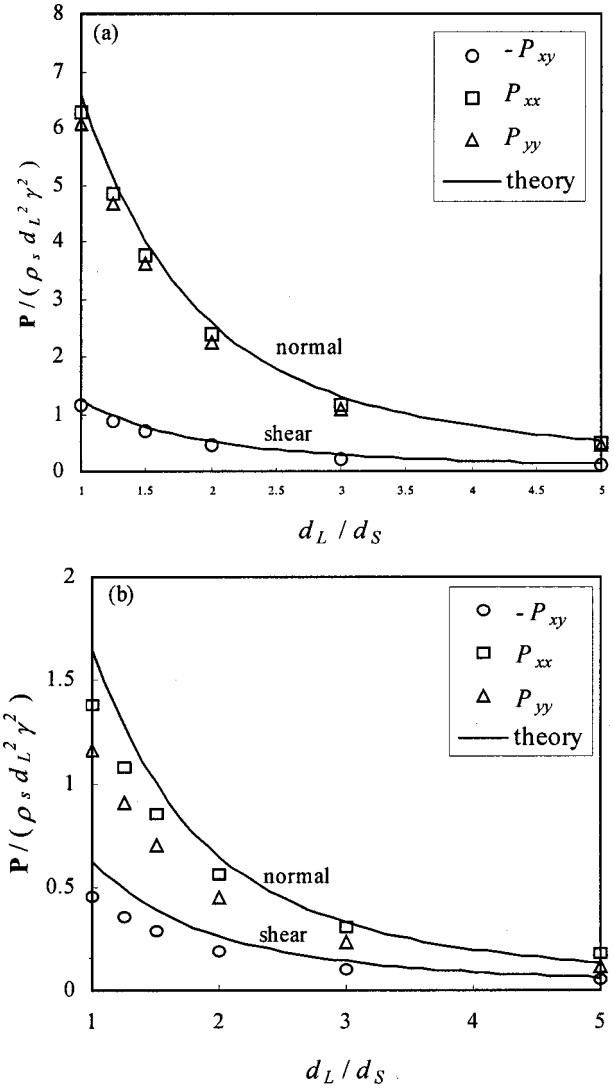

FIG. 3. Stresses in binary systems with kinetic-theory predictions of Willits and Arnarson [9] for $\nu=0.3$, $\nu_L/\nu_S=1.0$ and (a) $e=0.95$ and (b) $e=0.8$.

monodisperse systems over a range of solids fractions and coefficients of restitution. In Fig. 2, a comparison between the dimensionless stresses determined from simulation and those obtained using kinetic theory (for monodisperse systems) is given for two different coefficients of restitution. In this diagram, the MD results are represented by individual points and the kinetic-theory predictions of Jenkins and Richman [16] are indicated by lines. Note that because an assumption of the Jenkins and Richman theory is $P_{xx}=P_{yy}=P$, a single line denoting the kinetic-theory prediction of P is shown for comparison with both the P_{xx} and P_{yy} simulation results. As illustrated in Fig. 2(a) for $e=0.95$, very good agreement between theory and simulation is obtained for both the shear (lower line and data points) and normal (upper line and data points) stresses. For example, at a solids fraction of 0.3, the kinetic theory overpredicts the simulation results for P_{xx}, P_{yy}, and $-P_{xy}$ by 5%, 9%, and 9%, respectively. As the value of e is lowered to 0.8 [Fig. 2(b)], however, the theoretical predictions become substantially higher than the simulation data, and a significant anisotropy of the normal stresses is observed in the simulations. For the same solids fraction of 0.3, the discrepancy between the theory and simulation data has increased to 20%, 41%, and 38% for P_{xx}, P_{yy}, and $-P_{xy}$, respectively. Such a behavior is consistent with the limitations of the theory, which was developed in the nearly elastic limit ($e\sim 1$) under the assumption of an isotropic normal stress tensor.

The molecular-dynamic simulations of the binary mixtures were carried out over a broad parameter space, namely, $e=0.8-0.99$, $\nu=0.1-0.5$, $\nu_L/\nu_S=0.5-4$, and $d_L/d_S=1-5$. The results of these simulations for $\nu=0.3$ are displayed in Figs. 3–7; the other solids fractions that were investigated exhibit similar characteristics and are not shown for the sake of brevity.

Figure 3(a) depicts the variation of the dimensionless stresses with the particle diameter ratio (d_L/d_S) for $\nu_L/\nu_S=1$ and $e=0.95$. In this diagram, the molecular-dynamic results are compared to the kinetic-theory predictions of Willits and Arnarson [9] for binary mixtures. For both the shear

and normal stresses, the kinetic theory correctly captures the qualitative nature of the MD simulations. In particular, both stresses are seen to decrease with an increase in particle size ratio. [Note that an increase d_L/d_S is attained by decreasing d_S and thus increasing N_S according to Eq. (4). Thus, the *average* particle diameter decreases as d_L/d_S increases.] From a quantitative standpoint, good agreement is obtained for both the normal and shear stress components. Specifically, at the highest diameter ratio investigated ($d_L/d_S=5$), the theoretical predictions for P_{xx}, P_{yy}, and $-P_{xy}$ are respectively 8%, 19%, and 26% higher than the simulation values, which are slightly larger than the discrepancies obtained at the monodisperse limit (5%, 9%, and 9% respectively). This observation is consistent with the known limitations of the theory (i.e., the second Enskog approximation is expected to be valid for mixtures of particles characterized by *similar* size and mass).

A similar comparison is shown in Fig. 3(b) for the more dissipative case of $e=0.8$. Near $d_L/d_S=1$, the kinetic-theory predictions are inferior to those obtained at the higher coefficient of restitution [Fig. 3(a)]. This behavior is similar to that of the monodisperse system displayed in Fig. 2. However, the level of agreement between the theoretical predictions and simulation data is found to generally *increase* as the diameter ratio increases. Namely, the discrepancies between the theory and simulation for P_{xx}, P_{yy}, and $-P_{xy}$ are 20%, 41% and 38% at $d_L/d_S=1$ and -23%, 17%, and 19% at $d_L/d_S=5$. This trend is opposite to that observed for the more elastic case of $e=0.95$ [Fig. 3(a)]. A possible explanation for this behavior may be linked to the size of the system used in the simulations. As was initially observed by Hopkins and Louge [17] for a monodisperse, simple shear system, the stresses obtained in MD simulations are known to increase with H/d (where d refers to the diameter of the single particle size). These stresses eventually reach an asymptotic value at high H/d, as was recently shown by Liss and Glasser [18]. The former behavior is traced to the increasing prevalence of particle microstructures or ''clusters'' (i.e., inhomogeneities in the spatial distribution of particles), which occur due to the inelastic nature of particle collisions. Once the domain size is made large enough for the clusters to ''fully form,'' further increases in stress with H/d are no longer observed. For all of the binary-sized simulations performed in this work, recall that a fixed system size of $H/d_L=19.817$ has been used. Although this system size is fairly small, the effect of particle clusters is expected to become more pronounced at higher values of d_L/d_S due to the increased number of particles in the domain (i.e., although H/d_L is kept constant, H/d_S increases with d_L/d_S). Since the effect of clusters is *not* incorporated in the development of kinetic-theory models, a reasonable consequence of more pronounced clustering at higher d_L/d_S is an increase in the simulation stresses relative to those of the theoretical predictions, as is observed in Fig. 3(b). Furthermore, the magnitude of the observed effect is of the same order as that which has been linked to clustering. For example, simulations of a monodisperse system with $\nu=0.3$ and $e=0.8-0.95$ indicate that stresses obtained at $H/d\sim 20$ are greater than 90% of their asymptotic value. Finally, previous investigators have found that clustering is more prevalent at lower coefficients of restitution [17], which appears to explain why an increase in the simulation stresses relative to the theoretical predictions with increased d_L/d_S is evident for the more dissipative system of $e=0.80$ [Fig. 3(b)] but not for the system with $e=0.95$ [Fig. 3(a)].

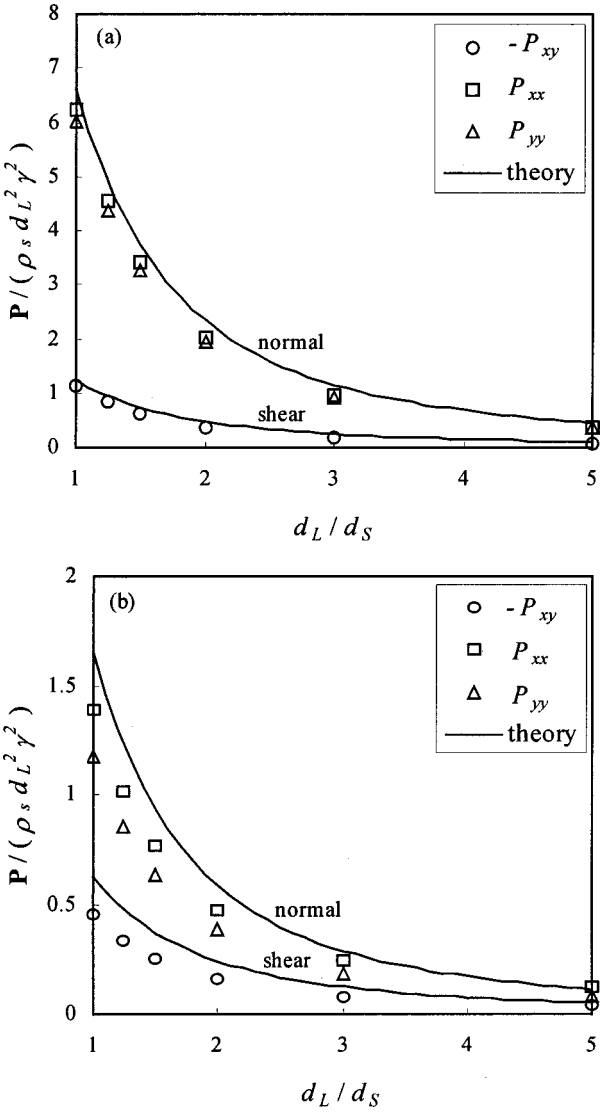

FIG. 4. Stresses in binary systems with kinetic-theory predictions of Willits and Arnarson [9] for $\nu=0.3$, $\nu_L/\nu_S=0.5$ and (a) $e=0.95$ and (b) $e=0.8$.

The dependency of the stress behavior on the solids area fraction ratio (ν_L/ν_S) can be ascertained via a comparison of Figs. 3–5. In particular, Fig. 3 represents a system composed of a 50/50 mix (by particle area) of large and small particles ($\nu_L/\nu_S=1.0$), whereas Figs. 4 and 5 show analogous results for a 33/67 ($\nu_L/\nu_S=0.5$) and 80/20 ($\nu_L/\nu_S=4$) mix of large to small particles, respectively. A comparison of these plots indicates that the Willits-Arnarson theory [9] correctly captures the qualitative dependency of the stresses on ν_L/ν_S. Namely, for a given diameter ratio, stresses are observed to increase with an increase in ν_L/ν_S. Furthermore, both the simulations and theory indicate that this effect becomes more

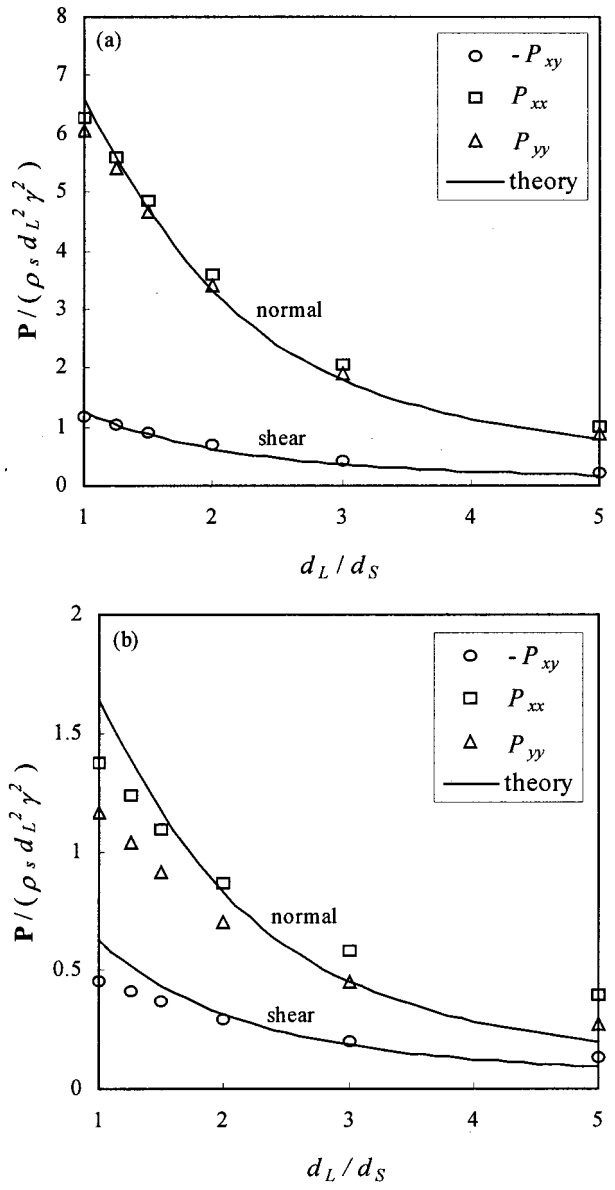

FIG. 5. Stresses in binary systems with kinetic-theory predictions of Willits and Arnarson [9] for $\nu=0.3$, $\nu_L/\nu_S=4.0$ and (a) $e=0.95$ and (b) $e=0.8$.

pronounced for higher values of d_L/d_S. Quantitatively, a comparison of Figs. 3–5 shows that the level of agreement between theory and MD simulation is similar over the range of volume fractions investigated. Nonetheless, the observation of increased simulation stresses relative to theoretical predictions with an increase d_L/d_S becomes more apparent as ν_L/ν_S increases. For example, at the $\nu_L/\nu_S=0.5$ and $e=0.95$ [Fig. 4(a)] the simulation stresses are lower than theoretical predictions for all d_L/d_S investigated; for the same restitution coefficient and $\nu_L/\nu_S=4.0$ [Fig. 5(a)], the simulation stresses become larger than the predictions at higher values of d_L/d_S.

At this point, comments on an additional aspect of the stress comparisons portrayed in Figs. 3–5 are worthwhile. Namely, the qualitative nature of the comparisons as presented in these figures is different than that previously observed by Karion and Hunt [13] in their soft-sphere simulations of systems near the dense limit. Their simulations of binary mixtures exhibited normal and shear stresses that were considerably *higher* than the predictions obtained using the kinetic theory developed by Jenkins and Mancini [3]. This behavior was found over the entire range of size and volume fraction ratios considered. Recall, however, that this particular kinetic theory was developed based on the assumption of a Maxwellian velocity distribution, which was later demonstrated by Willits and Arnarson [9] to result in a substantially lower shear viscosity than that obtained using a non-Maxwellian distribution (by roughly a factor of 2 or more). This observation, as well as those made by the authors (e.g., comparison of simulations for spheres and theory for disks), may help to explain the qualitative differences that exist between the current comparisons and those presented by Karion and Hunt [13].

As mentioned earlier, with the exception of the earliest Jenkins and Mancini [3] effort and the Huilin *et al.* effort [4], each of the kinetic theories that have been developed for binary systems [5,8,9] rely on the assumption of an equipartition of granular energy. In other words, it is assumed that average kinetic energy associated with fluctuating motion of each particle size is equal (i.e., $E_L=E_S$). The validity of this assumption can be determined from the simulation data displayed in Fig. 6(a) that demonstrates the dependency of the granular energy ratio (E_L/E_S) on d_L/d_S and e for the case of $\nu_L/\nu_S=1$. An equipartition of energy is not observed for values of $d_L/d_S>1$ and $e<1$. More specifically, as was observed in the simulations of Karion and Hunt [13], the granular energy of the larger particle increases relative to that of the smaller particle as d_L/d_S increases. Furthermore, the current simulations also reveal that the energy difference is a strong function of the coefficient of restitution. For example, at a diameter ratio of 3, E_L is 26% larger than E_S for $e=0.95$, and more than 100% larger than E_S for $e=0.80$. Analogous plots are shown in Figs. 6(b) and 6(c) for $\nu_L/\nu_S=0.5$ and 4, respectively. Similar trends are observed for each of these area fraction ratios. Hence, the MD results indicate that the assumption of equipartition of energy is only valid in a limited range near the perfectly elastic, monodisperse limit. A related finding for a binary mixture undergoing homogenous cooling (i.e., an unforced system) has been reported by Garzo and Dufty [19]; their theoretical analysis indicates that such systems also display an energy difference between particles of different type.

Related information is portrayed in Fig. 7, where the ratio of the square of the fluctuating velocities associated with each particle size is given as a function of d_L/d_S and e. Simulation results for $\nu_L/\nu_S=1$, 0.5, and 4 are shown in subplots (a)–(c) respectively. As expected, the magnitude of the velocity fluctuations associated with each particle size is essentially equal in the monodisperse limit. As the size ratio between particles increases, however, $\langle V_L'^2\rangle/\langle V_S'^2\rangle$ is observed to drop off rapidly (i.e., the velocity fluctuations of the small particles become greater than those of the large particles) until $d_L/d_S\sim 3$, at which point changes in the ratio become more gradual. Furthermore, the effect of inelasticity also becomes more prominent at higher d_L/d_S. More spe-

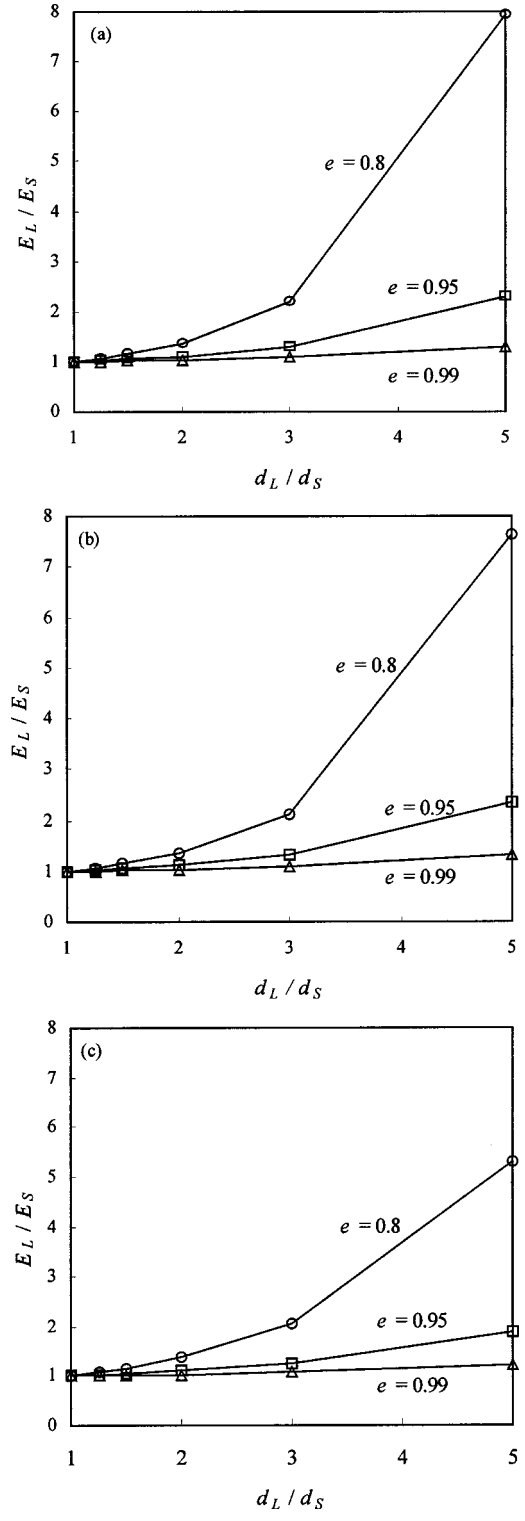

FIG. 6. Dependency of granular energy ratio (E_L/E_S) on diameter ratio and restitution coefficient for $\nu=0.3$ and (a) $\nu_L/\nu_S=1.0$, (b) $\nu_L/\nu_S=0.5$, and (c) $\nu_L/\nu_S=4.0$.

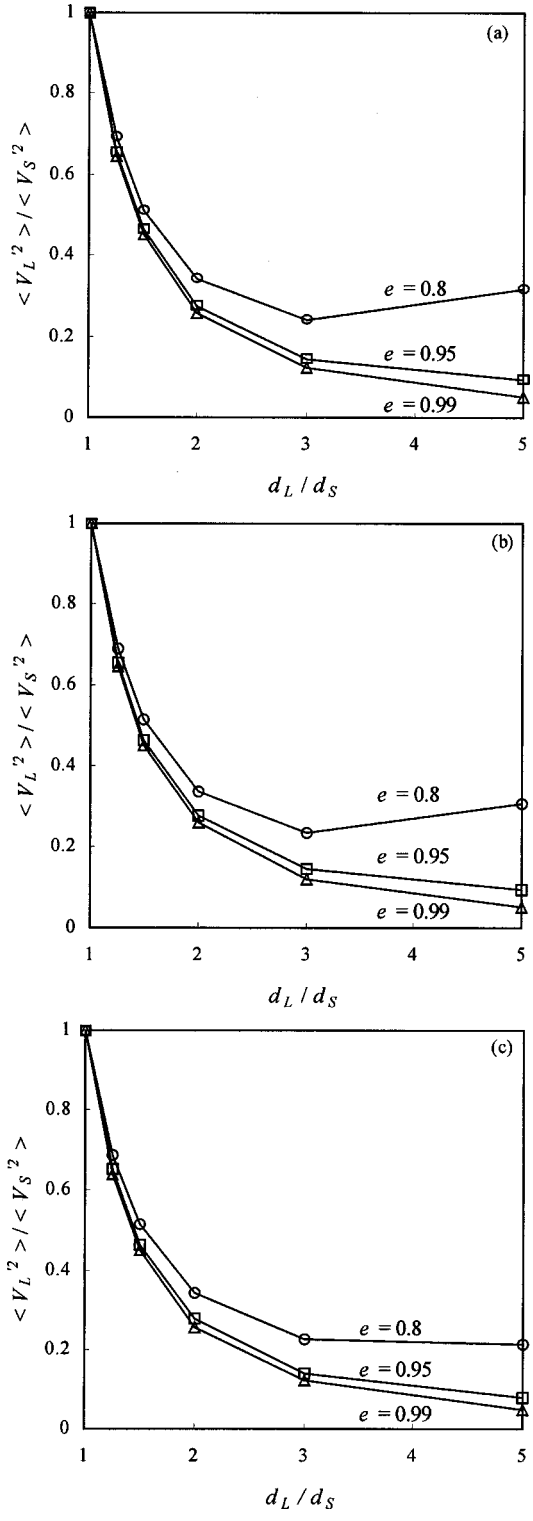

FIG. 7. Dependency of square of fluctuating velocity ratio ($\langle V_L'^2\rangle/\langle V_S'^2\rangle$) on diameter ratio and restitution coefficient for $\nu=0.3$ and (a) $\nu_L/\nu_S=1.0$, (b) $\nu_L/\nu_S=0.5$, and (c) $\nu_L/\nu_S=4.0$.

cifically, a larger difference between $\langle V_L'^2\rangle$ and $\langle V_S'^2\rangle$ occurs in systems characterized by a higher e. Interestingly, for the case of $\nu_L/\nu_S=0.5$ and 1, Figs. 7(a) and 7(b) indicate that the fluctuating velocity ratio for $e=0.8$ *increases* at the highest value of d_L/d_S, whereas similar behavior is not observed for the higher coefficients of restitution, nor for the other solids fraction ratio investigated [Fig. 7(c)].

In Fig. 8, the simulation data and kinetic-theory predictions for dynamic friction coefficient (i.e., $-P_{xy}/P_{yy}$) are plotted against overall solids fraction. For the case of

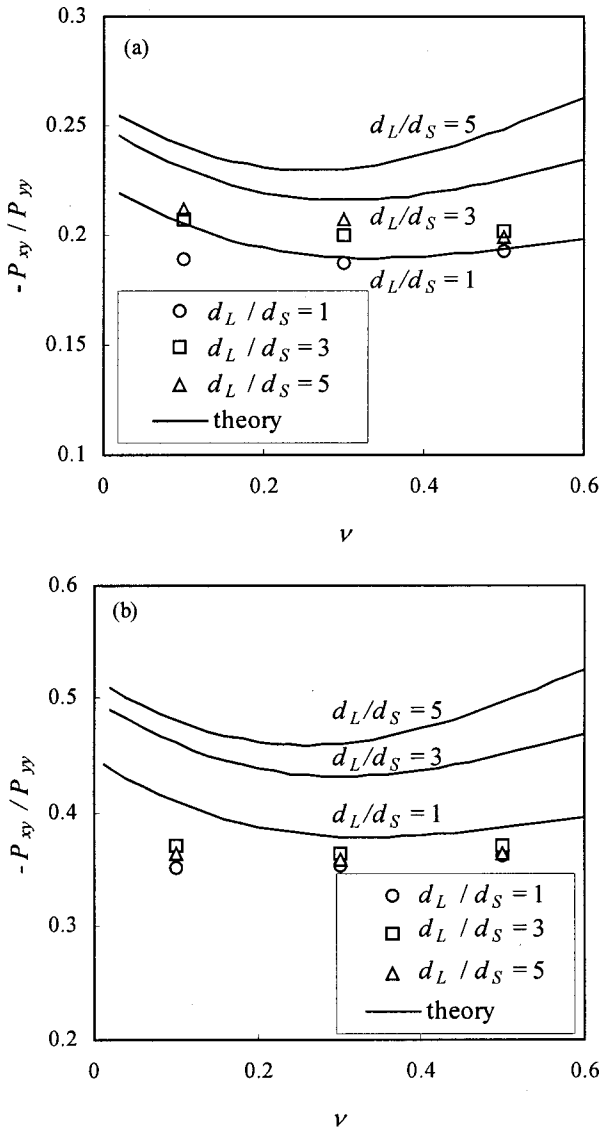

FIG. 8. Dynamic friction coefficients for binary systems with kinetic-theory predictions of Willits and Arnarson [9] for $\nu_L/\nu_S = 1.0$ and (a) $e = 0.95$ and (b) $e = 0.80$.

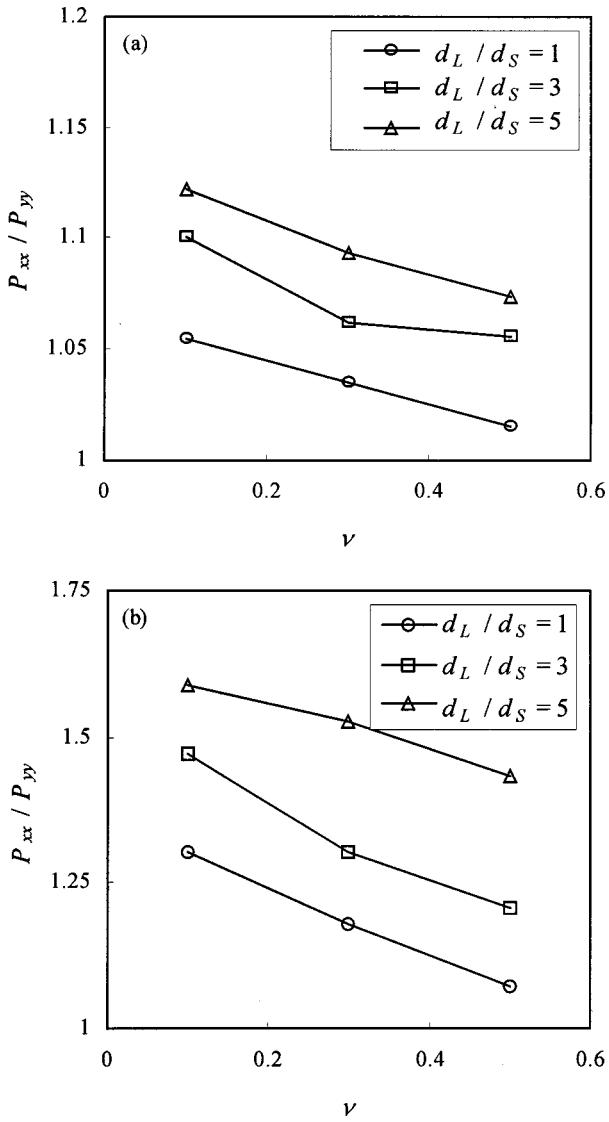

FIG. 9. Normal stress ratios for binary systems with $\nu_L/\nu_S = 1.0$ and (a) $e = 0.95$ and (b) $e = 0.8$.

$\nu_L/\nu_S = 1$ and $e = 0.95$ [Figure 8(a)], the kinetic-theory predictions of Willits and Arnarson [9] exhibit a minimum at moderate values of ν, which is similar to the behavior predicted by kinetic theories for monodisperse systems (see, for example, [20]). (Previous simulation data for monodisperse systems has shown a further decrease in the dynamic friction coefficient at solids fraction near the packing limit due to a layering of particles that forms in the streamwise direction [21]. Since the current simulations were not carried out for values of $\nu > 0.5$, this effect is not observed in either the monodisperse ($d_L/d_S = 1$) or binary ($d_L/d_S > 1$) systems.) As is evident from Fig. 8(a), the kinetic-theory predictions for $-P_{xy}/P_{yy}$ demonstrate a larger dependence on both the particle size ratio and overall solids fraction than is exhibited for the simulation data. Similar observations also hold for $e = 0.8$ (Fig. 8(b)), though the MD data indicates that $-P_{xy}/P_{yy}$ has an even smaller dependence on d_L/d_S at the lower restitution coefficient. The results obtained for the other ν_L/ν_S investigated are similar to those obtained at $\nu_L/\nu_S = 1.0$, and thus are omitted for the sake of brevity.

Finally, the normal stress ratio (P_{xx}/P_{yy}) observed in the MD simulations is presented in Fig. 9 as a function of the overall solids fraction and particle size ratio. Similar to monodisperse systems ($d_L/d_S = 1$), P_{xx}/P_{yy} decreases toward an asymptotic value of unity with increasing ν due to the increased importance of the collisional mode of granular energy generation. More specifically, at low solids fractions where collisions are infrequent, the kinetic mode dominates. Since the kinetic mechanism is only capable of *generating* a velocity fluctuation in the streamwise direction of the shear flow (i.e., the x direction), it follows that $P_{xx} > P_{yy}$ at low solids fractions. (A more rigorous analysis of the origin of the normal stress difference in the dilute limit is given in [22].) At higher particle concentrations, however, the collisional mode becomes more important. As the collisional mechanism generates velocity fluctuations that are relatively isotropic, $P_{xx} \sim P_{yy}$ in the collision-dominated regime. For

the case of binary systems, Fig. 9 illustrates the dependency of the normal stress ratio with particle size ratio. Namely, P_{xx}/P_{yy} increases with d_L/d_S over the entire range of ν_L/ν_S and e that were investigated.

IV. SUMMARY

Molecular-dynamic simulations of inelastic, smooth, hard particles have been used to determine the behavior of binary-sized particles engaged in simple shear flow and to compare this behavior with an existing kinetic theory for binary systems. For the range of parameters investigated, the qualitative nature of the simulation results and the theoretical predictions are found to be consistent. Specifically, both the simulations and theoretical predictions of Willits and Arnarson [9] indicate that the dimensionless stresses decrease with an increase in d_L/d_S or a decrease in ν_L/ν_S. Both the simulations and theory also indicate that the dynamic friction coefficient increases with d_L/d_S. Quantitatively, the stress predictions obtained using kinetic theory are in good agreement with the theory over the range of parameters investigated.

Despite the good match between the simulation stresses and the corresponding theory, the simulation results do indicate an area for possible improvement to existing theory for binary systems. In particular, the assumption of equipartition of energy is observed to worsen with increased inelasticity, particularly at larger values of d_L/d_S. Although this equipartition-of-energy assumption does not appear to have a negative impact on the ability of the existing theory to predict the stress tensor in simple shear flows, the presence of an energy difference is anticipated to lead to additional contributions to the constitutive relations. If such effects manifest themselves in more complicated flows (e.g., flows that exhibit size segregation), a multitemperature theory may be more appropriate.

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