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COMPUTER SIMULATION OF RAPIDLY FLOWING GRANULAR SOLIDS

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Abstract. New research tools in the form of two- and three-dimensional discrete-particle computer models that calculate the motion of each individual grain in assemblies of hundreds of particles in steady shearing flows with either periodic or real boundaries have been developed and are being utilized to study granular flow behavior. The models are similar to molecular-dynamics models except that the particles are inelastic, frictional, macroscopic grains. The particle interaction models reproduce experimentally measured recoil trajectories for colliding frictional spheres, including rotational effects. Time and space averages of particle positions and forces can be utilized to obtain almost any desired macroscopic quantity. Stresses calculated in steady shearing flow simulations agree with laboratory measurements where such data are available and they agree with theories when comparable approximations are made in the model (such as assuming frictionless and nearly elastic particles). These discrete particle simulation calculations are providing new insight into the micro-mechanisms occurring during deformation and flow of granular solids.

INTRODUCTION

Understanding the flow properties of granular solids has broad scientific and industrial applications ranging from soil mechanics to process control. The science of granular flow includes not only the study of natural geologic phenomena like landslides and avalanches, but also the development of technologies for a variety of new synthetic fuels including coal gasification/liquefaction, oil shale retorting, and tar sand processing. The development of commercial-scale synthetic fuel processing

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plants will, of necessity, involve the processing of large quantities of solids. Unfortunately, industrial plants which process solids have historically been much less reliable than those that utilize only gases or liquids. Almost always physical or mechanical reliability—not chemistry—has been the problem. In recent studies of industrial plants in the United States and Canada, researchers have concluded that, over the past 20 years, we have not significantly improved our ability to design reliable new industrial plants that include solids handling or processing. This lack of progress reflects primarily a lack of theoretical understanding of the behavior of particulate materials, combined with a tendency for process engineers to emphasize chemistry problems in the early design stages [Merrow, 1986]. All too often, design engineers consider the movement of solids a minor operational problem; yet when plant operations start, solids flow problems occur, causing major disruption in the system and resulting in expensive redesigns and delays.

In petroleum and refining technology, involving primarily gases and liquids, engineers are often able to design reliable large-scale units from first principles and small-scale experiments. Scale-up factors of 50000 are not uncommon in going from laboratory chemistry studies to commercial plant designs. In contrast, most solids-handling processes, must go through an empirical series of scale-up designs, typically involving scale-up factors of two to five for each stage, in order to obtain effective, reliable designs [National Research Council, 1988]. Major unanticipated problems often occur that require months of effort to resolve at the larger scale units. The later stages of such scale-ups (going, for instance, from pilot-plant to semi-works to commercial-scale module) can be very costly, requiring from tens to hundreds of millions of dollars for each step. An improved understanding of solids behavior could significantly reduce the time delays and costs that result from such scale-up problems.

Despite more than a century of sporadic scientific and engineering research including notable progress by such researchers as Reynolds [1885], Janssen [1895], Bagnold [1954], Rowe [1962], Jenike [1964] and many others [Savage, 1984], we have only a limited understanding of the deformation and flow behavior of granular solids. One of the problems that has hampered researchers is the difficulty of making meaningful measurements of pertinent flow parameters without intrusively disturbing the flow itself. Progress has also been hampered by lack of widespread recognition of granular solids flow as a scientific field worthy of significant fundamental study. While this view has significantly changed in the past few years, the general tendency has been to look for immediate engineering solutions to individual flow problems as they arise.

To develop a thorough understanding from a microstructural viewpoint we need to know the spatial and temporal distributions of velocity, porosity and forces acting within the flowing material. Such data are extremely difficult to obtain. Molecular-dynamics-like methods are being applied to the study of one very simplified model of a flowing granular solid (namely, a rapidly deforming assembly of inelastic spheres). The structural details of granular flows are being obtained in these simulations. Once those are more thoroughly understood, phenomenological, or theoretical relationships can be developed, relating the structural details to the stresses acting within the material. In the spirit of this conference, such constitutive relations will provide the 'bridge between structure and function' for granular materials. For quasi-statically deforming granular materials, the deformation behavior is dominated by structure; not only the geometric "fabric" of the material, but, also the "invisible" structure of locked-in stresses due to past deformation history. Rapid shearing flows, in contrast, are much simpler, depending primarily on "structure" characterized by statistical averages over space and time of such quantities as the deviatoric velocity, and the pair distribution function at contact. For steady shearing flows granular materials can usually by characterized by such parameters as the solids packing (density) and the shear rate (which determines the mean vibrational kinetic energy density). Material and particle interaction parameters determine the response to the applied shear. New theoretical models that incorporate phenomena observed in the computer simulations described here, such as anisotropic velocity and stress distributions, are currently being developed [Richman & Jenkins, 1988], and new experimental measurements are providing detailed velocity profiles in specialized cases. Understanding the rapid shearing flow behavior of spheres is only a small part of the entire problem, but it is an important first step toward understanding more general granular flows.

IDEALIZED MODELS FOR MACROSCOPIC GRANULES

Several new theoretical models being developed to describe granular solids are based on concepts similar to those used in the statistical theory of dense gases, wherein molecules of a gas are treated as tiny, perfectly elastic, frictionless spheres. A system of macroscopic granules can be treated in much the same manner as gas dynamics theory. The major difference being that when laboratory sized granules collide not all of their (precollision) kinetic energy is recovered as postcollision kinetic energy. Some of the energy goes into vibrations of the molecules that make up the grains, that is, it becomes internal heat. The magnitude of this temperature rise is usually quite small and does not significantly alter the properties of the granules, but the inelastic nature of the collisions significantly affects the macroscopic behavior of *assemblies* of such particles.

An isolated system of perfectly elastic spheres tends to approach a state with a uniform temperature and pressure throughout the system. A similar system of inelastic spheres, in contrast, loses kinetic energy with every collision; so, as successive collisions dissipate energy, it approaches a state with no relative velocity between particles. In the absence of gravity such a system would eventually approach a condition with the granules merely floating, stationary. If we ignore the interval vibrations of the molecules making up each particle and make the usual gas-dynamic identification of pressure and temperature [Reif, 1965], we would say that such a system approaches a state of zero pressure (no momentum) and absolute zero *granular temperature* (no kinetic energy). This is the "equilibrium" state for inelastic particles.

Systems of inelastic particles in thermodynamic equilibrium, which have essentially no pressure and do not interact with bounding walls have little bearing on practical engineering problems. Granular flow problems of practical interest all involve inelastic particles that are far from their equilibrium state. Thus, non-equilibrium statistical theories are required for flowing granular solids rather than the more usual thermodynamic equilibrium theories of gas dynamics. Advancement of new non-equilibrium statistical theories for inelastic particles has been hampered by lack of information on the particle velocity, and position distributions in such systems. Computer simulations of such flows are now providing, new detailed information on flow parameters that is aiding in the development and validation of new statistical theories for granular solids.

COMPUTER MODELS

The term "molecular-dynamics" has become synonymous with numerical simulation of the motion of individual particle trajectories in systems of particles, and the subsequent determination of bulk material properties from various averages of the particles coordinates, momenta and energies. Since the pioneering studies in molecular-dynamics at Livermore and at Los Alamos more than three decades ago, these techniques have been developed extensively. Techniques have been devised for non-equilibrium systems that enable us to make efficient determinations of transport coefficients such as viscosity and thermal conductivity [Ciccotti, *et al.*, 1987]. Most of this work has, however, been only for systems of perfectly elastic particles. Our contribution has been primarily to adapt recognized techniques from molecular dynamics to systems of inelastic, frictional particles. In these simulation calculations, the differences between the behavior of assemblies of macroscopic particles and assemblies of molecules is determined primarily by the differences in the interparticulate forces assumed to act between the particles being simulated. Much work has been done modeling molecules as *smooth, elastic, rigid* spheres. Analogously, we can describe granules as *frictional, inelastic, rigid* spheres. Even simpler, we could ignore friction and assume that granular materials are simply composed of assemblies of *smooth, inelastic, rigid* spheres. We have done just that, and have used computer simulations of such systems to determine the properties of the simulated granular material. We have then added various additional features to the interaction models (such as friction and finite stiffiness) and determined the sensitivity of the stresses in rapidly shearing flows to the effects of each new parameter.

SIMULATION OF RAPID SHEARING FLOWS

This paper describes initial simulation studies which focus on rapid shearing flow conditions, conditions that occur in channels, chutes, pipes or near the exits of hoppers and also occur naturally in landslides and avalanches. Under rapid deformation conditions granular materials are often vibrationally fluidized and resemble a flowing liquid in many aspects of their behavior. In such flows, the behavior of the material is strongly influenced by the collisions or impacts between granules that transmit momentum and vibrational kinetic energy from boundaries or free surfaces to the interior of the flowing layer, and thus maintain the material at a density (solids packing) much lower than would exist if the material were at rest in the earth's gravitational field.

The simulation calculations model a representative region or "cell" of material in the middle of a flowing layer. If we consider such a representative "cell" of material inside a landslide or an inclined chute flow or in an annular-shear-cell test, we find that the material above the cell moves more rapidly, while the material below moves more slowly than the material in the cell. If we then attach a moving coordinate system to our cell, we find that, in terms of that coordinate system, the material above appears to be moving in one direction, while the material below appears to be moving in the opposite direction.

In the computational model this is simulated as steady, rectilinear shear flow and periodic boundaries are used on all sides of a primary calculational cell of fixed volume containing a fixed number of particles. Periodic image cells above and below the primary calculational cell replicate the particles in the primary cell, except that each image cell is moving at constant velocity with respect to the primary cell with the cell above moving to the right and the one below moving to the left (see Figs. 1a and 1b). This configuration causes a steady shearing flow to exist in the simulated material; the moving image particles above interact with the particles near the upper boundary of the primary cell causing these particles to move nearly at the speed of the image cell passing by. Likewise for the lower image cell and particles located near the bottom of the primary calculational cell.

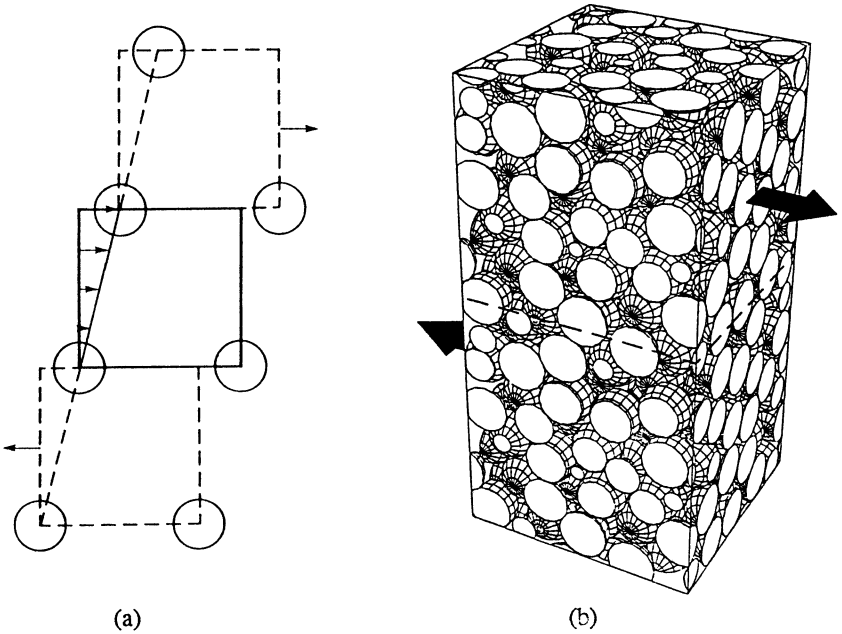
(a) (b)

Fig. 1. (a) A steady shearing flow calculational cell and two moving image cells showing one particle and its periodic images. Notice that one complete particle (i.e., one half-particle and two quarter-particles) appear inside each cell shown. (b) Perspective view of 125 particles in the primary calculational cell and their periodic images in the cell below the primary cell in a steady shearing flow calculation of inelastic spheres.

This method is one of several methods of generating a uniform shear field that have been developed for nonequilibrium molecular-dynamics simulation [Hoover, 1983]. During these steady shearing simulation calculations, bulk flow properties such as stress, velocity and porosity distributions are obtained by taking time and space averages of the forces, velocities and positions of the particles in the primary calculational cell. The most notable diagnostic quantity is the stress tensor, the components of which are determined from cumulative time averages of the momentum-flux-density. Within a flowing material the momentum flux in each direction can be calculated from the velocities of the particles and from the instantaneous values of the forces acting between the particles. An expression commonly used for the instantaneous space average of components of the momentum-flux-density tensor is:

$$p_{ij} = \frac{1}{V} \sum_{i}^{n} m_i(\boldsymbol{v}_i - \boldsymbol{u}_i)(\boldsymbol{v}_i - \boldsymbol{u}_i) + \frac{1}{V} \sum_{i \neq j}^{n} \boldsymbol{R}_{ij}\boldsymbol{F}_{ij}$$

where each of the two terms on the right hand side are dyads, and V is the volume of the cell, m_i is the mass of the ith particle, $\boldsymbol{v}_i$ is the (vector) velocity of the ith particle, $\boldsymbol{u}_i$ is the mean (vector) velocity field evaluated at the location of the ith particle, $\boldsymbol{R}_{ij}$ is a vector between the centers of two contacting particles i and j, and $\boldsymbol{F}_{ij}$ is the (vector) force acting between the two contacting particles; (If the force is along the line of centers then this expression is symmetric; however, if tangential friction forces are acting, then non-symmetric terms exist).

Stresses in Shearing Flows

Ultimately our concern with the physical properties of flowing granular solids is aimed at knowing what forces the material will exert on the containers it flows through and also knowing the internal forces acting to cause changes in the flow direction or velocity. In an ordinary (i.e., Newtonian) fluid, the shear stress that the fluid can develop is proportional to the shear rate. The proportionality constant being the *viscosity* of the fluid, with its value often determined by measuring the torque transmitted through a thin layer of fluid between a rotating cylinder and a coaxial stationary cylindrical container (Couette flow).

One of the first studies of shearing flows of colliding inelastic spheres was done by Bagnold [1954] with neutrally buoyant wax spheres suspended in water between rotating and stationary cylinders similar to Couette flow measurements in a fluid. He found that at high shear rates the shear stresses transmitted through such a suspension were dominated by the momentum carried by the inelastic particles, with the viscosity of the water adding a negligible contribution to the total shear stress in the suspension. He also found that the shear stress at these high shear rates increases in proportion to the square of the shear rate, not linearly as it would in a simple fluid. Reasoning that this stress was primarily caused by particle collisions (i.e., the forces acting during momentary contacts), Bagnold explained the observed behavior by noting that the frequency of collisions should increase linearly with the rate of shearing and that the relative velocity of typical colliding particles should also increase with the shear rate. Thus, both the momentum transferred per collision and the frequency of collisions would be higher at higher shear rates, resulting in the second power dependence of the "solids contribution to the stress". Combining these arguments with dimensional analysis, Bagnold further deduced that stresses in steady shearing flows of inelastic particles should also vary with the square of the particle size and linearly with the material density of the particles. Subsequent annular shear cell tests with glass and plastic beads (in air) have demonstrated stresses varying nearly as Bagnold predicted [Savage & Sayed, 1984; Hanes & Inman, 1985].

More thorough statistical theories for inelastic particles have been developed in recent years, and numerical models have been used to directly determine stresses in rapid shearing flows. Numerical simulations of such flows (without any interstitial fluid) have essentially verified the relationship that Bagnold developed for the dependence of shear stress on shear rate, particle size and material density for inelastic particles in steady shearing flow. (Each of the two terms contributing to the stress in systems of colliding particles described above, namely a term due to the momentum carried by the particles themselves, and a term resulting from the instantaneous forces acting between contacting or colliding particles—increases with the square of the mean vibrational velocity in the system. This vibrational velocity increases nearly linearly with the shear rate, thus producing a second-power dependence on shear rate for each of the two terms contributing to the total stress in the system) [Walton & Braun, 1986b].

These simulations have shown, however, that Bagnold's shear-rate dependence is only strictly valid for a special class of inelastic particles, namely, for particles that collide with a constant coefficient of restitution (i.e., the ratio of relative normal-direction incident velocity to recoil velocity) independent of the magnitude of the relative velocity of the colliding particles. Collisions between most real particles, in contrast, become less and less elastic as the relative collision velocity increases. The simulations have shown that this changing coefficient of restitution causes the stresses in shearing systems of inelastic particles to increase with the strain rate at a power somewhat less than the square predicted by Bagnold and more modern theories using constant coefficients of restitution. Such behavior is also predicted by recent theories incorporating velocity dependent inelasticity [Lun & Savage, 1986].

Numerical results

Computer simulations are being used to map the stress, density, and strain-rate dependence of simulated materials and to gain a microstructural understanding of deformation and flow behavior. These simulation results will help up to develop appropriate continuum constitutive relationships and to check out predictions of various new statistical theories for granular materials. Simulation models allow us to determine the sensitivity of predicted stresses to various assumptions made about the particles and, thus, to focus attention on the parameters that have the strongest effect on the calculated stresses. Generally, we have found that the details of the particle-particle interaction models (i.e., the exact force-time history during collisions) play a significant role in determining the stresses in rapid shearing flows. However, these effects are not nearly as important as changes in porosity, shear rate, and the degree of inelasticity [Walton & Braun, 1986a, b].

(We expect that the details of interaction models will prove to be much more important for quasi-static deformations. In such situations "locked-in stresses" that are dependent on past strain history can also be quite important. Such hidden stresses cannot be observed or detected simply from an examination of the geometry or fabric of the particles and contacts. Instead either the forces at each contact need to be known or a significant portion of the recent deformation history must be known in order to establish the static internal forces. When quasi-static deformation behavior is studied it will be necessary to reexamine the sensitivity of these simulations to the details of the force-displacement models used.)

Stresses in steady shearing flows at different solids packings and for particles with different material properties have been determined in numerically simulated flows. Figure 2 shows a plot of the calculated shear stress, p_{xy}, for a range of solids loadings [Walton & Braun, 1986b]. The solid curve is drawn through the results from several calculations at the same constant shear rate at a variety of different solids packings for particles with a constant coefficient of restitution, e=0.8. The same number of particles were used in each simulation; the lower solids packings were achieved by using a larger volume calculational cell. To obtain the same shear

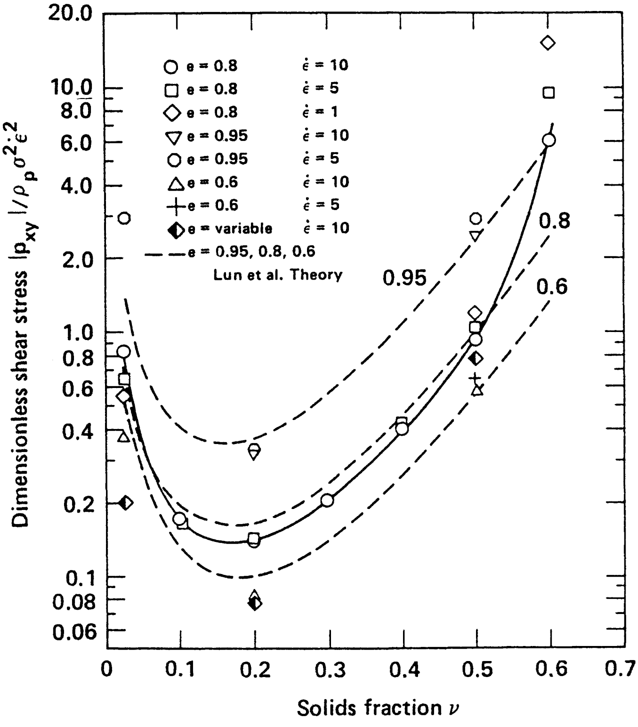

Fig. 2. Calculated shear stress for steady shearing flows of smooth (i.e., frictionless) equal sized spheres [Walton & Braun, 1986b] (non-dimensionalized by dividing by the square of the particle diameter, the square of the shear rate, and the material density) compared with predictions of the dense-gas-like theory of Lun *et al.* [1984] for various values of the coefficient of restitution of the colliding spheres (dashed curves).

rate (horizontal deformation rate per unit height) it was necessary to use higher velocities for the image cells at the lower solids packings. Each calculation was done in a steady-state, that is, the energy being added to the system by moving the image cells past the primary cell was balanced, on average, by the dissipation due to the collisions between particles, resulting in constant average values for all pertinent parameters such as translational kinetic energy, shear rate, stress, density, etc.

The characteristic "U" shape to the shear stress curve shown in Fig. 2 is also exhibited by all other stress components. It can be best understood by recognizing that the curve represents stresses generated at the same shear rate at various densities. However, the average vibrational kinetic energy is not constant along the curve. Thus, it does not correspond to an "isotherm" of an ordinary equation-of-state. The simulations show that at high solids packings, the average kinetic energy of the particles in steady shearing flow changes very little as the solids packing initially decreases. At these high solids packings the typical distance a particle can move between collisions is extremely short and the stresses are almost entirely due to the momentum transmitted through collisions (i.e., by the forces acting for a brief instant during each impact). As the solids packing is initially decreased, the mean free paths increase rapidly and the stresses decrease primarily because the frequency of collisions is decreasing as these free-flight path lengths increase.

At very low solids packings, another effect dominates. Below solids packings of 0.15 or so the mean-free-path of particles is very large, collisions are infrequent, and stresses are caused almost entirely by the momentum carried by the particles as they travel between collisions. Since the constant shear rate is achieved in the simulations by moving the image cells at higher and higher velocities, we find that as the cell size increases (i.e., as the density decreases) the average particle velocities are correspondingly higher. This increase in velocity coupled with a decrease in the frequency of dissipative collisions leads to much higher vibrational kinetic energies at the low solids packings and accounts for the increase in all stress components with decrease in solids packing for systems shearing at the same rate.

Less elastic particles, interacting with lower coefficients of restitution, dissipate more energy per collision and thus generate less pressure at the same shear rate than more elastic particles. This behavior is apparent in Fig. 2 where the results of representative simulations with various coefficients of restitution are plotted as individual symbols above and below the solid curve (coefficient of restitution=0.8). Figure 2 also shows three dashed curves which are predictions of one proposed kinetic theory for smooth, inelastic spheres [Lun *et al.*, 1984]. The theoretical curves (which are based on perturbations of dense gas kinetic theory) show the same general trends as the simulation calculations, and are quantitatively close to, our calculated results when the simulated particles are made frictionless and nearly elastic. However, for frictional particles, and as the degree of inelasticity increases, the deviation between theory and simulation becomes significant.

During each simulation calculation not only is the average pressure monitored but also a variety of other diagnostic quantities are calculated, such as average vibrational kinetic energy, the distribution of velocities and the relative magnitudes of various contributions to the total stress components. This additional information allows a detailed comparison with kinetic theory models to be made, and allows us to determine why deviations occur between the calculations and theoretical predictions.

Among the more interesting differences noted between the calculations and these initial theories is the anisotropic nature of the stress and velocity distributions we find in simulations of steady-shearing flows. This effect was unexpected for two reasons. First, the initial statistical theories proposed for granular solids assumed that the vibrational velocity distribution was isotropic—this precluded any prediction of anisotropies in velocities or resulting stresses. Second, previous non-equilibrium molecular dynamics simulations of rectilinear shear flows did not exhibit significant anisotropic velocity or stress distributions. (Minor deviations from isotropy had been seen in such simulations, but were usually considered a flaw in the method caused by the extremely high shear rates simulated or produced by improper scaling of the velocities during application of the constant kinetic energy constraint.)

However, at low solids packings, where the material was expected to behave much like a kinetic theory gas, the stresses in the direction of the induced shearing are found to be much higher than the stress components perpendicular to the shear. This difference increases in magnitude as the degree of inelasticity increases or as the solids packing decreases. This effect, which is illustrated in Fig. 3, is a direct result of the localized kinetic energy loss during particle collisions and can be explained by considering the details of what happens during inelastic collisions. In steady shearing flows, kinetic energy and momentum are "pumped" into the system in the direction of the shearing. If all collisions are perfectly elastic they soon redistribute

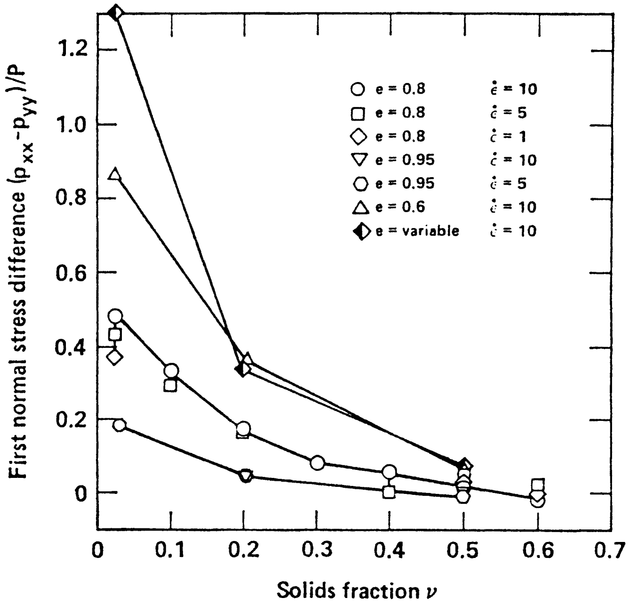

Fig. 3. Calculated ratio of first normal stress differences $(p_{xx}-p_{yy})$ to pressure $(p_{xx}+p_{yy}+p_{zz})/3$ for 125 inelastic spheres in uniform shearing flow [Walton & Braun, 1986b]. Large first normal stress differences at low solids fractions are a direct result of localized energy loss during collisions.

the new momentum equally in all directions. However, because these particles are inelastic, much of energy is dissipated before it can be redistributed (via collisions) into directions perpendicular to the direction of shearing. Thus, equipartition-of-energy in each available degree of freedom is not attained in these flows. This is further evidence of the non-equilibrium nature of flows involving inelastic particles.

Such behavior was only noticed as a minor perturbation in previous non-equilibrium molecular-dynamic simulations with perfectly elastic particles because the kinetic energy added to the system due to the shearing motion was isotropically removed by scaling all velocity components of all particles so as to keep the total kinetic energy in the system constant. In inelastic-particle simulations the energy input is naturally balanced by the energy loss occurring in the collisions and, this localized energy loss results in anisotropic velocity and pressure distributions with much higher values in the direction of the shearing. (Such high stresses in the direction of shearing have not been observed in annular shear cell tests primarily because there is no convenient method available to measure the hoop stress around the annulus.)

Figure 4 shows experimental measurements of stress obtained in annular-shear-cell measurements on assemblies of glass beads [Savage & Sayed, 1984; Campbell, 1986] and the results of discrete-particle simulation calculations for inelastic frictional spheres [Walton & Braun, 1987]. The measurements show a decrease in

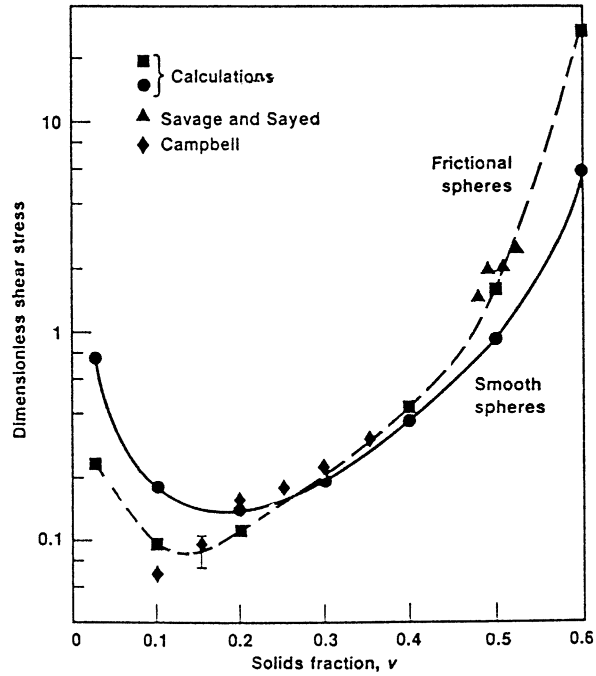

Fig. 4. Calculated shear stress for steady shearing flows of inelastic frictional spheres (i.e., including particle rotations) compared with measured shear stresses obtained in annular shear cell tests [Savage & Sayed, 1984; Campbell, 1986].

stress with decreasing solids loading, but do not exhibit the left hand side of the characteristic "U" shape produced both in kinetic theory and in our simulations for spheres with constant coefficients of restitution. This lack of a minimum in the laboratory data is primarily a result of the fact that the low solids packing measurements can only be obtained employing very high velocities for the moving boundaries inducing the shear in the granular material. This means that the low density measurements are made on systems with much more energetic collisions than the high density measurements, and almost all real particles exhibit less elastic behavior as the collision speed increases. Simulation calculations with a variable coefficient of restitution have demonstrated that the location of the minimum in the characteristic "U" shaped stress-vs-packing curves moves noticeably toward lower solids loadings if the coefficient-of-restitution decreases with increasing impact velocity. Such a shift in the location of the minimum could prevent it from being observed to date in the laboratory measurements.

In addition to shear rate, density and inelasticity, the effects of interparticulate friction, and particle stiffness on calculated stresses have also been examined. These simulations have shown that the inclusion of friction introduces another energy loss mechanism and can thus lower stresses if much sliding occurs. However, if the friction coefficient is high the stresses at high solids packings can actually increase. The two sets of calculations shown in Fig. 4 illustrate this effect as they exhibit a decrease in stress at low density and an increase at high density when going from smooth to frictional particles.

COMPARISON WITH GRAVITY FLOW TESTS

In addition to simulation calculations aimed at determining the constitutive behavior of rapid shearing granular solids, another concern is verifying that the somewhat simplified particle interaction models in these calculations are adequate to simulate the behavior of real granular flows. One of the methods of validating our models has been through comparison with measurements of stresses in annular shear cells mentioned above. Much more detailed comparisons with a series of gravity flow tests conducted at the University of California at Los Angeles (UCLA) have also been made. Researchers at UCLA have supplied us with detailed information on individual particle collisions, density profiles, velocity profiles and material properties for a series of nearly two-dimensional inclined channel tests. In these tests identical plastic spheres were confined to a single vertical layer by parallel glass sidewalls. The UCLA researchers observed and documented the motions of individual "grains" within the flows using high-speed motion pictures; they then digitized the films, frame-by-frame, to obtain the density, velocity, kinetic energy and collision information desired [Drake & Shreve, 1986]. Simulation calculations of similar configurations were performed. Figure 5 is a perspective view of particle positions in a simulation of one of the UCLA tests. The "horizontal" axis of this figure is tilted 42.72 deg. so that gravity drives the flow from right to left "down" the incline. A layer of fixed particles lie along the bottom of the channel, and glass side walls are simulated on the front and back of the single layer of frictional inelastic spheres. Because of the steep angle of the particular flow shown in the figure the

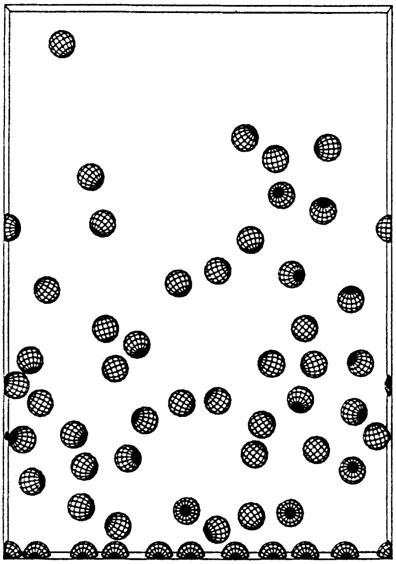

Fig. 5. Perspective view of inelastic frictional spheres in computer simulation of UCLA inclined channel flow test. The horizontal axis is tilted 42.75 deg so that gravity drives the flow from right to left.

particles are quite disperse (and also quite energetic). Input parameters to the model were obtained from direct measurement of the stiffness, surface friction and energy loss in collisions of pairs of particles. The resulting flow simulations not only were able to reproduce the measured mean flow velocity, but also produced velocity and density profiles that were very close to the measured curves [Walton & Drake, 1988].

Simulation calculations of gravity flow of inelastic, frictional spheres falling through an array of horizontal cylinders have also been compared directly with laboratory tests of glass beads falling through a similar array of steel cylinders. The mean velocity was found to be in agreement with the measurements (within a few percent) over a wide range of solids packings [Walton *et al.*, 1988].

CONCLUDING REMARKS

We have just begun to understand granular flow on a microstructural level. This research has been directed toward understanding rapidly shearing flows of systems of spherical particles at various shear rates and solids packings. Spheres with various properties were considered: smooth or frictional, elastic or inelastic, uniform sized set or binary mixture, and perfectly rigid or slightly deformable. The sensitivity of various stress components to each of these parameters were examined. While we have learned a great deal, there is much still to be done.

All flow stoppages and reinitiations of flow involve material that is stationary or deforming quasi-statically. The slightly deformable particle models used for many of the simulations described in this article can be applied to such low strain-rate deformations. Nonsymmetric particles, in the form of sphere-clusters, would be a natural extension of the current models so that realistic particle shapes could be investigated. In future work we plan to add such particles and also to add new boundary conditions so that converging and axisymmetric flows can be modeled. Such additions will enable us to make a thorough investigation of cohesionless, dry, granular solids.

However, most engineering problems are even more complex and include mixed phases, cohesion, aeration, and other phenomena. For instance, a large fraction of industrial solids processing involves multiphase flows with an interstitial fluid flowing through the particulate material, sometimes in the same direction as the solids and sometimes in the opposite direction. A gas or liquid not only passes through a bed of particles; it also can act as a fluidizing agent, a suspending medium or a source of momentum for transport. Researchers at LLNL and elsewhere have begun examining various techniques for including interstitial fluid effects in simulation models [Ladd, 1988a, b, c]. As such models are developed it will become possible to simulate flow behavior of slurries and suspensions.

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