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COMPUTER SIMULATION OF SHEAR FLOWS OF GRANULAR MATERIAL

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ABSTRACT

The purpose of this paper is to present results from computer simulations of Couette flows of granular materials and to examine the detailed rheological behavior inherent in these simulations. Comparison is made with the experimental results of Bagnold (1954) and Savage and Sayed (1980, 1982) as well as with the various theoretical constitutive models (see below).

INTRODUCTION

In recent years there has been a significant increase of interest in the detailed mechanics of granular material flows and considerable progress had been made toward understanding the different regimes of flow. The present state of knowledge has recently been reviewed by Spencer (1981) and Savage (1982). The latter comprehensively reviews the recent experimental and theoretical work in higher speed granular flows which lie in the so-called "grain inertia" regime. It is clear that the experimental work in this area is hindered by lack of well-proven, non-intrusive instrumentation necessary to document precisely the velocity, solid fraction and granular temperature distributions within such flows. On the other hand most of the existing theoretical work is limited to modest solid fractions of the order of 0.3 to 0.4. Considerable work is required to extend theories to solid fractions approaching the critical value. An alternative approach is to utilize the kind of computer simulations which have been quite successful in the analogous problems in molecular gas dynamics (eg. Bird (1976), Barker and Henderson (1976), Wood (1975)).

The purpose of such computer simulations is threefold. First they can provide insights and detailed results which can be used to suggest appropriate assumptions and validate theoretical models particularly at higher solid fractions. At the present time this is best accomplished using simple shear flows or Couette flows. This is the specific objective of the present paper. Two other objectives may, however, be mentioned in passing. One is to compare the simulation results with experimental measurements in order to establish appropriate models of the mechanics of particle/particle and particle/wall interactions. Efforts in this direction are reported elsewhere (Campbell (1982), Campbell and Brennen (1982)) with specific attention to the simulation of chute flows for which some experimental results exist. Parenthetically one might add that a third use of computer simulations might be the exploration of the effects of additional forces (such as those due to the interstitial fluid or electrostatic effects). For simplicity, such effects are not included in the simulations presented here. Discussion of interstitial fluid effects can be found in other recent works (eg. Savage (1982)).

Other computer models of granular material flows include the work of Cundall (1974), Davis and Deresiewicz (1977), Cundall and Strack (1979), Trollope and Berman (1980) and Walton (1980). Most of these are directed toward the simulation of slower flows and smaller deformations. However, in his original work Cundall (1974) did extend his methods to some higher speed but transient flows such as rockfalls and the emptying of a hopper. Also the versatility of Walton's (1980) computer program is readily apparent from the excellent movies which the Lawrence Livermore Laboratory has produced. However to our knowledge none of the existing models have been used to produce continuous "steady" flows which could be used for basic rheological purposes. The intent of the present model was to minimize the complexity of the geometry and the interactions so that steady flows of sufficiently long duration for rheological analysis would be produced. Thus the simulations are just two-dimensional and the particles are circular cylinders. Though extension of the simulation to the third dimension is possible, the necessary computer time would be considerably greater.

Granular material flows in the grain inertia regime have much in common with molecular gas dynamics (Chapman and Cowling (1970), Ferziger and Kaper (1972)) and the recent theoretical work of Blinowski (1978), Kanatani (1979 a,b, 1980), Ogawa and Oshima (1977, 1978a,b, 1980), Savage and Jeffrey (1981), Ackermann and Shen (1982, 1982) and Jenkins and Savage (1982) has drawn extensively from that source. An advantage in granular media flows is that the hard sphere model is appropriate provided the interstitial fluid and electrostatic effects can be neglected. Difficulties do however arise from the dense packing and the inelasticity of the collisions.

Extensive work has, of course, been done on the computer simulation of molecular gas dynamic flows. In that arena, Monte Carlo methods (Bird (1976)) have proved particularly efficient. In the future, such methods may also prove valuable for granular material flow simulations. However the present simulation is entirely mechanistic.

COMPUTER SIMULATION

The present method for the computer simulation of granular material flows has been documented elsewhere (Campbell (1982)) and will only briefly be described in the present paper. Two dimensional unidirectional flows of inelastic circular cylinders are followed mechanistically. The flow solutions sought have no gradients in the flow direction (x-direction, Figure 1). Though both Couette flows and inclined chute flows have been examined the present paper is confined to discussion of Couette flows in the absence of gravity (see Campbell and Brennen (1982) for inclined chute flows). The simulation is initiated by placing a number of cylindrical particles (radius, R; mass, m) in a control volume bounded by the solid boundaries and two perpendicular "periodic" boundaries (see Fig. 1). A particle passing out of the control volume through one of the periodic boundaries immediately re-enters the control volume through the other periodic boundary at the same distance from the solid boundaries and with the same instantaneous velocity. Thus the number of particles initially placed within the control volume remains constant. Simulations with different distances, L, between the periodic boundaries were performed until further doubling of this length had little effect upon the results. In the Couette flow simulations values of L/R of about 10 were found to be acceptable (see Fig. 2).

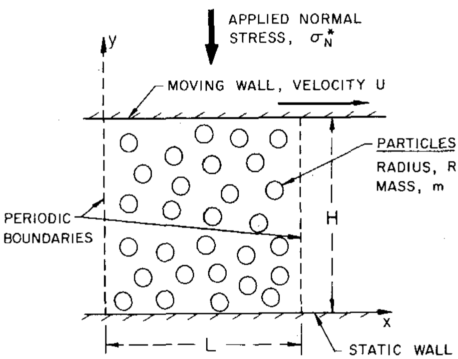

Figure 1. Schematic of computer simulation.

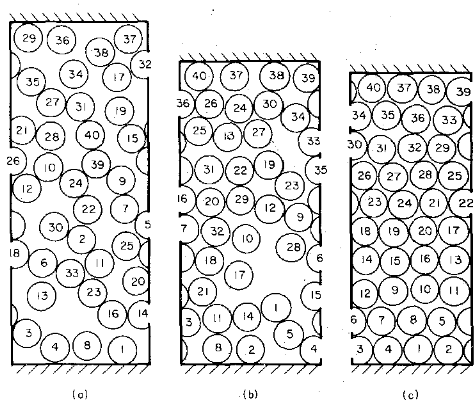

Figure 2. Typical snapshots of the Couette flow simulations for (a) ν=0.56 (b) ν=0.63 (c) ν=0.76.

All simulations were begun with a randomly perturbed square lattice array of particles in the control volume and randomly chosen instantaneous translation velocities (u,v, in the x,y, directions of Fig. 1) and rotational velocity (ω). This entire assemblage of particles is followed mechanistically as the particles collide with each other, the static lower wall and the moving upper wall (velocity, U, in the x direction) until a final asymptotic state is reached in which the flow is steady in the sense of being invariant over long time scales. The first Couette flow simulations attempted maintained a constant wall separation, H, as well as a constant moving wall velocity, U; the intent was to evaluate the asymptotic normal and shear stresses generated at the walls. However it was found that simulations specified in this way were unstable particularly at the lower solid fractions; all the particles tended to migrate to a localized region so that they no longer came into contact with one or both walls. The simulation was then altered to maintain a predetermined normal stress, σ^*_{yy}, on the walls (as well as a given moving wall velocity, U). This required continuous adjustment of the gap, H, according to whether the normal stress exerted by the particles on the walls was greater than or less than the prescribed normal stress (for details see Campbell (1982)). Such a procedure is, of course, analogous to the manner in which the experiments of Savage and Sayed (1980,1982) were performed. These simulations consistently converged, typically requiring 20,000 collisions to reach an asymptotic state.

After convergence a substantial extension of the simulation (of the order of 20,000 collisions) was required to obtain sufficient duration of "steady" flow for meaningful statistical analysis. Since the simulations exhibited fluctuations typical of small thermodynamic systems (Landau and Lifshitz (1958)), this duration had to be longer than one might otherwise anticipate.

SIMULATION DETAILS

Each individual particle/particle or particle/wall collision is assumed to be instantaneous and conventional means are used to solve for the departing linear velocities (u,v in the x,y directions, Fig. 1) and angular velocity, ω, given the incident velocities. In the process, impulses normal and tangential to the contact surfaces are evaluated. In addition to the linear and angular momentum/impulse equations two further relations are required to close a collision solution. First the relative approach and departure velocities normal to the contact surface are related by a coefficient of restitution to represent the inelasticity of the collisions. Different coefficients (denoted by ε_p and ε_w respectively) can be used for particle/particle and particle/wall collisions. Secondly a frictional closure condition pertaining to the relative tangential velocities of the contact points upon departure is necessary. The present simulation assumed that relative tangential motion is destroyed by a collision and hence that the tangential velocities of the contact points are identical upon departure. Parenthetically it should be noted that this choice of the final closure condition is somewhat arbitrary; other choices are possible. However, this second closure condition is used for particle/particle collisions in all the simulations reported here.

On the other hand, for reasons discussed later, two separate types of particle/wall collision (Types (A) and (B)) were investigated. The above mentioned second closure condition is used for particle/wall collisions in the type (A) Couette flows; this choice approximates "smooth" interior surfaces of the walls (see Campbell and Brennen (1982)). In addition simulations (type (B)

Couette flows) were run with an alternative second closure condition intended to approximate "roughened" interior surfaces. In this case a particle colliding with a wall departs with a particle center velocity whose tangential or x component is equal to that of the wall.

ANALYSIS OF THE SIMULATION RESULTS

The results of the Couette flow simulations are presented non-dimensionally by dividing the velocities by the upper wall velocity, U, the stresses by mU^2/R^2, and lengths by either H or R. Consequently the only parameters which affect the results are (i) the wall spacing to particle size ratio, H/R (which is only indirectly specified by fixing the number of particles in the control volume) (ii) the non-dimensional normal stress $\sigma_{yy} = \sigma^*_{yy}R^2/mU^2$ (iii) The coefficients of restitution, ε_w and ε_p and (iv) the ratio of radius of gyration of a particle to its radius, β. This last parameter was maintained at the value for solid cylinders (0.5) throughout.

All flow properties (say, p) were assessed as functions of y/H by dividing the control volume into strips parallel to the x-axis and computing the particle area weighted mean of that property in each strip. The time-averaged value of this is denoted by $<p>$. Mean velocity, $<u>$, and solid fraction profiles are evaluated. In addition, the squares of the components of both the fluctuating translational and rotational components of velocity (as opposed to the velocities, $<u>$, associated with the mean shear flow) were evaluated as

$$<u'^2> = <u^2> - <u>^2 \quad ; \quad <v'^2> = <v^2> \quad ; \quad <\omega'^2> = <\omega^2> - <\omega>^2 \qquad (1)$$

Hence the kinetic energy associated with the random motion of the particles (as opposed to that of the mean shear flow) is given by

$$\tfrac{1}{2}m(<u'^2> + <v'^2> + \beta<\omega'^2>) \qquad (2)$$

and, for convenience, this is termed the "total granular temperature". The part of this associated with fluctuating translational motions (i.e. without the last term of the expression (2)) is termed the "translational granular temperature". Both temperatures are non-dimensionalized by $\tfrac{1}{2}mU^2$.

In the existing theoretical studies (see Savage (1982)) the parameter, S, (Savage's R) is used as a measure of the ratio of the typical velocity difference associated with the mean shear flow, $2R\,d<u>/dy$ and the typical translational fluctuating velocity. Here S values are assessed as

$$S = 2R\frac{d<u>}{dy} \Big/ [<u'^2> + <v'^2>]^{\frac{1}{2}} \qquad (3)$$

In the converged state, Couette flows have normal and shear stresses, σ_{yy} and

σ_{xy}, which are uniform throughout the flow and are equal to the stresses exerted by the walls. In the results which follow they are both evaluated simply by summation of the normal and tangential impulses applied to the walls by particle collisions.

VELOCITY, SOLID FRACTION AND TEMPERATURE PROFILES

Three typical instantaneous snapshots of the arrangement of particles in the control volume are presented in Fig. 2. The mean solid fraction in these examples vary from $\nu = 0.56$ to $\nu = 0.76$. For future reference note the increased tendency for the particles to arrange themselves in layers at the higher solid fractions.

Typical velocity and solid fraction distributions for the type (A) (or "smooth wall")Couette flows are presented in Fig. 3 for, $\varepsilon_w = 0.8$, $\varepsilon_p = 0.6$ and various normal stresses and H/R. The velocity distributions are characteristic of all such simulations indicating "slip" at both walls amounting to about 20% of the relative velocity and regions of higher shear close to the walls. The solid fraction profiles exhibit a corresponding decrease in ν in these regions of higher shear.

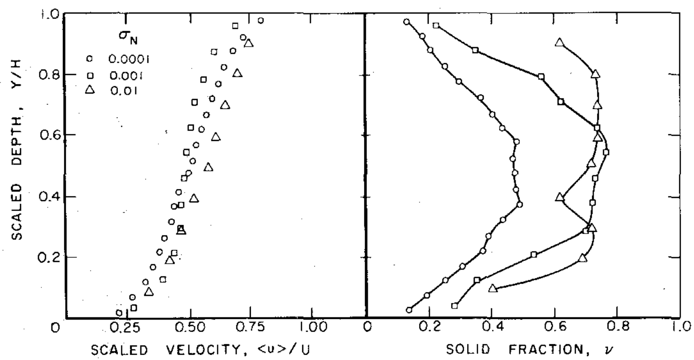

Figure 3. Typical velocity and solid fraction profiles for the type A Couette flow simulations for $\varepsilon_p = 0.6$, $\varepsilon_w = 0.8$. Data is shown for $\sigma_{yy} = 0.0001$ and H/R = 39.6, $\sigma_{yy} = 0.001$ and H/R = 23.9, $\sigma_{yy} = 0.01$ and H/R = 19.5.

Typical type B (or "rough wall") Couette flow profiles are presented in Fig. 4 for three different normal stresses, σ_{yy} (and H/R though this does not vary much in this set of data). The resulting linear velocity profiles have no slip and the solid fractions are virtually uniform across the flow. The total granular temperature profiles are more scattered but do indicate a temperature which is fairly uniform over the central core of the flow; there is however some indication of a reduced temperature near both of the walls. Globally it is clear that the solid fraction increases and the temperature decreases as the normal stress increases. In fact the type B simulations closely approximate simple shear flow and are therefore well suited for rheological investigations. Therefore the remainder of the paper concentrates on the type B simulations.

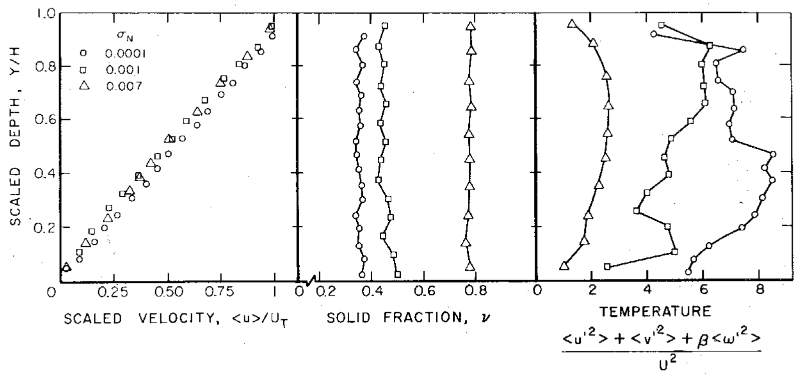

Figure 4. Typical velocity, solid fraction and total granular termperature profiles for the type B Couette flow simulations for $\varepsilon_p = 0.6$, $\varepsilon_w = 0.8$. Data is shown for $\sigma_{yy} = 0.0001$ and $H/R = 39.7$, $\sigma_{yy} = 0.001$ and $H/R = 29.2$, $\sigma_{yy} = 0.007$ and $H/R = 20.8$.

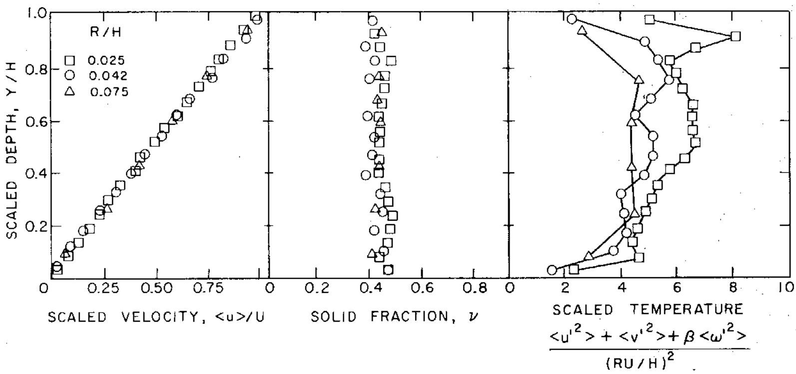

Figure 5. Comparison of type B Couette flow simulation data for different H/R as indicated but all with $\sigma_{yy} = 0.567(R/H)^2$. Note the temperature scale in this figure has been divided by $(R/H)^2$.

Figure 5 presents a comparison of typical results for different values of H/R. Specifically the three cases shown all have a dimensionless applied normal stress equal to 0.567 $(R/H)^2$. According to the existing constitutive models discussed below this should yield the same solid fraction and a temperature proportional to $(R/H)^2$ in all three cases. We note that this indeed appears to be the case.

COMPARISON WITH EXISTING CONSTITUTIVE MODELS

In the absence of interstitial fluid, electrostatic or other additional effects, dimensional analysis requires that the normal and shear stresses (σ^*_{yy} and σ^*_{xy}) in a simple shear flow must be given by

$$\sigma^*_{ij} = \rho_p [R \frac{d<u>}{dy}]^2 f_{ij} \tag{4}$$

where ρ_p is the particle density and the quantities f_{yy} and f_{xy} can only be functions of S, ν and ε_p. This relation agree with Bagnolds (1954) original heuristic constitutive laws. We have already demonstrated in Fig. 5 that the scaling implicit in the relation is indeed manifest by the present simulations.

In non-simple shear flows (such as the type A Couette flows or the chute flows of Campbell and Brennen (1982)) temperature gradients can exist in the y direction; steady flows can be generated in which granular heat is conducted in the y direction and introduced or removed through solid boundaries. Both Ogawa, Oshima et al. (1977, 1978a,b , 1980) and Kanatani (1979a,b, 1980) have explored such phenomena theoretically. However since their results for f_{ij} are not in very good agreement with the measurements (Savage (1982)) an appropriate form of the granular energy equation which would be required in order to model non-simple shear flows remains to be established. We have previously shown (Campbell and Brennen (1982)) that such a relation is necessary to understand the development of plugs in chute flows.

Therefore we concentrate here on the less ambitious task of establishing the functions f_{yy} and f_{xy} in simple shear flows. Values of f_{yy} and f_{xy} obtained from the simulations are presented in Figs. 6 and 7 as functions of the solid fraction (and for several values of $\varepsilon_p, \varepsilon_w$). The ratio f_{xy}/f_{yy} which is the

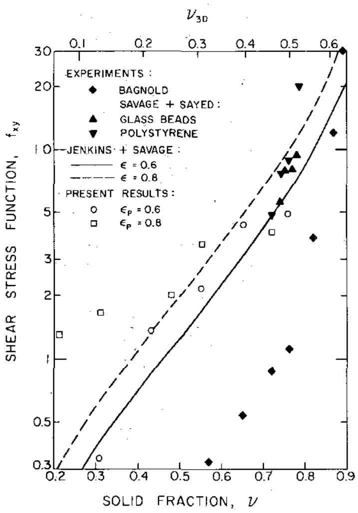

Figure 6. The shear stress function, f_{xy}, as a function of ν.

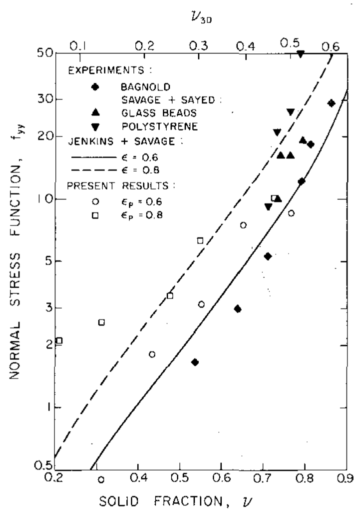

Figure 7. The normal stress function, f_{yy}, as a function of ν.

effective coefficient of friction for the material is presented in Fig. 8. For reference, the corresponding values of S are presented in Fig. 9.

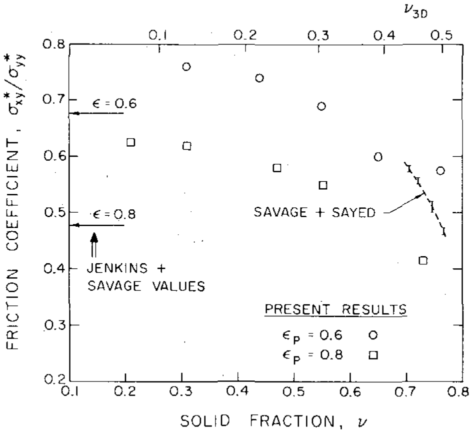

Figure 8. The friction coefficient, $\sigma^*_{xy}/\sigma^*_{yy}$ or f_{xy}/f_{yy}, as a function of ν. Also shown are the theoretical values from Jenkins and Savage which are independent of ν.

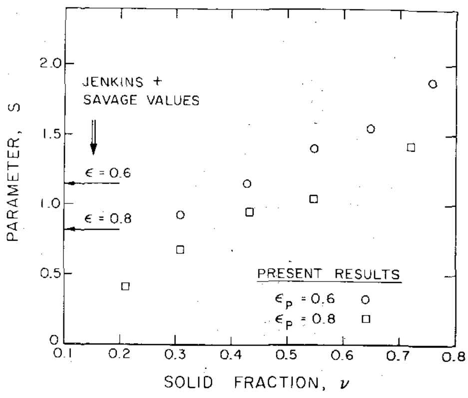

Figure 9. The parameter, S, as a function of ν. Also shown are the theoretical values of Jenkins and Savage which are independent of ν.

In order to make comparisons with the existing experimental and theoretical results for three dimensional near-spherical particles it is necessary to define an approximate equivalent three dimensional solid fraction, ν_{3D}. Here we somewhat arbitrarily choose to define ν_{3D} so that the average interparticle gap is the same as that in the two-dimensional simulation so that $\nu_{3D} = 0.752\nu^{3/2}$. The experimental data of Bagnold (1954) and Savage and Sayed (1980, 1982) as well as the theoretical predictions of Jenkins and Savage (1982) are thus displayed in Figs. 6 to 9.

Though an exact comparison with the three dimensional results is inappropriate it seems clear that the values of f_{xy} and f_{yy} from the simulation (Figs. 6 and 7) are comparable with those from the experiments and from the theory of Jenkins and Savage (1982). The values of these functions increase almost exponentially with the solid fraction and presumeably asymptote to infinity at some maximum packing or critical solids fraction. The values also increase with coefficient of restitution, ε_p.

Though the simulation data of Figs 6 and 7 is somewhat erratic, the ratio of f_{xy}/f_{yy} which is the effective coefficient of friction and the value of the parameter S (which is an inverse measure of the translational temperature for a fixed $Rd\langle u\rangle/dy$ are less erratic and are displayed in Figs. 8 and 9. Contrary to the three dimensional theory of Jenkins and Savage both the friction coefficient and S proved to be functions of ν. As seen in Fig. 8, the values of the friction coefficient are of the same order as those of Jenkins and Savage and, indeed, they decrease as ε_p increases in a similar manner. Moreover they are relatively independent of solid fraction at the lower values of ν where the theory of Jenkins and Savage is most appropriate. However the friction coefficient does appear to decrease as ν reaches higher values. As seen in Fig. 8 this decrease is consistent with the experimental data of Savage and Sayed (1980,1982).

The values of the parameter, S, which can be conveniently envisaged as an inverse measure of the granular translational temperature (for the same $Rd\langle u\rangle/dy$) also exhibit a substantial increase with ν over the whole range of ν examined. Indeed it appears to be a linear function of ν with lower values for a higher coefficient of restitution.

STATISTICAL PROPERTIES OF THE COUETTE FLOWS (TYPE B)

Most of the existing theories assume that the random motions in granular material flows have velocities with Maxwellian distributions. For this reason both translational and rotational velocity distributions were constructed from the Couette flow (type B) simulations (see Campbell (1982)). Since all of these distributions are qualitatively similar we present only one in this paper, namely the distribution of the magnitude of the translation velocity with the mean velocity removed. The abscissa, X, of Fig. 10 is therefore defined as

$$X = \left[\frac{(u-\langle u\rangle)^2 + v^2}{\langle u'^2\rangle + \langle v'^2\rangle}\right]^{\frac{1}{2}}$$

Figure 10 shows that the translation velocity distribution at lower void fractions (and smaller S) is essentially Maxwellian. However the distribution tends to deviate from Maxwellian at higher values of ν (and S).

The collision angle distribution is also of considerable importance in determining the rheology of a granular material flow. The orientation of two particles involved in a collision is non-isotropic due to the fact that the differential velocities inherent in the mean shearing motion are of the same order of magnitude as the random motions. Figure 12 presents the distribution of collisions over the orientation or collision angle, θ, as defined by the inset in that figure. Results are shown for Couette flows (type B) of five different solids fraction. There is clearly a substantial change in the form of this distribution as the solids fraction is increased. At low solids fractions ($\nu \sim 0.35$) or low S where the random motions dominate there is a relatively smooth skewness caused by the shearing motion. This distribution (at $\nu = 0.35$) is very similar in form to that proposed by Savage and Jeffrey (1981) and also used in other theoretical models. Quantitatively these low solids fraction distributions are somewhat different from those proposed by Savage and Jeffrey (1981) and also used in other theoretical models. Campbell (1982) has suggested a modification to their theoretical distribution which results in better quantitative agreement with the simulation results.

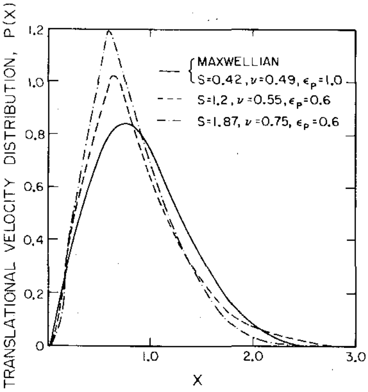

Figure 10. Translational velocity distribution functions from some Couette flow (type B) simulations.

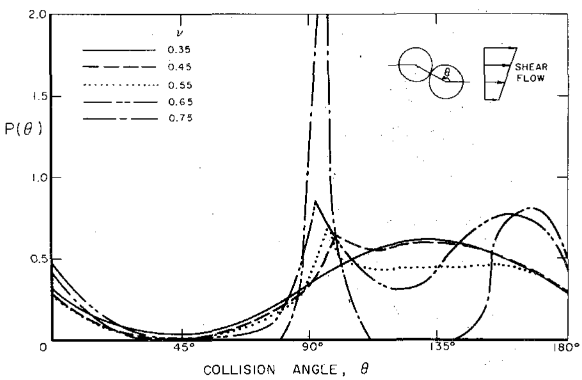

Figure 11. Collision angle distributions for various solid fractions from Couette flow (type B) simulations.

However, the main point of Fig. 12 is to demonstrate that the collision angle distribution undergoes substantial changes as ν increases to higher values. Two peaks around $\theta \approx 90°$ and $\theta \approx 180°$ develop and ultimately dominate the distribution at solids fractions larger that 0.6. These higher solids fraction distributions result from increased geometric order or "microstructure" within the flow. Probability distributions for the relative positions of two particles within the flow(Campbell (1982)) show that as ν increases from 0.35 to 0.75 there is an increased likelihood that particles arrange themselves in layers. Thus the peak at $\theta \approx 90°$ represents glancing collisions between particles in neighboring layers while the peak at $\theta \approx 180°$ represents collisions between particles in the same layer. It seems clear that any rheological model capable of predicting flows over the entire range of solids fraction must incorporate or reflect such substantial variations in the collision angle distribution.

CONCLUSIONS

In summary, this paper has presented results for the computer simulation of Couette flows of a "two-dimensional" granular material consisting of circular cylinders characterized by coefficients of restitution for cylinder/cylinder collisions and for cylinder/wall collisions. Interstitial fluid and gravitational effects are neglected as are other possible forces (eg. electrostatic) that can occur in the rapid flows of granular materials.

Results for two different kinds of wall boundary condition are first presented. The first type corresponds roughly to "smooth walls" and the simulations exhibit slip at both walls. The flow in the neighborhood of the walls has a lower solid fraction and granular temperature than in the core. On the other hand an alternative boundary condition corresponding to "rough walls" yielded linear velocity profiles without slip and uniform solid fractions.

The latter were therefore used to examine the effective constitutive relations for the flowing material. The veracity of a generalized form of Bagnold's constitutive laws was first demonstrated and the problem reduced to establishing the normal and shear stress functions f_{yy} and f_{xy} which may be functions of the solid fraction and coefficient of restitution. It is shown that the simulations yield values of these functions similar to those in the experiments of Savage and Sayed (1980, 1982) and to the theory of Jenkins and Savage (1982). The effective coefficient of friction, f_{xy}/f_{yy}, decreases with increasing solid fraction, ν, and with increasing coefficient of restitution. The former trend is consistent with the experiments of Savage and Sayed.

The statistical properties of the flow are also examined. It is shown, for example, that the velocity distributions tend to deviate from Maxwellian at the higher solid fractions. This is accompanied by an increased microstructure or layering of the particles. This, in turn, radically alters the collision angle distribution function.

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