Impulse strengths in rapid granular shear flows

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Summary. This paper describes measurements of the impulses that particles experience while undergoing rapid shear. These were performed with an eye towards understanding the processes that lead to particle attrition and fracture. The measurements were taken from a discrete particle computer simulation of a simple shear flow of spheres. Special attention is paid to the strongest impulses as these will do the most damage. The results indicate that the largest impulses arise, not from the mean shear flow, but from the random particle velocities that are characterized by the so-called “granular temperature”. Measurements of the largest impulses are presented as functions of particle properties and solid concentration. Histograms of the impulse strengths illustrate the effect of concentration and particle surface friction. Finally, geometric distributions are presented that illustrate the shear induced anisotropy in the impulse strengths.

1 Introduction

In any type of flow situation, the particles that make up a bulk granular material will exert forces on one another, either by collision or through long duration contacts. The largest of these forces may be sufficient to cause the particles to fracture, but, even if breakage does not occur, the impacts may alter surface properties, and, in particular, affect the surface activity. An example of this is the “negative grinding” phenomenon (see, for example Jimbo et al. [12]); they show that after grinding for a long period of time, the surface of the particles become activated to the point that agglomeration occurs and further grinding will actually cause the average particle size to increase. Another is the “mechanical activation” of solid surfaces (Boldyrev [1]) by which chemical reaction rates are enhanced by mechanical preprocessing. To further understand these phenomena requires some understanding of the forces that a particle experiences. These are largely unknown (Isherwood [11]) in real systems due to the complexity of making such a measurement. Many rheological studies, (e.g. Campbell [3], Campbell and Gong [8], Savage and Sayed [13], Hanes and Inman [9]) have studied the average stresses generated within a shearing granular mass, both by direct measurement and by computer simulation. Immersed in that data is information about the average forces that a particle experiences, but, unfortunately, it is the largest force, which may be many times the average force, that will do the most damage to the particles. Thus, it is the distribution of impulses, not the average values that are of importance here.

2 Computer simulation

Other than the statistics that are gathered, the simulation used for this study is identical to that used to make stress tensor measurements by Campbell [3]. Throughout the simulation, spherical particles (of mass \(m\) and radius \(R\)) are confined within a control volume of dimension \(L\) in the
x-direction, $H$ in the $y$-direction and $B$ in the $z$-direction, such as that shown schematically in Fig. 1. (Here and in the following discussion, the $x$-direction will refer to the direction of mean motion. The boundaries of the system generate a mean field velocity gradient in the $y$-direction. The $z$-direction refers to the out of the shear plane coordinate.) All of the sides of the control volume are bounded by "periodic" boundaries; as a particle passes through one periodic boundary it reenters its opposite number with exactly the same position and relative velocity with which it left. This type of boundary gets its name because it simulates a situation in which the control volume and its particles are periodically repeated, infinitely many times, upstream, downstream, above, below, and beside, the central control volume. This setup greatly enhances the computational efficiency of the simulation by permitting the simulation of an infinite volume while limiting the number of particles to the finite number initially placed in the control volume. It has the drawback that it is only applicable to flows with no gradients in the flow direction (i.e. steady, unidirectional flows). To impose a shear rate $\gamma = U/H$, the periodic images that bound the top and bottom of the control volume are set in motion with velocities $\frac{1}{2}U$ and $-\frac{1}{2}U$, respectively, in the $x$-direction. That is, when a particle exits the bottom of the central control volume, it reenters the top with its $x$-direction velocity increased by $U$ and a displaced $x$-coordinate that reflects the displacement of the origin of the moving periodic image. The opposite path is followed by particles that exit through the top of control volume. With this setup, uniformly shearing flows are assured. Most of the current work was performed on control volumes of 216 particles which were originally arranged in a $6 \times 6 \times 6$, (referring to the $x$, $y$ and $z$ directions) cubical array.
The particles interact by colliding with one another. Each collision is assumed to occur instantaneously once the particle surfaces come into contact — this is essentially the hard-sphere approximation often used in the kinetic theory of gases — and the collision result is computed from a standard center-of-mass collision solution. Because the particles rotate as well as translate, two conditions are required to close the system of equations: one for the relative particle velocities normal and one for the velocities tangential to the particle surfaces at contact. The normal velocity condition assumes that the particles are “nearly elastic” in the sense that energy is dissipated as a result of the collision but the particles retain their spherical shape. This is realized in the simulation through a coefficient of restitution, $\varepsilon$, ($\varepsilon < 1$), which is the ratio of the approach to recoil velocities, and is specified as an input parameter to the program. For the tangential condition, the particle surfaces are assumed to interact frictionally. The impulse $\mathbf{J}$, exerted by the collision may be divided into the contributions normal and tangential to the point of contact

$$\mathbf{J} = \mathbf{J}_N + \mathbf{J}_T.$$  

Here $\mathbf{J}_N$ represents the collisional impulse normal to the point of contact

$$\mathbf{J}_N = \frac{1}{2} \frac{m}{m(1+\varepsilon)} \left( \mathbf{q} \cdot \mathbf{k} \right) \mathbf{k},$$ \hspace{1cm} (2)

where $m$ is the mass of the particle, $\varepsilon$ is the coefficient of restitution, $\mathbf{q} = \mathbf{u}_1 - \mathbf{u}_2$ is the relative velocity of the particles just before collision, and $\mathbf{k} = (x_2 - x_1)/\|x_2 - x_1\|$ is the unit vector pointing along the line connecting the particle centers at the instant of collision. (Here, $x_1$ and $x_2$ are vectors pointing from the origin to the centers of particles 1 and 2 respectively and $\mathbf{u}_1$ and $\mathbf{u}_2$ are the translational velocities of the particles immediately prior to collision.) $\mathbf{J}_T$ is the impulse tangential to the point of contact and is computed in a two-step process to incorporate a surface friction coefficient. First of all, the impulse is computed assuming that there would be no tangential slip between the particle surfaces. This test case will be called $\mathbf{J}_T'$ and is defined as

$$\mathbf{J}_T' = \frac{m\beta}{2(1+\beta)} \left( \mathbf{q} - (\mathbf{q} \cdot \mathbf{k}) \mathbf{k} + R(\omega_1 + \omega_2) \times \mathbf{k} \right),$$ \hspace{1cm} (3)

where $\omega_1$ and $\omega_2$ are the particle angular rotation rates, $\beta$ is the ratio of the square of the particle radius of gyration to the square of the particle radius. The value of $\|\mathbf{J}_T'\|$ is then compared against the value computed for $\|\mathbf{J}_N\|$ to see if the ratio exceeds a specified surface friction coefficient $\mu$. If the surface friction is not exceeded, then there will be no slip between the particle surfaces and $\mathbf{J}_T$ is set equal to $\mathbf{J}_T'$. I.e.

$$\text{if} \quad \frac{\|\mathbf{J}_T'\|}{\|\mathbf{J}_N\|} < \mu \quad \text{then} \quad \mathbf{J}_T = \mathbf{J}_T'. \hspace{1cm} (4)$$

However, if $\mu$ is exceeded the tangential impulse is set to have a magnitude of $\mu\|\mathbf{J}_N\|$ in the direction of $\mathbf{J}_T'$. I.e.

$$\text{if} \quad \frac{\|\mathbf{J}_T'\|}{\|\mathbf{J}_N\|} > \mu \quad \text{then} \quad \mathbf{J}_T = \mu\|\mathbf{J}_N\| \frac{\mathbf{J}_T'}{\|\mathbf{J}_T'\|}. \hspace{1cm} (5)$$

Most of these simulations were run using a value of $\mu = 0.5$.

After the initial configuration and velocities of the particles and boundaries are chosen, the simulation is allowed to proceed as it will, with no outside intervention, until it converges to a steady state. (For these simulations, a converged state was assumed to occur when the total system kinetic energy achieves nearly constant values. However, like all small thermodynamic
systems, the kinetic energy will fluctuate slightly with time, making the determination of convergence somewhat difficult.) Starting from the initial state, convergence was achieved after as little as 500 collisions per particle for most of these simulations, although they were typically run for over 1100 collisions per particle before statistics were gathered. The averaging period covered at least 8000 collisions per particle, but for some cases, at large concentrations where collisions are frequent, it was extended to as much as 40000 collisions per particle.

3 Impulses and impulse distributions

There are two attributes of a granular shear flow that can account for the relative velocity between particles which, in turn, determine the strength of the impact. The first is the shear flow itself. Imagine two particles that move with exactly the mean velocity expected from their location within the shear flow. An impact can occur between the particles whenever their centers are less than a particle diameter (2R) apart and thus have a maximum shear flow induced relative velocity of 2Rγ, where γ is the shear rate. Note that this mechanism only generates relative velocity in the direction of the mean flow (the x-direction). But the actual velocity of particles will in most cases deviate from the mean in a random, fluctuating manner. This is reflected in the “granular temperature” T, which is defined as the mean square magnitude of the fluctuating particle velocities; the temperature is, itself, generated by particle collisions and is, thus, in some sense, also related to the shear rate. Now there are also two mechanisms that lead to the generation of the granular temperature. The first is directly related to collisions as any collision between particles — even two particles that initially move with exactly the mean velocities appropriate to their positions — will result in the generation of random components of velocity. The direction of the velocity change depends on the geometry of the collision and will, thus, in the large, be randomly distributed. The second mode of temperature generation is, itself, a byproduct of the random particle velocities. Following its random path, a particle moving parallel to the local velocity gradient will pick up an apparently random velocity that is roughly equal to the difference in the mean velocity between its present location and the point of its last collision. Note that, like the first mode of temperature generation, the magnitude of the random velocities so generated will also be proportional to the local velocity gradient. However, unlike the collisional temperature generation, this “streaming” mechanism can only generate one component of random velocity — the component that lies in the direction perpendicular to the mean velocity gradient (which, in this case, is the x-direction). Consequently, the granular temperature will be anisotropic with its largest component in the direction of mean motion. (This may be clearly seen in the results of Campbell [3]).

As the collisions between particles dissipate energy, the granular temperature cannot be self-sustaining. Thus, the energy of the random motion can only come from the mean motion — that is, from the imposed shear flow — through the mechanisms described in the last paragraph. One can imagine an internal energy flow beginning with the energy of the imposed motion; part of that energy is converted to granular temperature through the mechanism of shear work only to eventually be dissipated away to real heat by the inelasticity of the collisions. (For more details on the energy flow patterns, see the discussion in the review article by Campbell [4].) Thus, one expects some relationship between the granular temperature and the shear rate. This is represented by the dimensionless parameter S, which is plotted in Fig. 2 and defined as

\[ S = \frac{2R\gamma}{T^{1/2}}. \]
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II

\[ A = o \]

\[ 0 \]

\[ o \]

7

\[ \frac{2R^2}{T} \]

\[ \epsilon = 0.4 \]

\[ \epsilon = 0.6 \]

\[ \epsilon = 0.8 \]

\[ \epsilon = 1.0 \]

Fig. 2. The parameter $S$, plotted as a function of the solid fraction $\nu$

(Note: The temperature, $T$, is defined as the mean square average of the fluctuating velocity components: $T = \langle u'u' \rangle$. In this paper, it includes only the translational components of the random velocity and not the rotational components.) One obvious feature of this curve is that the larger the coefficient of restitution $\epsilon$, the smaller the value of $S$, indicating a larger relative value of the granular temperature. This reflects the fact that the larger the coefficient of restitution, the smaller the rate of dissipation of the energy associated with the random particle velocities. Also, for small values of the solid fraction $\nu$, the value of $S$ is small, indicating that the granular temperature $T$ is large compared to $(2R^2) T$; but for most of the range of the solid fraction $S$ is of order one, indicating that the two are of the same magnitude. The rapid decline in $S$ as $\nu \rightarrow 0$, can be understood as follows: As mentioned before, the granular temperature is a result of shear work, which, in the simple shear configuration, is represented by $\tau_{xy}$. At such low densities the shear stress is generated by the “streaming mechanism”, (see [3], [4], [8]) in which the shear stress takes the form of a Reynolds' stress, $\tau_{xy} = q \langle u'u' \rangle$, where $q = \rho \nu$ is the local density, (here $\rho$ is the density of the solid material) and $\langle u'u' \rangle$ is the average of the fluctuating velocity components in the $x$- and $y$-directions respectively. Thus, the generation of granular temperature is proportional to the solid fraction $\nu$. Now, the dissipation of granular temperature is proportional to the collision rate, which, in turn, is proportional to the probability of finding two particles in contact. At small concentrations when the position of one particle has an insignificant effect of the position of any other, the probability of finding a particle at any location is proportional to $\nu$ and, consequently, the probability of finding two particles in contact is proportional to $\nu^2$. As a result, the ratio of generation to dissipation of granular temperature is proportional to $1/\nu$ and goes to infinity as $\nu \rightarrow 0$. Thus, the granular temperature must asymptote to infinity as the solid fraction is reduced, and, consequently, $S \rightarrow 0$ as $\nu \rightarrow 0$. This is clearly the case for the data plotted in Fig. 2. The lowest concentration points plotted here correspond to $\nu = 0.005$, indicating that the asymptote to zero occurs very rapidly. (Note that this behaviour is a byproduct of the assumption that the only energy dissipation comes about from the inelasticity of the particles. Any other dissipation mechanism, such as drag from an interstitial fluid, would severely curtail this asymptotic behavior.) The upshot of this is that, at small concentrations, the greatest
contribution to the relative velocity and, consequently, to the impulses between particles at collision will result from the granular temperature. However, at moderate to large densities — like those commonly found in a granular flow — the relative velocities due to the shear rate and the granular temperature will be of roughly the same magnitude.

The collision impulse $J$ has the units of momentum. As the mechanisms that lead to the relative velocity between particles ultimately depend on the shear rate $\gamma$, it seems reasonable to use $\gamma$ to scale the impulse. Consequently, it seems logical to present the following data in dimensionless form as

$$\frac{J}{mR\gamma}$$

where $J = ||J||$ is the scalar magnitude of the vector impulse $J$. Simple dimensional analysis indicates that the scaled impulse should be a function only of the solid fraction $\nu$, and the material properties represented by the coefficient of restitution $e$, and the coefficient of friction $\mu$.

Figure 3 shows histograms of the scaled collision impulse. The distributions were taken from a large array, each element of which contains the fraction of collisions which fell into a small range of scaled impulse strength. Separate distributions were calculated for the total impulse $J$, its normal component $J_N$, and tangential component $J_T$, all of which are drawn in each plot. The data was separated in this fashion because the two mechanisms may lead to different modes of

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**Fig. 3.** Histograms of the normal, tangential and total collision impulses for $e = 0.8$, $\mu = 0.5$. a $\nu = 0.56$, b $\nu = 0.35$, c $\nu = 0.15$, d $\nu = 0.05$
particle damage. In particular the normal impulse may tend to cause large scale fracture of the particles while the tangential impulse may lead to an abrasive shearing of the microroughness on the surface of the particle. These particular distributions were taken from simulations with particle properties $\varepsilon = 0.8$ and $\mu = 0.5$. Notice that, throughout, the tangential impulse is significantly smaller than the normal impulse. In fact, the tangential impulse becomes such a large tight peak confined to the lower end of the impulse distribution, that it is plotted at one quarter its actual magnitude.

The principle feature of this figure is that the scaled impulses are not randomly distributed but are highly peaked. However, the peaks become shallower and much wider as the solid fraction is reduced. As the mean shear flow cannot generate a relative velocity greater than $2R_\gamma$, the normal impulse attributable directly to the velocity gradient cannot exceed $m(1 + \varepsilon)R_\gamma$ (as given by Eq. 2). As all of the plots shown in Fig. 3 correspond to $\varepsilon = 0.8$, the impulses attributable to that mechanism conceivably can cover the range from $J/mR_\gamma = 0$ to 1.8. However, the impulses generated by the granular temperature is not so confined and it has long been known (Campbell [2], Campbell and Brennen [6]) that the magnitude of the random particle velocities roughly obeys a Maxwellian velocity distribution based on the granular temperature. Consequently, there is a non-zero probability that the random particle velocities may be many times that which can be attributed to the mean velocity gradient and any values of $J/mR_\gamma$ larger than 1.8 must be attributed to the random components of velocity. Note that the most probable impact strength lies within the range attributable to the velocity gradient for any concentration greater than

![Fig. 4](image.png)

Fig. 4. Histograms of the normal, tangential and total collision impulses for $\varepsilon = 0.8$, $\mu = 0.35$. a $\mu = 0.1$, b $\mu = 0.2$, c $\mu = 0.5$, d $\mu = \infty$
\(v = 0.15\). However, at the lowest concentrations studied, the scaled impulse is typically much larger than 1.8 and, consequently, must be a byproduct of the granular temperature. This is consistent with the plot of \(S\) shown in Fig. 2 which shows that the granular temperature may be many orders of magnitude larger than the shear rate at small concentrations. The form of the histograms shown in Fig. 3 can now be understood in terms of these arguments. At large concentrations, the granular temperature is roughly of the same magnitude as \((R/T)^2\) and, consequently, the histograms show tight peaks near the lower values of the scaled impulse, while, at the lower concentrations, the granular temperature is large compared to the shear rate so that the scaled impulses are widely distributed.

Figure 4 shows similar histograms for various values of the surface friction coefficient \(\mu\). Changing \(\mu\) will only directly affect the tangential impulses, but, as friction is a dissipation mechanism, it will also have an indirect effect on the magnitude of the granular temperature. Still, one might expect that, as the tangential impulse is only a small fraction of the whole, changing \(\mu\) will have a minimal effect on the total impulse. At \(\mu = 0.1\), the tangential impulse is a tall narrow peak centered around small impulse levels and the normal and total impulse distributions overlay one another almost exactly. Increasing \(\mu\) causes the peak for the tangential impulse to become shorter and broader and the normal impulse becomes noticeably different from the total impulse. Note for future reference that there is little difference between the \(\mu = 0.5\) and \(\mu = \infty\) histograms.

Remember, however, that this work was performed with an eye towards the fracture problem and that it is the largest impulses that will do the most damage, not the most probable. Consequently, the most important part of the histograms are the large impulse tails as particle fracture can largely be attributed to the collisions between particles whose random velocities lie at the extreme ends of the velocity distribution. With this in mind, Fig. 5 shows the scaled magnitudes of the maximum particle impulses. Three separate plots are shown for the normal, tangential and complete contributions to the impulse. The values plotted in Fig. 5 correspond to the largest magnitudes of the collision impulses experienced during the averaging period of each simulation. However, the maximum impulses are somewhat ill-defined quantities. As the impulses are statistically distributed, they could, theoretically, approach infinity with a vanishing probability. Thus, the more samples that are taken, the larger the values of the maximum impulse that is likely to be experienced and, consequently, the values of the maximum impulse become dependent on the period over which statistics are taken. It makes sense, then, to define the values of the impulse in a statistical manner. To this end, Fig. 6 shows the corresponding values of “99.99%” impulses; i.e. 99.99% of collisions fall below the plotted values which, then, are exceeded by those exerted in only 1 in 10000 collisions. These values are determined by integrating along the impulse histograms. Consequently, relative to the maximum impulses, the 99.99% values are better defined measures of the largest impulse strengths in the sense that increasing the sampling period will not substantially change the measured values. However, precision in the determination of the value is attained at the expense of some arbitrariness in the choice of the limit — i.e. why 99.99% and not 99% or 99.999%. The 99.99% choice was made to be representative of the largest impulses as was felt to be possible without sacrificing reasonable statistical accuracy of the results. Now the averaging period of the results shown here encompasses anywhere from 2000000 to 10000000 collisions with most cases lying in the range of 5000000 collisions. This means that anywhere from 200 to 1000 collisions have impulses that exceed the 99.99% criterion, which should provide a reasonable evaluation of the value of the limit. Any higher value, say 99.999%, would cut these values by a factor of ten and introduce additional uncertainty in the result. It was on this basis that the choice of the 99.99% limit was, still somewhat arbitrarily, made.
Fig. 5. The distribution of the maximum impulses as a function of the solid fraction, $v$ for various values of the coefficients of restitution $\epsilon$: a normal, b tangential and c total impulses.
Fig. 6. The distribution of the 99.99% impulses as a function of the solid fraction \( \nu \) for various values of the coefficients of restitution \( \varepsilon \); (a) normal, (b) tangential and (c) total impulses.
Fig. 7. The distribution of the 99.99% impulses as a function of the solid fraction \( \nu \) for various values of the surface friction coefficients \( \mu \); a normal, b tangential and c total impulses.
The maximum impulses shown in Fig. 5 differ from the 99.99% impulses plotted in Fig. 6 by factors of 3 to 10. Still both sets of data show many of the same general features. Collectively and individually, they demonstrate the effect of the granular temperature on the impulse. All the data asymptotes to infinity very rapidly as $v \to 0$, reflecting the asymptotically increasing granular temperatures and are all relatively independent of $v$ at moderate concentrations. This latter point should be expected as the values of $S$, shown in Fig. 2, indicate that the ratio of the shear rate to the granular temperature does not change with $v$ except at the smallest concentrations. The maximum impulses can be attributed to the largest relative velocity of the particles, which, in turn, are related to the square root of the granular temperature and should be proportional to the shear rate. Thus, one expects that the dimensionless impulses plotted in Fig. 5 should be independent of $v$ at the larger concentrations as the shear rate dependence has already been scaled out. The slight drop in the impulse at the largest values of the solid fraction can be attributed to the particles becoming trapped in a crystalline microstructure. (The microstructure development will be made apparent in the next section.) The other notable feature in these figures is the strong dependence on the coefficient of restitution $\epsilon$. Changing $\epsilon$ from 0.4 to 1.0 causes a variation in the impulses that ranges from at least a factor of two to at most a factor of ten. This is, again, a reflection of the fact that the granular temperature is the primary driving force behind the impulse. As the impulse attributable to the shear rate varies as $1 + \epsilon$, the maximum corresponding variation is limited by the range of coefficients of restitution $(0.4 < \epsilon < 1.0)$ to maximum variation by a factor of $(1 + 1.0)/(1 + 0.4) \approx 1.4$, much smaller than is apparent in any figure. However, as the dissipation rate of the granular temperature is strongly dependent on the coefficient of restitution, increasing $\epsilon$ has a strong effect on $T$. This is apparent in the behaviour of the factor $S$ plotted in Fig. 2. Consequently, the larger $\epsilon$, the larger the granular temperature and the larger the corresponding collision impulses. Thus, it is the effect of $\epsilon$ on the dissipation of granular temperature, not its direct effect on the collision impulse, that determines the magnitudes of the largest impulses.

A much weaker effect is attributable to the surface friction coefficient $\mu$. Varying $\mu$ has two effects. First of all, the larger the friction coefficient, the larger the tangential impulse that can be transmitted between the particle surfaces during a collision; but as the coefficient of friction only places a limit on the ratio of tangential to normal impulses that can be exchanged, it has a rather complicated effect on the actual value of the tangential impulse. Figure 7 shows the 99.99% impulses exerted as a function of $\mu$. A single coefficient of restitution, $\epsilon = 0.8$, was used for all of this data. Since Figs. 3 and 4 indicate that the tangential impulse is such a small fraction of the total, one would expect that changing the friction coefficient would have only a very weak effect on the total impulse and, indeed, that appears to be the case. The only instance in which an effect of the coefficient of friction might be expected is in the tangential component. Again, this is true, but probably to lesser extent than many would have anticipated. Notice that there is essentially no difference between the $\mu = 0.5$ and the $\mu = \infty$ data. (Similar observations have been made previously in measurements of the stress tensor in a uniform shear flow and this has led many, including myself, to argue that $\mu = \infty$ is a good model for reasonable values of the surface friction. However, Campbell [5] shows that this is not the case near flat solid boundaries and there may be other instances for which such an assumption also breaks down.)

4 Angular distribution of collision impulses

In a shear flow, one does not expect impacts to be evenly distributed over the surface of the particles. This is illustrated, schematically, in Fig. 8. Due to the velocity gradient, one might anticipate that a particle is most likely to collide with faster moving particles from behind and
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Fig. 8. An illustration of the collision geometry and its relation to the shear flow

above or with slower moving particles from below and in front. Thus, if one imagines a cut through the vertical center of a sphere, as shown in Fig. 8, one expects a preference for collisions in the second and fourth quadrants, i.e. in the range of $\pi/2 \leq \theta \leq \pi$ and $3\pi/2 \leq \theta \leq 2\pi$. It is easy to see that there is a simple symmetry in this problem as, in a collision between two particles, one particle experiences the collision at an angle $\theta$ and the other at an angle $\pi + \theta$. Consequently, it makes sense to exploit this symmetry and to fold the first and third, and the second and fourth, quadrants over one another when presenting the results. Note that this restricts the applicable range of the angle $\phi$ to $-\pi/2 < \phi < \pi/2$. The dependence on $\phi$ is also somewhat complicated because of the velocity gradient in the $y$-direction. The case discussed above corresponds to $\phi = 0$, in which, changing $\theta$ rotates the contact point through the plane $z = 0$ and, consequently, through values of $-R \leq y \leq R$; as the velocity gradient points in the $y$-direction, this movement brings corresponding changes in the mean flow velocity. However, at $\phi = \pi/2$, changing $\theta$ only moves the contact point around the plane $y = 0$ with no corresponding change in the mean flow velocity. Thus, at $\phi = \pm \pi/2$, one expects no shear flow induced preference for values of $\theta$. Note, however, that this effect is symmetric about $\phi = 0$ so that one expects the same behaviour at $+\phi$ as at $-\phi$. Consequently, it also makes sense to exploit this symmetry by presenting the results plotted against the absolute value of $\phi$, which lies in the range $0 \leq |\phi| \leq \pi/2$. (For simplicity, $\phi$ will be used to represent $|\phi|$ from now on.)

During the course of this investigation, the simulation compiled information on the spatial distribution of the collisions and the impulses they exerted. This is accomplished by dividing the range, $0 \leq \theta \leq \pi$ into 50 segments and the range $0 \leq \phi \leq \pi/2$ into 25 segments, yielding a $25 \times 50$ array into which the various statistics are assembled. The quantities sampled include the collision frequency distribution and the maximum and average values of the total, normal and tangential collision impulses. The collision frequency represents the probability that a collision will occur at a given angular position. This is calculated by counting the number of collisions that occur
Fig. 9. The geometrical distribution of collisions about a particle for $\epsilon = 0.8$, $\mu = 0.5$ and $\nu = 0.25$. a Collision frequency distribution, b maximum impulse distribution, c average impulse distributions
within each angular range and scaling the result by dividing by the number of collisions and the surface area associated with each element. The maximum impulse distributions were collected by simply storing the maximum values that occurred in each element. The average impulse distributions are assembled by separately summing the impulses and accumulating the number of collisions that occurred within each element so that the average impulse may be found as the ratio of these two values.

One further note should be made about the following figures. The important point here is the spatial distribution of impulses and their absolute magnitudes are not terribly important. Thus, they were plotted using autoscaling on the vertical coordinate which maximizes the spatial resolution, but with the consequence that the span of the vertical scale is arbitrary. Thus, the reader should be aware that it is the shape of the figures that is emphasized here, and should not draw inferences from the apparent relative magnitudes of different plots.

As a point of reference, consider Fig. 9. Plotted here are (a) the collision frequency distribution, (b) the distribution of maximum impulses and (c) the distribution of average impulses for $\varepsilon = 0.8$, $\mu = 0.5$ and $v = 0.25$. Figure 9a demonstrates the features described in the first paragraph of this section. Along the $\phi = 0$ face, one can clearly see an almost sinusoidal shape of the distribution, reflecting the shear induced preference for collisions in the range $\pi/2 \leq \theta \leq \pi$ over those in the range $0 \leq \theta \leq \pi/2$. Furthermore, the distributions appears nearly uniform along the $\phi = \pi/2$ face, just as was anticipated. While these features are reflected in the distribution of the maximum total impulses shown in Fig. 9b, it is very difficult to discern any features because of the highly spiked nature of the surface. This is an unfortunate side effect of plotting the maximum impulse which, as it reflects unlikely collisions far out the tail of the probability distribution, may show a wide variation between neighboring elements along the surface. It is much easier to discern the details in the average distributions shown in Fig. 9c. There the effect of the mean shear flow on the applied impulse can be clearly seen along the $\phi = 0$ face in mimicry of its effect on the collision frequency distribution. Thinking back to Fig. 8, one can see that the portion of the collision impulse that can be ascribed to mean shear flow, drives particles together and strengthens these impulse in the second and fourth quadrants ($\pi/2 \leq \theta \leq \pi$), and, at the same time, drives particles apart and weakens the impulse in the first and third quadrants ($0 \leq \theta \leq \pi$) — precisely as seen in Fig. 9c. At the same time, the effect of the shear rate is much weaker on the collision impulse than on the collision frequency which is an indication that the average impulse is strongly influenced by the randomly distributed granular temperature. Furthermore, as with the collision frequency, the effect of the shear rate disappears as $\phi \to \pi/2$, and the average impulse becomes uniformly distributed with $\theta$.

Figures 10–14 show the collision frequency and the distribution of the average values of the total and tangential impulses for $v = 0.56$, 0.50, 0.35, 0.15 and 0.005. All were computed for the material properties $\varepsilon = 0.8$, $\mu = 0.5$. The maximum impulse values are not shown — even though these would be most important in determining particle fracture — as it is simply too difficult to discern important features in figures such as 9b. Also, it would be too difficult to try and evaluate a quantity according to some criterion — like the 99.99% criterion in the last section — as this would require computing a histogram for each of the surface elements, which would, in turn, require that a histogram be determined for each element and, thus, require tremendous simulation times and extraordinary computer resources to realize a statistically significant number of samples in each element. Instead, the average values are plotted as they are well defined and relatively easy to compute. The distribution of normal impulses was also assessed, but is not plotted since it does not differ substantially from the total impulse (as would be expected from the results in the last section).
Figure 10 shows these distributions for a large concentration, \( v = 0.56 \). Here, the mean separation of particle centers is 2.05 particle radii and the particles are nearly in perpetual contact. The particles are locked into a crystalline microstructure which permits them to maintain a fluid-like shear flow at a concentration at which, if the positions of particles were randomly distributed, they would most likely exhibit solid behavior. In this case, the particles are arranged in lines oriented parallel to the direction of mean motion (the \( x \)-direction) and these lines are distributed in a hexagonal pattern so that the immediate neighbors of a given line are distributed in the \( y - z \) plane at intervals of \( \pi/3 \). As a result, the shear flow may be maintained by the relative motion of lines of particles rather than individual particles. Please note that this microstructure did not occur naturally; instead, it corresponds to the manner in which the particles are initially loaded into the control volume. However, it is clearly a stable structure as the particles do not break out of their initial configuration. It should be pointed out that this may not be the only possible microstructure that the particles might assume, but it is much the same as has been observed by Heyes [10] in molecular dynamics models of shearing fluids and it is the only one that I can think of that will permit a shear flow at such a large concentration. One effect of this microstructure development is that the possible angles for collisions between particles becomes restricted by the precise arrangement of their neighbors. These ideas are reflected in the collision frequency distribution plotted in Fig. 10a. In this case one expects collision between a particle and other particles within its own string; these are represented by the large probability of collisions at \( \theta = 0 \) or \( \theta = \pi \). Collisions will also occur with particles in neighboring strings which should be restricted to small regions about the relative positions of the strings. Remember that the strings are positioned at intervals of \( \pi/3 \). Relative to \( \phi = 0 \), strings may be found at \( \phi = \pi/6, \pi/2, 5\pi/6, 7\pi/6, 3\pi/2 \) and \( 11\pi/6 \). Using the symmetries of the problem, those collisions from the strings at \( \pi/2 \) and \( 3\pi/2 \) map onto the twin peaked structure at \( \phi = \pi/2 \) and the others map onto the peak at \( \phi = \pi/6 \). Thus, one can see how the microstructure is reflected in the strongly restricted regions at which collisions are possible. An interesting feature is the saddleback peak at \( \phi = \pi/2 \). At this angle, changing \( \theta \) only rotates the contact point through the plane at \( y = 0 \) for which the velocity gradient has no effect on the relative velocity of the particles and cannot affect the collisional distribution; consequently, whatever leads to the twin peaks must arise as a byproduct of the granular temperature. But, remember that the “streaming” mode of temperature generation only contributes to random motion in the \( x \)-direction — although the mechanism must be very weak at such a large concentration where the freedom of particle motion is so limited. Yet, such an anisotropy would tend to lead to an increased collision rate, slightly on either side of the \( \theta = \pi/2 \) plane of the sphere and could account for the observed saddleback distribution.

At such large concentrations, the distribution of collision impulses shown in Fig. 10b does not follow the same pattern as the collision frequency distribution. Remember, however, that these are the average values of the impulses that occur at a given location and are not directly related to the number of collisions that occur there (as is the collision frequency). In this case, the collision frequency is bound by the microstructure and not significantly affected by the velocity distributions, while the average impulse depends only on the velocity distribution and is affected by the microstructure only by the restrictions it places on the geometry of collisions (and through any indirect effect on the velocity distribution). The shape of the collision island at the center of the figure, surrounding \( \phi = \pi/6 \), shows much larger impulses exerted toward the larger values of \( \theta \), reflecting the effect of the velocity gradient expected from the mechanism illustrated in Fig. 8. But this does not carry over to collisions at \( \theta = 0 \) and \( \pi \) which correspond to collisions within a particle’s own string. For those collisions, all the particles involved occupy roughly the same position within the velocity gradient and move with much the same mean velocity. There, the
Fig. 10. The geometrical distribution of collisions about a particle for $\epsilon = 0.8$, $\mu = 0.5$ and $v = 0.56$. a Collision frequency distribution, b average impulse distributions, c average tangential impulse distribution.
Fig. 11. The geometrical distribution of collisions about a particle for $e = 0.8$, $\mu = 0.5$ and $\nu = 0.50$. a Collision frequency distribution, b average impulse distributions, c average tangential impulse distribution.
Fig. 12. The geometrical distribution of collisions about a particle for $e = 0.8$, $\mu = 0.5$ and $v = 0.35$. 

a) Collision frequency distribution, 
b) average impulse distributions, 
c) average tangential impulse distribution
Fig. 13. The geometrical distribution of collisions about a particle for $\phi = 0.8$, $\mu = 0.5$ and $v = 0.15$. a Collision frequency distribution, b average impulse distributions, c average tangential impulse distribution
Fig. 14. The geometrical distribution of collisions about a particle for $\varepsilon = 0.8$, $\mu = 0.5$ and $\nu = 0.005$. a Collision frequency distribution, b average impulse distributions, c average tangential impulse distribution
Fig. 15. The geometrical distribution of the components of the tangential impulse across the surface of a particle. **a** Impulse $J^{\text{lin}}_{\text{tang}}$ due to the relative linear velocities of the particle, **b** impulse $J^{\text{rot}}_{\text{tang}}$ due to the rotational velocity of the particles. **a1, b1** $v = 0.56$, **a2, b2** $v = 0.35$, **a3, b3** $v = 0.05$
collision impulse is controlled solely by the magnitude of the granular temperature. The same can be said of the small central ridge at $\phi = \pi/2$ and explains why the collision impulses there are independent of $\theta$ and are not controlled by the velocity gradient. (Note, in compiling the average impulse figures, only those surface elements within which more than 50 collisions occurred were used in the figure; to eliminate statistical noise, the rest were set to zero. This significantly clarifies the picture by eliminating elements with too few collisions to obtain a proper average. The effects of an insufficient number of collisions can still be seen in the spiked regions that form the outer edges of the collision islands in Fig. 10b. These spikes should be interpreted as scatter due to averages over a small sample size and are not an indication of some unexplained internal flow phenomenon.)

As the concentration is reduced, the effect of the microstructure disappears and gives way to conditions, such as those shown in Fig. 8, in which both the collision distribution and the collision impulse are controlled by the flowfield. The appearance of the microstructure is still apparent at $v = 0.50$ in Fig. 11, but has disappeared completely by $v = 0.35$ shown in Fig. 12 at which point the collision distribution and average impulses have assumed all of the attributes described in the discussion surrounding Fig. 9. In Figs. 13 and 14, where the concentration is further reduced to $v = 0.15$ and beyond, one might notice the distributions becoming flatter on the right face of the distributions. Remember that the almost sinusoidal behavior of the right face is attributable to the relative velocities between particles that are induced by the velocity gradient. Thus, the observed behavior may be understood as different values of $\theta$ correspond to different values of the shear induced relative velocity, $u = \gamma y = R\gamma \sin \theta \cos \phi$. The flattening of the distributions indicates that the velocity gradient is becoming less important relative to the randomly distributed granular temperature in determining the relative velocity of the particles at collision. This should have been anticipated from the plot of $S$ versus $v$ in Fig. 2 which indicates that, as the solids concentration becomes small, the granular temperature is much larger than the relative velocity induced by the shear rate.

Examining the tangential components of the collision impulse in Figs. 12–14 shows that, for the most part, it is evenly distributed over the surface of the particle. The only recognizable feature is a small peak around $\theta = \pi/2$. This, again, may be attributed to the velocity gradient. In that context, a collision at $\theta = \pi/2$ indicates a glancing blow across the edge of the particle. If the relative velocity between the particle surfaces were wholly due to the mean velocity field, such a blow would transmit the maximum tangential impulse. But such a small peak indicates that the velocity gradient is not the major contributor to the tangential collision impulse. This is true regardless of concentration and thus cannot be a result of the randomly distributed granular temperature, as it holds at large concentrations where Fig. 2 indicates that $2R\gamma$ and $T^{1/2}$ are of the same magnitude. The only remaining explanation is that the majority of the tangential impulse arises from the relative surface velocities induced by particle rotation. The mean rotational velocity of particles in a simple shear flow is roughly one half the shear rate, regardless of the particle position (this has long been known to be the case for almost any shear flow and was demonstrated explicitly for granular flows by Campbell [3]). Thus, the rotationally induced impulses so induced will be independent of the angular position and is clearly the dominant effect in the tangential impulse figures. Note that the tangential impulse $J_{T\theta}$ given by Eq. (3) can be decomposed into the portion due to the relative linear particle velocities tangential to the point of contact

$$J_{T\theta} = \frac{m \beta}{2(1 + \beta)} (q - (q \cdot k) k)$$  (8)
and that due to the particle rotation

\[ J_{T\omega} = \frac{m\beta}{2(1 + \beta)} R(\omega_1 + \omega_2) \times k. \]

Plots of these two contributions are shown in Fig. 15. Again, the autoscaling feature has been employed in making these plots so that they show the maximum spatial resolution, but with the consequence that all the vertical scales are different. Examining these plots verifies the speculation that the centrally located peak previously seen in the average tangential impulse distributions arises from the relative tangential linear velocities while the — usually more important — impulses contributed by the rotational velocity are uniformly distributed. It is a bit surprising that the tangential \( J_{T\omega} \) impulse plotted in Fig. 15a3 is so tightly peaked at \( v = 0.05 \) where one would expect that the relative velocity induced by the velocity gradient is insignificant compared to the granular temperature. The explanation lies in the anisotropy of the temperature distribution that, due to the streaming mode of temperature generation, favors random motion in the \( x \)-direction. Relative velocity in the \( x \)-direction will induce the largest tangential impulses around \( \theta = \pi/2 \), just as it is apparent in the figure. However, as this is a byproduct of the temperature and not the velocity gradient, it should be independent of the relative \( y \)-coordinate of the colliding particles, which in the spherical coordinates used here, means that the tangential impulse should be independent of \( \phi \) — just as is apparent in Fig. 15a3.

5 Conclusions

This was a first attempt to try and understand attrition and fracture of particles in the light of flow-induced interparticle forces. The data was compiled from a discrete particle computer simulation of a granular flow of spheres undergoing simple shear — the simplest possible flowfield. The collision impulses are related to the relative velocities, both normal and tangential to the point of impact. The results show that the impulses scale with the shear rate \( \gamma \), although this scaling reflects the contribution of two mechanisms. First of all is the direct effect of the velocity gradient, which induces relative velocity between particles as a consequence of differing locations within the mean velocity field. The rest of the collision impulse may be attributed to the granular temperature — the random, almost thermal, particle velocities which are themselves a result of the mean velocity field. (The relationship between the granular temperature and the shear rate is quantified by the parameter \( S \), shown in Fig. 2.) However, the random particle velocities are statistical quantities that are distributed in a nearly Maxwellian manner. Consequently, the largest impulses, which lead to the largest degree of particle damage, can only be attributed to that small fraction of particle velocities that lie far out on the tail of the velocity distribution. Several representative histograms were presented for the collision impulses as well as plots that showed the dependence of the largest impulses as a function of concentration and material properties. Due to the relationship between the collision impulse and the granular temperature, the largest impulses occur at small densities when the granular temperature is the largest.

Finally, the angular distribution of collision impulse about a particle reflects the contributions of the granular temperature and the velocity gradient and, in addition, the effect of an internal microstructure that affects the angular distribution of contacts. The effects of the microstructure disappear at concentrations below \( v = 0.50 \), leaving the velocity gradient and temperature as the only sources of anisotropy. Below \( v = 0.15 \), the granular temperature grows
exponentially, and, only then, do the collisions take on spatially uniform characteristics. Interestingly, the tangential impulses are largely by products of the relative tangential velocities induced by particle rotation.

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