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Stress Calculations for Assemblies of Inelastic Spheres in Uniform Shear*

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With 6 Figures

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Summary

Previous work on assemblies of inelastic, frictional disks is extended to three dimensions in a molecular-dynamics study of steady shearing flow of an idealized granular material consisting of equal-sized spherical particles that are smooth but inelastic. Cumulative time and space averages are calculated for several diagnostic quantities including the kinetic and potential energy densities, the R.M.S. (deviatoric) velocity and both the kinetic and potential contributions to each component of the stress tensor. Under steady-state shearing deformation the kinetic-energy-density (granular temperature) generally is found to increase as the solids fraction is decreased and decrease as the binary-collision coefficient-of-restitution is decreased. For constant coefficient-of-restitution interactions the calculated stresses increase generally with the square of the strain rate, with exceptional behavior noted at extremes in solids loadings. The general trends of the calculated stresses and velocities are in substantial agreement with the Lun et al. linearized perturbation of Chapman-Enskog theory for slightly inelastic spheres. However, some significant differences are noted at very low ($\nu < 0.1$) and very high ($\nu > 0.5$) solids fractions. A variable coefficient-of-restitution interaction model (decreasing as the impact velocity increases) results in calculated stresses that deviate from the constant coefficient-of-restitution behavior in a manner similar to that predicted by Lun and Savage. The calculated stresses are in rough agreement with experimental measurements; however, the calculated shear-stress to normal-stress ratio for spheres with coefficients of restitution between 0.8 and 0.95 are significantly below experimentally measured values for glass and polystyrene beads in annular shear cell tests. Based on effects seen in two-dimensional calculations, the inclusion of interparticulate friction and particle rotations are expected to significantly reduce the discrepancy.

1. Introduction

The statistical mechanics of a system of inelastic particles differs from traditional gas-dynamics. Inelastic particles have a natural equilibrium state with a granular-temperature of absolute zero. Unless some energy source is provided

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to maintain vibrational kinetic energy, any system of inelastic particles will, through energy dissipating collisions, tend toward this natural zero-energy state. Except at high solids packings (i.e. $\nu > 0.6$) the equilibrium state is of little interest scientifically or practically, but many steady-state non-equilibrium (i.e., shearing) flow situations are of concern and, at present, are not fully understood. Among these are familiar laboratory configurations for studying granular solids flow behavior such as annular shear cells, incline chute flows, vertical channel flows, and converging hopper flows in which energy is provided to the granular material through a combination of gravitational potential and/or boundary interactions. Ultimately a complete understanding of granular solids flow behavior must include boundary interactions and energy transport from boundaries. With some notable exceptions (e.g. Jenkins and Richman [1]), most theoretical studies (as well as this calculational study) of granular solids flow have concentrated on understanding the constitutive and transport properties of the material itself and have deferred the study of boundary interactions. Because laboratory measurements inevitably include both boundary effects and frictional interactions, neither of which is included in the present study, we make most of our comparisons in this paper with theories that have also ignored these effects. Future calculations (in progress) will inlcude these effects and will be compared directly with existing experimental measurements.

Microstructural theories for granular materials based on perturbations to established equilibrium kinetic theories of gases and liquids are complicated by the necessity to account for the inelasticity of the particle interactions as well as simultaneously dealing with a system that is in a non-equilibrium state. Several microstructural and/or kinetic theories have been proposed recently to decribe flowing granular materials ([2]—[6]). Many of these treat an idealized granular material composed of equal-sized, smooth, inelastic spheres that have a constant coefficient of restitution, independent of impact velocity. However, each theory contains assumptions not shared by others (usually either involving the collision integral or the non-equilibrium contact distribution function). The present calculational study treats an idealized granular solid composed of equal-sized, smooth, but inelastic, spheres with a constant coefficient of restitution in rectilinear shear flow; the same material as in many kinetic theory studies of granular materials. No a priori assumptions are made about the velocity-, particle- or pair-distribution functions. Instead, the motion of each particle is calculated in a cell with periodic boundaries on all sides, maintaining a state of uniform shear, while statistically monitoring the stress tensor and the velocity and energy densities in the cell. Since the calculated pair interaction model closely resembles the collision operator assumed in many of the present theories, the results of these calculations can be utilized to aid in discriminating between competing non-equilibrium theoretical approximations for steady shearing flow. We compare our calculated stresses with those predicted by Lun et al. [3] for slightly inelastic particles in a general flow field. We find that for a wide range of solids packings (from $\nu = 0.1$ to 0.5) many of our results are in substantial agreement with that theory. We also calculate the behavior of spheres with a velocity-dependent coefficient of restitution and find changes in calculated behavior from that obtained with a constant coefficient of restitution that are qualitatively similar to the changes in predicted behavior proposed by Lun and Savage [7] in their recent theory based on an exponentially varying coefficient of restitution. Finally, we discuss the changes in behavior that occurred in two-dimensional calculations when the effects of friction and particle rotations were included [8] and infer how these same effects will change the calculated behavior in three dimensions.

2. Uniform Shear Model

The steady-state shearing algorithms for inelastic frictional disks of Walton and Braun [8] are extended to three dimensions for smooth, inelastic spheres. The calculational technique is patterned after the non-equilibrium molecular dynamics methods of Hoover [9], Hoover and Ashurst [10], and Evans [11]. Uniform shearing is achieved by moving periodic image particles above the primary calculational cell to the right and moving those below the primary cell to the left at a velocity v_x' given by $v_x' = v_{x0} + n_s \dot{\varepsilon} l_y$ where v_{x0} is the x-velocity of the particle (or image) in the primary calculational cell; v_x' is the velocity of the particle's image located n_s cells above (n_s positive) or below (n_s negative) the primary calculation cell; $\dot{\varepsilon}$ is the shear rate, du_x/dy, and l_y is the height of the calculational cell.

Spheres are initially randomly placed in the calculational cell, then moved to minimize initial potential energy (i.e. particle overlap) and assigned random deviatoric velocities. Shearing flow is then initiated and, once steady-state is achieved, various diagnostic cumulative time-and-space averages are calculated. Each particle's deviatoric velocity is obtained by subtracting the mean shearing field $u_x = \dot{\varepsilon} y$ from the calculated particle x-velocity, v_x, so that the mean deviatoric speed $\langle \boldsymbol{v}^2 \rangle^{1/2}$, is given by

$$\langle \boldsymbol{v}^2 \rangle^{1/2} = \left\langle \frac{1}{n} \sum \left[(v_{xi} - u_{xi})^2 + v_{yi}^2 + v_{zi}^2 \right] \right\rangle^{1/2}.$$

Cumulative time averages are calculated for both the kinetc and potential contributions to each of nine components of the momentum-flux-density tensor (i.e. the stress tensor), $\boldsymbol{P}$, instantaneously given by the expression

$$\boldsymbol{P} = \frac{1}{V} \left[\sum_i m_i (\boldsymbol{v}_i - \boldsymbol{u}_i)(\boldsymbol{v}_i - \boldsymbol{u}_i) + \sum_{j>i} \boldsymbol{R}_{ij} \boldsymbol{F}_{ij} \right]$$

in which the first term on the right is a symmetric dyad representing the kinetic contribution to the tensor and the second dyadic term represents the collisional or potential contribution to the stress tensor. This term could contain antisymmetric components if non-central forces (e.g. friction) were included. In this calculational study however, only central forces are allowed so the stress tensor is always symmetric.

3. Comparison with Molecular-Dynamics

As a test of the accuracy of the integration scheme, the correctness of the cumulative time-averaging algorithms for the nine components of the stress tensor and the overall validity of our three-dimensional steady state shearing algorithms, the results of our model were compared with Hoover's molecular dynamics calculations of the stress tensor for soft spheres in plane Couette flow [12]. Using a 12th-power pair potential $\phi = \varepsilon(\sigma/r)^{12}$ with ε, σ and the particle mass, m, all set to 1.00, a 256 particle system with a constant kinetic energy of 1.465 per particle was calculated at a shear rate of one and at a solid packing of $\nu = 0.444288$ which corresponds to Hoover's reduced density, $\nu/\nu_{\max}$ of 0.600. The calculation was run for a total time of 100 using a time step of $\Delta t = 0.005988$. The parameters correspond to those of Hoover except his calculation was run to a final time of 500. The resulting mean total energy per particle was 3.654 compared to 3.656 for Hoover's calculation. The resulting kinetic and potential contributions to the total stress tensor are given in Table 1. The numbers in parenthesis are the deviation from Hoover's values. His stated uncertainties were "of order 0.002" in the kinetic part and "of order 0.005" in the potential part. As can be seen from Table 1 the values we obtained for the components of the stress tensor are quite close to those obtained by Hoover. The largest deviations appear in the potential contributions, yet the trace of the stress tensor we calculate is within 0.005 of the value obtained by Hoover. We did not run our calculation further to establish uncertainties in our calculated values; but, based on the values obtained, concluded that the basic integration and diagnostic algorithms in our model are essentially working properly. (It should be noted that we truncated the inter-

Table 1. *Stress tensor for 256 particles in steady shear (12th-power potential)*

Kinetic contributions to the stress tensor		
0.844 (−0.004)	−0.104 (+0.001)	0.000 (0)
−0.104 (+0.001)	0.829 (+0.002)	0.000 (0)
0.000 (0)	0.000 (0)	0.813 (+0.001)
Potential contribution to the stress tensor		
7.419 (−0.024)	−1.106 (+0.019)	0.002 (+0.002)
−1.106 (+0.019)	7.499 (−0.003)	−0.013 (−0.013)
0.002 (+0.002)	−0.013 (−0.013)	7.377 (+0.022)

particulate force at a center-to-center separation of 2.458. Hoover used a nearest image convention which resulted in a truncation distance of approximately 3.35 in his calculations.)

4. Inelastic Spheres in Uniform Shear

Inelastic interactions with a constant coefficient of restitution were modeled with a partially-latching spring model [8]. In this model, the normal force, F_n, is given by

$$F_n = K_1\alpha \qquad \text{for loading}$$

and by

$$F_n = K_2(\alpha - \alpha_0) \qquad \text{for unloading}$$

where α is the relative approach (overlap) after initial contact and α_0 is the value where the unloading curve goes to zero. No negative (tensile) values are allowed for F_n. The coefficient of restitution, e, for a binary collision with this force model is given by

$$e = (K_1/K_2)^{1/2},$$

where e is the ratio of the magnitude of recoil to incident normal velocities. For some of the calculations a more realistic impact velocity dependent coefficient-of-restitution model was used. This was modeled by making the unloading slope, K_2, a linear function of the maximum force achieved before unloading, $F_{\max}$, so that

$$K_2 = K_1 + SF_{\max}.$$

Using this model the coefficient of restitution for two spheres of mass, m, depends on the relative velocity of approach, v_0, as given by

$$e = [\omega_0/(Sv_0 + \omega_0)]^{1/2}, \qquad \text{where} \qquad \omega_0 = \frac{2K_1^{1/2}}{m}.$$

Such an impact velocity dependence is quite similar to experimental measurements reported by Goldsmith [13] and also is quite close to results obtained in dynamic finite-element calculation of impacts of spheres using an elastic/perfectly-plastic material model [8].

An initial parameter study examining the effects of coefficient of restitution, solids-packing fraction and shear rate on mean stresses and deviatoric velocities in the granular assembly was performed using the partially-latching-spring interaction model. We find that the resulting behavior is quite similar to that predicted by the linearized perturbation to Chapman-Enskog theory for slightly inelastic spheres of Lun et al. [3]. That theory, consistent with the original phenomenological arguments of Bagnold [14], predicts that stresses increase as the square of the shear rate for spheres interacting with a constant coefficient of restitution. The slope of the ln (P) vs. ln $(\dot{\varepsilon})$ results obtained in the present work (see Fig. 1) is almost exactly 2.0 for constant coefficient of restitution interactions at solids fractions between 0.1 and 0.5. At higher solids concentrations, where enduring contacts occur, the computer-simulated flows show a less steep variation with shear rate. At very low solids concentration (e.g. $\nu = 0.025$) the calculated stresses increase somewhat faster than the square of the strain rate. At these low solids concentrations the calculated deviatoric velocity in the direction of shear is substantially higher than in directions perpendicular to the shear. This effect becomes more pronounced as the coefficient of restitution deviates further from unity. This anisotropic velocity distribution results in substantial differences in the normal stress components of the stress tensor. Fig. 2 shows the calculated ratio of the first normal stress difference $(p_{xx} - p_{yy})$ to the pressure $(p_{xx} + p_{yy} + p_{zz})/3$ as a function of the solids fraction for various coefficients of restitution. As can be seen from this figure at very low solids packings the calculated normal stress components differ significantly. The calculated second normal stress difference

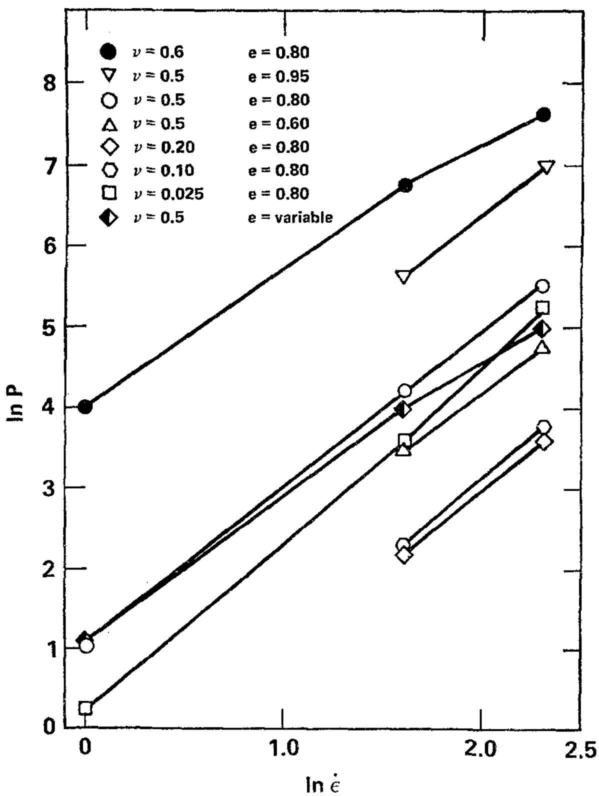

Fig. 1. Logarithm of the calculated pressure *vs.* logarithm of the shear strain rate at various constant solids loadings and with various coefficients of restitution for 125 inelastic spheres in uniform shearing flow. Theories predict constant slope of 2.0

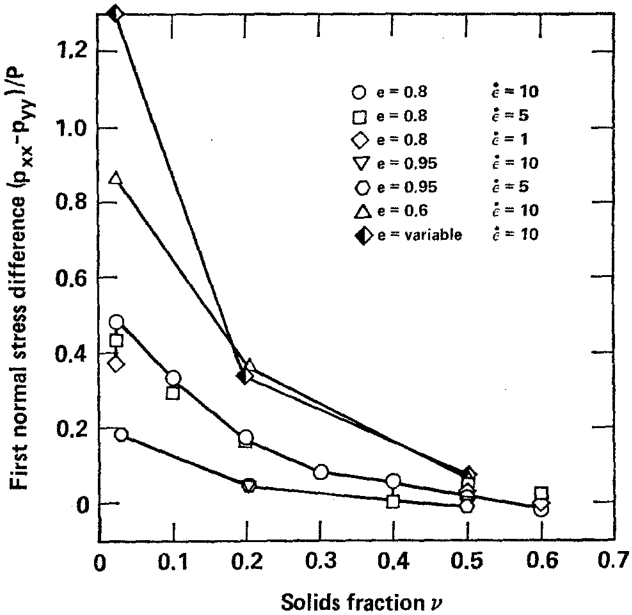

Fig. 2. Calculated ratio of first normal stress difference $(p_{xx} - p_{yy})$ to pressure $(p_{xx} + p_{yy} + p_{zz})/3$ for 125 inelastic spheres in uniform shearing flow

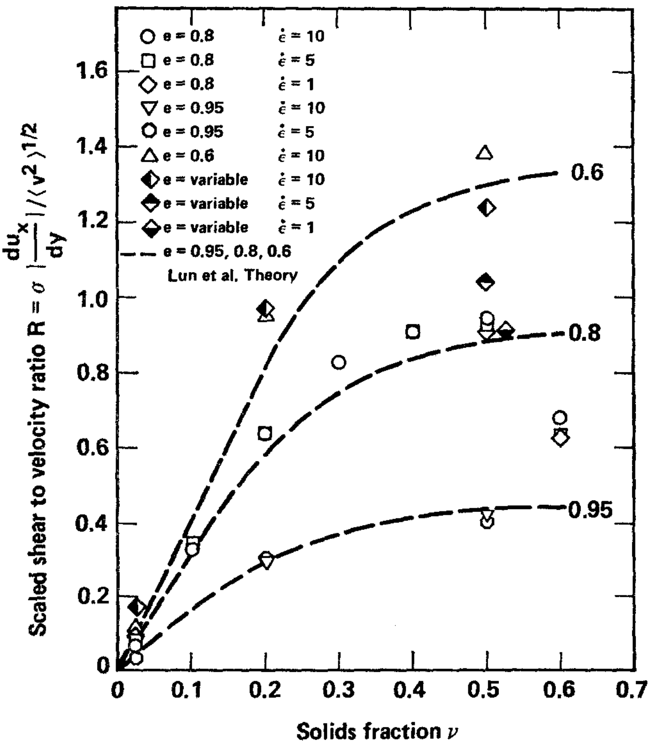

Fig. 3. Calculated variation of velocity ratio, R, with solids fraction for system of 125 inelastic spheres in uniform shearing flow (symbols); ——— Lun et al. theory [3]

$p_{yy} - p_{zz}$ also shows some variation with coefficient of restitution and solids fraction but it is generally relatively small, remaining at less than 10% of the pressure for almost all calculations performed.

Fig. 3 shows how the calculated Savage and Jeffery [5] velocity ratio, R, defined by

$$R = \sigma \left| \frac{du_x}{dy} \right| \Big/ \langle v^2 \rangle^{1/2},$$

where σ is the sphere diameter, varies with solids fraction and coefficient of restitution. Also shown on this figure is the predicted variation of R according to the theory of Lun et al. [3]. Values of R near 1 indicate that particles located one diameter apart vertically, in our uniformly shearing cell, have a relative velocity due to the mean shear field that is as large as their relative velocity due to random vibrational motion. Thus the shear rates being examined for cases with R near unity correspond to extremely rapid shearing by most fluid dynamic criteria. This occurs not so much because the actual shear rates are high as because the effective granular-temperature is so low. At low solids concentrations the mean free path between collisions increases substantially and the collision frequency decreases. This results in substantially higher deviatoric velocities since fewer energy absorbing collisions occur. This effect is reflected in Fig. 3 by the small values of R at low solids fractions, indicating high granular-temperature at these densities. This changing effective granular-temperature causes the material composed of variable coefficient-of-restitution spheres to behave differently at different solids packings. The calculated value of R for variable-e with $\dot{\varepsilon} = 10$ at a solids fraction of 0.5 lies between the values obtained for $e = 0.6$ and $e = 0.8$ under the same conditions. At a solids packing of 0.2 the variable-e point agrees very closely with the $e = 0.6$ calculation while at $\nu = 0.025$ the variable-e point is considerably larger than the $e = 0.6$ value. This indicates that the effective mean coefficient of restitution decreases as the solids packing decreases (because of the corresponding increase in granular temperature). A similar effect is seen in the three variable-e points at solids packing $\nu = 0.5$. Each point corresponds to a different shear rate. At a shear rate of $\dot{\varepsilon} = 1$ the calculated R value is the same for the $e = 0.8$ and variable-e cases. At a shear rate of $\dot{\varepsilon} = 5$ the R value has moved somewhat toward the $e = 0.6$ point, and at a shear rate of $\dot{\varepsilon} = 10$ the R value calculated is much closer to the $e = 0.6$ result than to the $e = 0.8$ result. This indicates that at the higher shear rate the variable-e material behaves like a material with a low effective coefficient of restitution and vice versa. Lun and Savage [7] report a qualitatively similar increase in R with increasing shear rate using their variable coefficient-of-restitution theory.

Fig. 4 shows the calculated normal stress component, p_{yy}, for systems composed of spheres with constant coefficients of restitution of 0.95, 0.80, and 0.60. Also shown are results obtained with a variable coefficient of restitution. The dashed lines on this figure are the predictions of the Lun et al. theory [3]. The stress has been non-dimensionalized by dividing by the quantity $\varrho_p \sigma^2 \dot{\varepsilon}^2$, where ϱ_p is the particle material density and σ is the sphere diameter. This normalization scales various shear rates to the same value if the stress component varies with the square of the strain rate, $\dot{\varepsilon}^2$, as assumed in the Lun et al. theory. The other normal stress components p_{xx} and p_{zz} exhibited behavior qualitatively very similar to that shown in Fig. 4. At low solids fractions, $\nu < 0.15$, the kinetic contributions to the various stress components exceed the collisional or potential contributions. These kinetic contributions continue to increase with decreasing ν, due to the already discussed increasing granular-temperature at low packings. At solid fractions greater than 0.15, the collisional or potential contributions to the stress tensor components dominate, and continue to increase as the solids fraction increases, since the collision frequency increases as the mean free paths decrease. The total stress which results from the sum of these two terms thus exhibits a minimum near $\nu = 0.15$ and increases with the change in solids packing from that value.

In the solids fraction range from $\nu = 0.1$ to 0.5 the calculated values of the present work are generally within 10% of the Lun et al. theory [3] for $e = 0.95$,

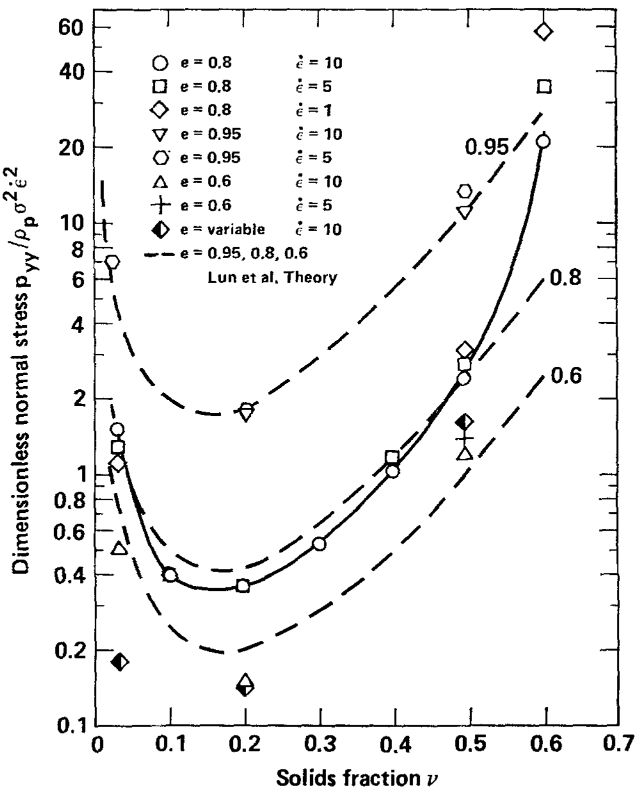

Fig. 4. Calculated variation of dimensionless normal stress with solids fraction for system of 125 inelastic spheres in uniform shearing flow (symbols); ——— spline fit through $e = 0.8$, $\dot{\varepsilon} = 10$ calculated points; – – – Lun et al. theory [3]

within 20% for $e = 0.80$ and within about 40% for $e = 0.60$. At extremes in solids concentrations we see substantial differences between the present work and the Lun et al. theory. Such differences are to be expected since the theory assumes only binary collisions, an assumption that is not valid at high solids concentrations, and it further assumes an isotropic deviatoric velocity distribution, a condition that is not seen in the present calculations for uniform shearing flow at very low solids concentrations or for highly inelastic particles. The deviation of the velocity dependence from the second power of the strain rate already noted at high solids concentration is exhibited in this figure by the non-coincidence of the three shear rates calculated for $\nu = 0.6$ with a constant coefficient of restitution, $e = 0.8$. We interpret this difference as arising because the enduring contacts, which cause the stress to exceed the theoretical value, are effective for a larger fraction of the time at low shear rates than at high rates. That is, at higher shear rates any bridging or short range order due to enduring multiple contacts is less effective at increasing the overall stress level because the higher deviatoric velocities involved at the higher shear rate tend to destroy the temporary order formed by such bridges or multiple enduring contacts.

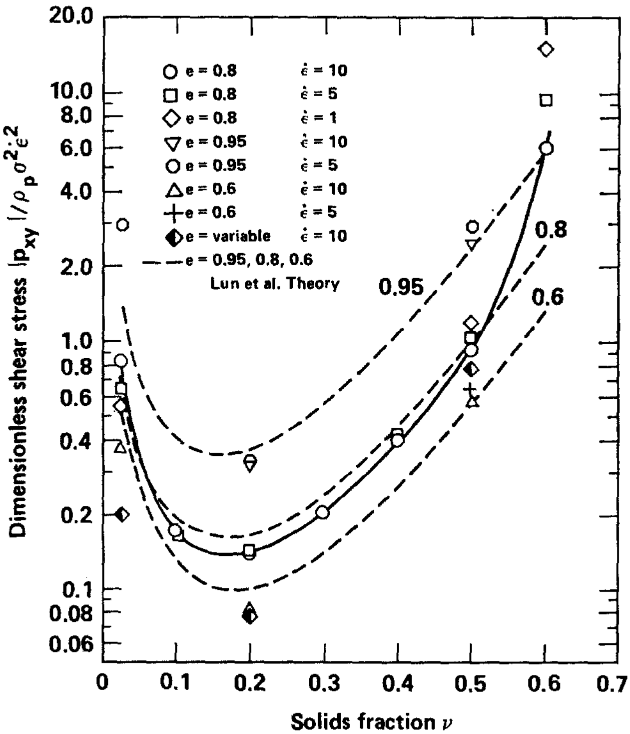

Fig. 5. Calculated variation of dimensionless shear stress with solids fraction for system of 125 inelastic spheres in uniform shearing flow (symbols); ——— spline fit to $e = 0.8$, $\dot{\varepsilon} = 10$ calculated points; — — — Lun et al. theory [3]

Fig. 5 shows calculated shear stress, p_{xy}, (non-dimensionalized in the same manner) and the theoretical curves due to Lun et al. [3]. The behavior is qualitatively the same as the normal stress component behavior seen in Fig. 4. Deviations between the present calculations and the Lun et al. theory for p_{xy} are of the same order as those seen for p_{yy} and for the same reasons.

Fig. 6 shows the variation of the dynamic friction coefficient $|p_{xy}/p_{yy}|$ with solids fraction for spheres interacting with constant coefficients of restitution of $e = 0.95$, 0.80, and 0.6 and also for the variable-e case. The calculated value of $|p_{xy}/p_{yy}| = 0.2$ for the $e = 0.95$ case agrees almost exactly with the Lun et al. theory, while at lower coefficients of restitution the calculated and theoretical values for the dynamic friction coefficient show some moderate deviation. Experimental values for the $|p_{xy}/p_{yy}|$ ratio for glass beads and polystyrene beads are in the range from 0.5 to 0.7 at solids packing near $\nu = 0.5$ and with measured coefficients of restitution on the order of 0.90 ([15], [16]). Both the present calculations and the theory of Lun et al. are significantly below these measurements. However, previous calculations of shearing flow in two-dimensions clearly indicate a significant increase in the friction coefficient $|p_{xy}/p_{yy}|$ when interparticulate friction and particle rotations were included. Walton and Braun [8] found $|p_{xy}/p_{yy}| = 0.36$ for smooth disks interacting with a constant coefficient of restitution $e = 0.8$. When friction and particle rotations were included in those two-dimensional calculations the stress ratio increased to a value between 0.55

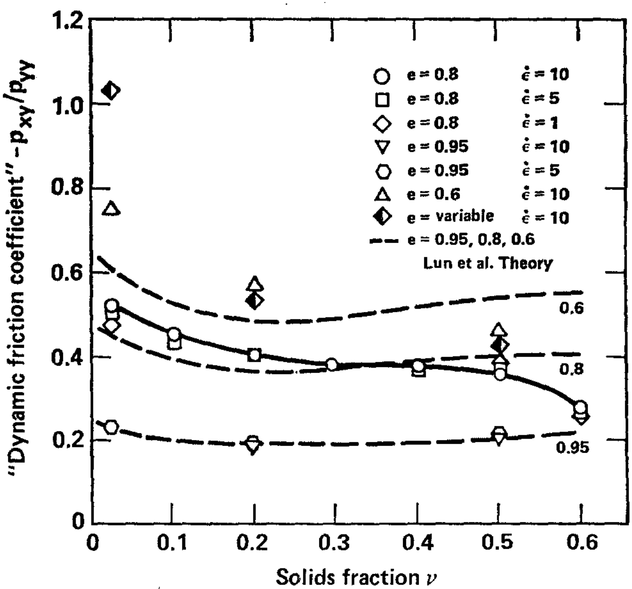

Fig. 6. Calculated variation of dynamic friction coefficient $|p_{xy}/p_{yy}|$ with solids fraction for system of 125 inelastic spheres in uniform shearing flow (symbols); ——— spline fit to $e = 0.8$, $\dot{\varepsilon} = 10$ calculated points; — — — Lun et al. theory [3]. See text for discussion of experimental measurements

and 0.65 depending on the solids fraction. We have every reason to expect a similar factor of 1.5 to 1.6 increase in the values calculated for $|p_{xy}/p_{yy}|$ when interparticulate friction and particle rotations are included in three dimensions. Such calculations are in progress.

5. Concluding Remarks

Non-equilibrium molecular-dynamics-like calculations of stresses in an idealized granular material in uniform shearing flow have provided heretofore unavailable detailed information on the mechanisms affecting those stresses. The sensitivity of the calculated stresses to the choice of coefficient of restitution was found at intermediate solids packings to be similar to the behavior predicted by the theory of Lun et al. [3] for constant coefficients of restitution and similar to Lun and Savage [7] for coefficients of restitution that decrease with increasing impact velocity. The anisotropic deviatoric velocity distributions obtained in these calculations at low solids packings differ significantly from equilibrium gas dynamics because of the uniform shear imposed on the system and the inelasticity of the modeled binary collisions. The long mean-free- paths at low solids packings allow particles with a vertical velocity to travel significant distances perpendicular to the shear before encountering another particle. The uniform horizontal shear imposed on the system ensures that when a collision occurs after significant vertical travel the particles involved will have a large relative velocity in the horizontal direction. If only perfectly elastic collisions occurred, the high relative x-momentum of one of these collisions would soon (i.e., in a few subsequent collisions) be nearly isotropically distributed in the x, y, and z directions. However, with inelastic collisions the redistribution of relative momentum is only partially completed before the dissipation essentially absorbs the kinetic energy of that original collision. For every pair of colliding particles with a relative velocity perpendicular to the shearing direction this process continues to repeat itself. New kinetic energy (and high deviatoric x-momentum) is continuously fed into the system by virtue of the shearing field and this x-momentum is dissipated before complete redistribution into an isotropic velocity distribution occurs. The resulting normal stress component parallel to the shear, p_{xx}, is thus much higher (by as much as a factor of two) than the normal stress components perpendicular to the shear, p_{yy} and p_{zz}.

The detailed information on the mechanisms affecting the stresses in an idealized granular material in uniform shear obtained in these calculations is an indication of the insight that can be provided by direct simulation computer calculations. As further parameter sensitivity studies are completed and more complete diagnostic algorithms written, such calculations can be expected to provide significant guidance in selecting appropriate approximate theories for flowing granular solids. In particular, the sensitivity of including or not including various interparticulate interactions are easily tested using this technique. For instance, the effects of interparticulate friction and particle rotations were not examined in this study but will be the subject of future calculations employing this method. It is expected that the inclusion of these important interactions will significantly affect the distribution of the stress components, as was found when similar calculations were performed in two dimensions [8].

Acknowledgments

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