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Monte Carlo Analysis of Polydisperse Microparticle Impacts with Surfaces

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ABSTRACT. The Monte Carlo method was applied to an impact model to investigate the impact of polydisperse microparticles with surfaces. The Monte Carlo results were compared to experiments. Two different situations were examined: the normal (90°) impact of microspheres with a molecularly-smooth silicon surface, and the oblique (< 90°) impact of microspheres with a *Formica* surface. In the former, the percentage of microspheres captured by the surface and the overall capture velocity distribution were determined given the statistical distribution of the microsphere diameters. In the latter, both the *Formica* surface roughness angles and the diameters of the microspheres were treated as statistical variables. The mean values of the Monte Carlo simulation of the coefficient of restitution and the impulse ratio were found to agree with the data at the 95% confidence level. Finally, this approach was applied to model the impact of *Lycopodium* spores with a *Formica* surface.

INTRODUCTION

Many practical situations involve the impact of microparticles with surfaces, such as airborne spores with room ceilings, walls, furniture surfaces, and filters. Such problems, however, are difficult to model because the microparticles are not uniform in size and the surfaces of both the microparticle and the substrate are not perfectly smooth. Further, little definitive empirical information such as capture velocity and capture percentage of microparticle impacts with surfaces is available. This paper describes how the Monte Carlo method used in conjunction with an empirically-verified microparticle impact model can be applied successfully to predict the impact response of microparticles with typical indoor surfaces.

Microparticle impact with surfaces has been studied both theoretically and empirically over the past 30 years. Experiments originally considered the impact of monodisperse (i.e., having one diameter) microspheres with smooth surfaces (Dahneke 1971). Since then, a variety of results have been reported including complicated conditions such as bioaerosols contacting biological surfaces (Paw U 1983). Existing theoretical impact models developed to date have been primarily those involving monodisperse microspheres and perfectly-smooth surfaces. Few attempts have been conducted so far

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to simulate effects of surface irregularities on impact response, although Dunn et al. (1996) have analyzed the significant influence of surface roughness on the coefficient of restitution.

Initially, the normal impact of monodisperse microspheres with smooth surfaces was studied by Dahneke (1971). His experiments suggested that below a critical incoming velocity, a.k.a. the "capture velocity," the microspheres did not rebound from the surface after the impact. Wall et al. (1990) examined particle size effects on the capture velocity. Their experimental results showed that for the same materials, the smaller the microsphere diameter, the larger the capture velocity. Li et al. (1999) investigated the impact of polydisperse (i.e., having different diameters) microspheres with ultra-smooth silicon surfaces. Their observations also indicated that particle size affects capture velocity.

An empirical model to predict monodisperse microsphere impact with surfaces also was introduced by Dahneke (1971) based on the conservation of energy using a coefficient of restitution. Rogers and Reed (1984) assumed that the energy loss was due to the plastic deformation at the center of contact. Applications of the Rogers and Reed model by Wall et al. (1990) resulted in an adhesion energy higher than expected. Brach and Dunn (1995) presented two models to simulate the microsphere impact problem. Both models were based on Newton's second law, one in the form of momentum the other using differential equations. The latter treats energy loss as dissipation due to adhesion hysteresis. The former is algebraic and is based on rigid body mechanics. All these models consider an impact of a single microsphere and a smooth surface and treat impacts in a deterministic fashion.

Analyzing the complex situation of polydisperse microparticle impact with a rough surface requires a somewhat different approach. The microparticle diameter and the incident trajectory angle relative to the surface normal are not deterministic. The true angle of incidence is expressed as a deviation from the apparent flat surface by a local surface angle, which is obtained from a sampled surface height database. Thus, variations in microparticle size and surface roughness angle require a statistical model for those practical impact situations.

In this paper, first the Monte Carlo method is applied to simulate the statistical characteristics of normal impact of polydisperse microspheres with rough surfaces. Experimentally measured normal impact data reported by Li et al. (1999) is used for comparison with the modeling results. Their experiments were conducted with polydisperse microspheres and molecularly-smooth silicon surfaces. The microsphere diameter distribution used in the Monte Carlo simulations is either Gaussian or empirical. The Monte Carlo simulation results show that the percentage of capture varies with incoming velocity and the larger the microparticle diameter, the smaller the capture velocity.

The Monte Carlo approach then is applied to simulate microparticle oblique impact with a *Formica* surface and then is compared to the corresponding experimental results. A method to characterize the surface roughness is proposed and the results are used in the Monte Carlo simulation. Both of the microparticle diameter and true angle of incidence are treated as statistical variables. The resulting distribution of the coefficient of restitution and the impulse ratio vary with apparent angle of incidence are found to agree well with the experimental data. Finally, the Monte Carlo approach is used to investigate roughness of both the microparticle and the substrate surfaces. For this situation, the Monte Carlo simulations are compared with the experimental results of *Lycopodium* spores impacting a *Formica* surface.

MODELING APPROACH

Rigid Body Model

The impact mechanics used in this Monte Carlo analysis were described in the rigid body model proposed by Brach and Dunn (1995, 1998). The term *rigid body* denotes the presence of rotational inertia (in contrast to a point mass) and does not imply inflexibility. This approach

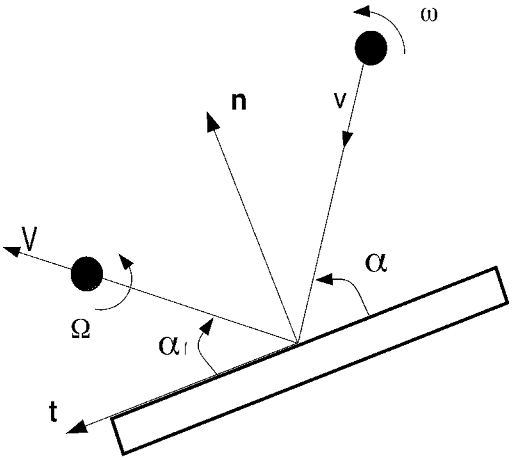

FIGURE 1. The definition of velocity components and angles of impact.

simplifies the analysis in that the rigid body model is based on algebraic equations and coefficients that govern collisions. For an impact event as depicted in Figure 1, the final normal and tangential velocity components (upper case symbols) can be determined from the initial velocity components (lower case symbols) and the coefficients R, ρ, and μ for planar impacts:

$$V_n = -R(1-\rho)v_n \tag{1}$$

and

$$V_t = v_t - \mu[1 + R(1-\rho)]v_n, \tag{2}$$

where R is the coefficient of restitution for internal material dissipation in the absence of adhesion and ρ is the adhesion coefficient (adhesion is negligible at high initial velocities and/or large diameters) with values ranging from 0 to 1 ($\rho = 0$ for no adhesion effects and $\rho = 1$ for capture). The ratio of the final rebound normal speed to the initial normal speed is the overall coefficient of restitution e, where $e = R(1-\rho) = -V_n/v_n$.

For a sphere, the impulse ratio, $\mu = (V_t - v_t)/(V_n - v_n)$, is determined from the motion status when it leaves the surface at the end of contact. If it is rolling without sliding at the end of contact, μ is equal to its critical value, μ_0, which is

$$\mu_0 = \frac{2\eta}{7[1 + R(1-\rho)]}, \tag{3}$$

where $\eta = (v_t - r\omega)/v_n$. If the particle is sliding at the end of contact, μ is equal to Coulomb's coefficient of friction. Previous studies have shown that coefficients R and ρ are not constants (Brach and Dunn 1998). Both coefficients are highly dependent on initial normal velocity, particle diameter, and material properties. To provide a practical, engineering model, the empirical equation for these coefficients are

$$R = \frac{k_1^p}{k_1^p + |v_n|^p}, \tag{4}$$

$$\rho = \frac{k_2^q}{k_2^q + |v_n - v_c|^q}. \tag{5}$$

The quantities k_1, k_2, p, q, and v_c are determined either empirically or from theoretical models. The quantity v_c is the capture velocity. The available experimental results suggest that these quantities depend on particle diameter, material properties, etc. Thus, they change from one application to another (Brach and Dunn 1998). For simplicity, in the present model it is assumed that $q = p = 1$. Thus, the overall coefficient of restitution is

$$e = \frac{k_1}{k_1 + |v_n|}\left(1 - \frac{k_2}{k_2 + |v_n - v_c|}\right). \tag{6}$$

In this paper, k_1, k_2, and v_c are obtained from a least-square regression analysis of the numerical simulations reported in Li et al. (1999).

Microparticle Size Distribution

One input variable in the Monte Carlo analysis is the diameter distribution of the micropsheres. In the actual Monte Carlo code, the diameter distribution can be either normal, log-normal, uniform, or empirical. In the present study, empirical diameter distributions were gathered using a Phase Doppler Particle Analyzer for three different distributions of polydisperse stainless-steel microspheres. These were SST65 (nominal

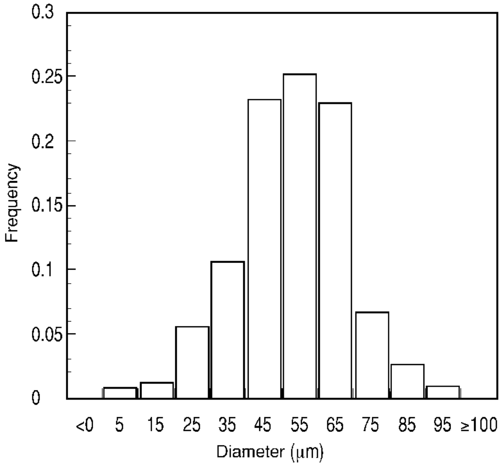

FIGURE 2. The frequency diameter distribution of SST65 microspheres.

diameter range from 10 to 65 μm), SST 76 (nominal diameter range from 10 to 65 μm), and SST125 (nominal diameter range from 64 to 76 μm). The frequency distribution of the SST65 microspheres is shown in Figure 2. Each diameter distribution was compared to a Gaussian distribution using a χ^2 analysis. From this it was determined that the SST65 distribution can be represented satisfactorily by a Gaussian distribution with a mean diameter of 52.8 μm and a standard deviation of 15.3 μm. For the other two cases, their empirical distributions were used because they deviated significantly from a Gaussian distribution.

Surface Roughness Characterization

Surface roughness can be considered as a local variation in the slope of the surface. Any variation in the local surface angle leads to an actual or true surface angle that differs from the apparent surface angle, as illustrated in Figure 3. This subsequently can lead to anomalous values of the impact parameters e and μ calculated from the experimental data. However, such local surface angle variations can be incorporated into the rigid body model using the angle ϕ, shown in Figure 3.

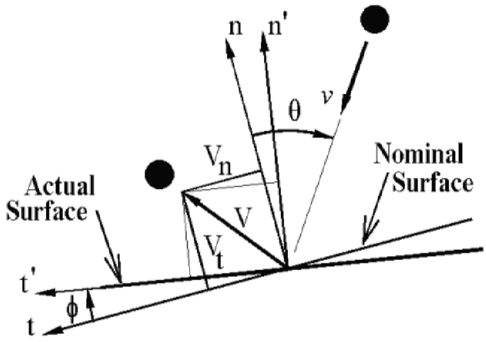

FIGURE 3. Coordinate systems of actual (n', t') and nominal (n, t) surfaces.

The values of the velocity components for the nominal coordinates can be expressed by those for the actual coordinates through the following matrix transformation:

$$\begin{pmatrix} v_n \\ v_t \\ V_n \\ V_t \end{pmatrix} = \begin{pmatrix} \cos\phi & \sin\phi & 0 & 0 \\ -\sin\phi & \cos\phi & 0 & 0 \\ 0 & 0 & \cos\phi & \sin\phi \\ 0 & 0 & -\sin\phi & \cos\phi \end{pmatrix} \times \begin{pmatrix} v_{n'} \\ v_{t'} \\ V_{n'} \\ V_{t'} \end{pmatrix}. \quad \textbf{(7)}$$

Thus, the measured (apparent) coefficient of restitution, e_m, and the impulse ratio, μ_m, are represented by

$$e_m = \frac{e - \tan\phi (V_{t'}/v_{n'})}{1 + \tan\phi (v_{t'}/v_{n'})}, \quad \textbf{(8)}$$

$$\mu_m = \frac{\mu - \tan\phi}{\mu \tan\phi + 1}. \quad \textbf{(9)}$$

In this study, the surface roughness angle, ϕ, was computed from the digitized surface profile data obtained by actual surface scans. The surface height data for a *Formica* surface was taken using a Surtronics 3+ profilometer. Ten scans at different locations on the surface were taken and all the data were combined together into one data file. For each scan, the scan length was set at 4 mm and the maximum amplitude at

150 μm, which was the highest possible value for this device. For each 1 μm of scan length, two data points of surface height were recorded. As a result, there were 8,000 points for each scan and 80,000 points total.

In order to determine the local surface roughness angle, the contact diameter was used as the horizontal scale length. For SST76 microspheres, the contact diameter was assumed to be 20 μm, which was estimated from the Hertzian contact mechanics equation $a^2 = rn$, where n is the particle's vertical mass center displacement, r its undeformed radius, and a its contact radius. Then, the surface roughness height was averaged within each 20 μm length, and the roughness angle for each 20 μm segment was determined as $\phi = \arctan(\bar{H}/200,000)$, where $\bar{H}$ was the average roughness height in Å. A code was written using MATLAB to determine the surface roughness angle distribution and its statistical parameters, such as the average roughness angle and standard deviation. It is important to note that this approach implicitly involves two major assumptions: that the surface roughness features on the order of the length scale of the microsphere's contact diameter primarily determine the microsphere's macroscopic response characteristics (rebound angle, etc.) and that average values of the involved quantites (e.g., microsphere contact diameter and surface roughness height) are sufficient to describe the process. The assumptions are somewhat arbitrary and justified mainly by their utility.

The empirical probability density function of the roughness surface angle is shown in Figure 4. A data file of 4,000 surface roughness angles was generated by random selection from this distribution for use in the Monte Carlo simulation.

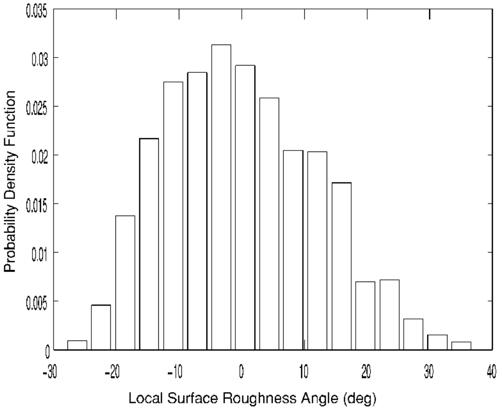

FIGURE 4. Empirical probability density function of the local surface angles of a *Formica* surface.

Monte Carlo Approach

Two empirical distributions already have been described: the microsphere diameter distribution and the surface roughness angle distribution. Another distribution that can arise in impact experiments is the microsphere's incident velocity distribution. In the normal impact experiments conducted by Li et al. (1999), the measured initial velocity variations were found to be small ($< \pm 10\%$ from the mean value). Thus, in this study, the incident velocity is treated as a constant and the surface roughness angle and the diameter of the microsphere are treated as statistical variables. All other parameters are treated as single-valued, which include the nominal incident angle and those parameters dependent on the microsphere diameter, such as k_1, k_2, and v_c.

The quantities k_1, k_2, and v_c depend on the diameter, material properties, and other factors. Usually, k_1, k_2, and v_c are obtained from least-squares regression analysis of empirical measurements. In this paper, the three quantities are obtained for different diameters using numerical simulations of normal impact as reported by Li et al. (1999). The least-squares regression analysis fit is used to express how k_1, k_2, and v_c vary with diameter. These functions are assumed to be the same for normal and oblique impact in the following simulations.

After determining the relations of the above three quantities with the particle diameter and specifying the distributions of the statistical variables, such as microsphere diameter and surface roughness angle, the Monte Carlo simulation can be carried out. Before the Monte Carlo approach was used, a convergence study was carried out to find out how many simulation points were necessary to get satisfactory outcomes. The capture percentage was chosen as a criterion. It was found that the percentage of capture beyond 4,000 simulations was constant to within ±3%. So, in the following studies, 4000 simulation points were chosen.

APPLICATION TO NORMAL IMPACT ONTO A MOLECULARLY-SMOOTH SURFACE

The Monte Carlo method was applied to study two normal (90°) impact cases of different diameter distribution microspheres with a molecularly-smooth silicon surface. The simulations were compared with the experimental results given by Li et al. (1999) for the SST65 and SST125 distributions. In their experiments, it was observed that the coefficient of restitution decreased with the decreasing of the initial normal velocity. In fact, the value of e decreased dramatically as $v_n \rightarrow v_c$. Although the approximate capture velocity can be determined, information such as the percentage of capture could not be obtained because it was beyond the capability of the experimental setup. However, using the Monte Carlo simulation, it is possible to determine the capture velocity and the percentage of capture for polydisperse microspheres.

The Monte Carlo results of the SST65 case are compared in Figure 5 with the experimental data, where the solid line denotes the Monte Carlo predictions. It is seen that the values of the coefficient of restitution generally agree for most of the normal impact velocity ranges. In this and subsequent figures presented in this paper, each symbol represents the average of 40–50 individual measurements and the error bars denote experimental uncertainty with 95% confidence. Because each data point constitutes a relatively small sample which probably is not normally distributed, some differences between the Monte Carlo simulation should be expected. The capture percentage is shown in the lower graph of Figure 5. It is seen that at 50% of capture, the corresponding normal velocity is approximately 0.20 m/s. This is the nominal value at which the particles were observed to begin to accumulate on the substrate surface, as reported in Li et al. (1999). It is seen that capture is reached suddenly as the normal velocity decreases. Likewise, the capture percentage increases very quickly as the impact velocity decreases to the capture value.

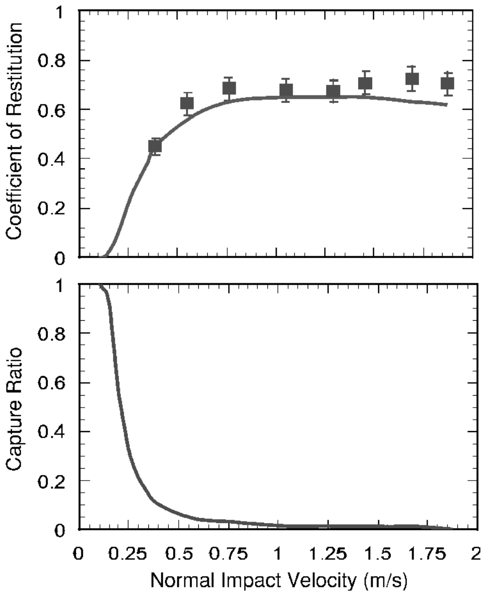

FIGURE 5. Results from Monte Carlo simulations of normal microsphere impact (SST65).

The simulations of the impact of SST125 microspheres are compared with the experimental results in Figure 6. Agreement between the empirical and predicted coefficient of restitution values are similar to those of the previous case. At 50% of capture, the critical velocity is approximately 0.13 m/s. This is less than the critical velocity of the SST65 case. These results, although they are not supported by actual measurements of the critical velocity, support the thesis of larger-diameter microparticles having smaller capture velocities.

APPLICATION TO OBLIQUE IMPACT ONTO A ROUGH SURFACE

To apply the Monte Carlo approach to simulate microsphere impact with a *Formica* surface, the parameters k_1, k_2, and v_c needed to be determined first. Ideally, these parameters should

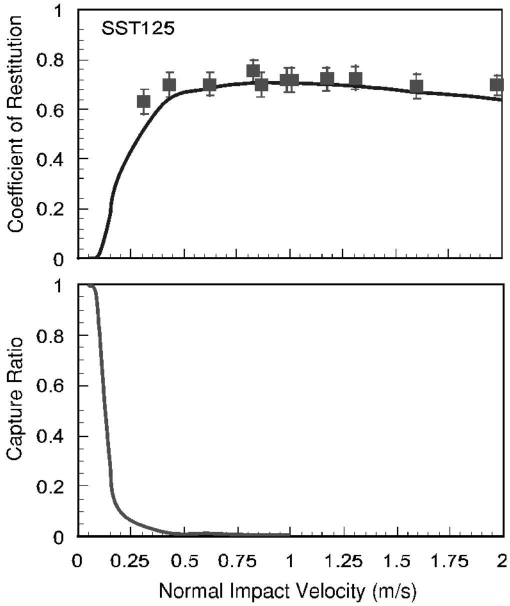

FIGURE 6. Results from Monte Carlo simulations of normal microsphere impact (SST125).

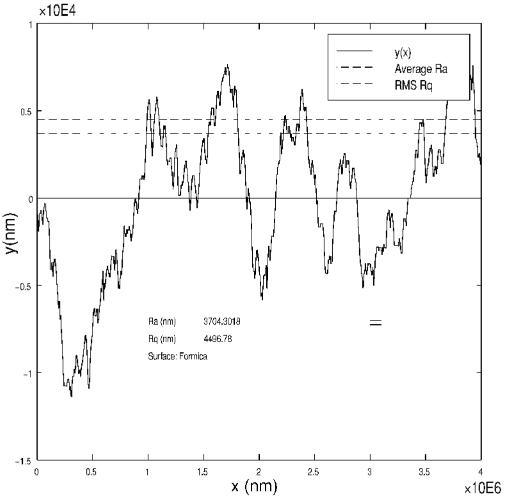

FIGURE 7. A surface profile of *Formica* substrate (note different scales for each axis).

be determined from the least-squares regression analysis of the results of the microsphere impact with a molecularly-smooth *Formica* surface. However, no experimental data are available for this case. Thus, for the purpose of this study, the behaviors of the three quantities, k_1, k_2, and v_c, with diameter were assumed to be the same as those used in the simulation of microsphere normal impact with silicon surface. This approach required that the coefficient of restitution values needed to be adjusted to compensate for initial differences due to the different material properties of Formica and silicon. This was accomplished by simply subtracting the coefficient of restitution values for each of the two cases by the respective values at the highest incident angle examined (here 85°). This results in what is termed the relative coefficient of restitution.

An example surface scan of the *Formica* surface is shown in Figure 7. The data from this particular scan and other similar ones were used to determine the local surface angle probability density function presented in Figure 4. This particular scan revealed that the standard deviation of surface height was approximately 45 μm, which was larger than the contact diameter of a SST76 microsphere (approximately 20 μm). In the Monte Carlo simulation, the SST76 microsphere diameter and the surface roughness angle were chosen as the statistical variables. Equations (7)–(9) were incorporated into the Monte Carlo analysis to calculate the apparent coefficient of restitution and apparent impulse ratio.

Some results of the Monte Carlo calculations are presented in Figure 8. The solid line represents the impact coefficients obtained using the surface roughness angle shown in Figure 4 and the diameter distribution of the SST76 microspheres shown in Figure 2. The dashed line in Figure 8 is a Monte Carlo simulation of the molecularly-smooth surface case using only the diameter distribution. Experimental data are plotted in the figure as open squares. It is seen that the calculations follow the data very well. From approximately 90° down to 45°, the molecularly-smooth and rough surface cases are similar. Below 45°, they differ. As the incident angle is decreased, the relative coefficient of restitution for the rough surface increases toward unity, whereas for the molecularly-smooth surface decreases due to the effects of adhesion. Impulse ratio values for the rough surface case

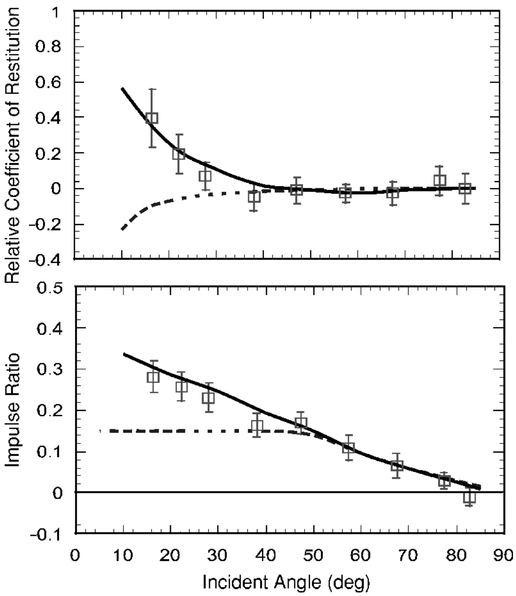

FIGURE 8. Monte Carlo simulations compared with experimental results. (Dashed line: simulations without considering roughness effects; solid line: simulations with roughness effects).

never become constant with decreasing incident angle, whereas for the molecularly-smooth surface case, they become constant and equal to 0.15. (Note that in this and subsequent figures, negative values of μ given by Equation 3 are plotted according to convention.)

The resulting frequency distributions of e_m and μ_m for apparent incident angles of 10° and 85° are shown in Figures 9 and 10, respectively. As shown in those figures, the shapes of the frequency distributions of e_m for both angles are asymmetric and similar. This asymmetry comes from the smaller diameter microspheres travelling at slightly lower incident velocities, where the effects of adhesion are more significant and result in relatively lower values of e_m. This asymmetry remains throughout all incident angles for the same reason. The shape of the frequency distribution of μ_m at 85° is relatively symmetric about zero, as expected. However, as the incident angle is lowered, the μ_m distribution becomes asymmetric. This asymmetry results from the "shadow" effect of the positive local surface angles, which skews the distribution and becomes more prevalent as the incident angle is lowered. That is, the microspheres began to "see" more and more of only those surfaces having negative local angles. For example, microspheres having an actual impulse ratio value equal to 0.3 that encounter a surface with a local angle of −20° will have an apparent impulse ratio value of 0.7 according to Equation (9). Similar arguments on the "shadow" effect by rough surfaces for larger particles at shallow impact angles have been developed independently by Sommerfeld and Huber (1999).

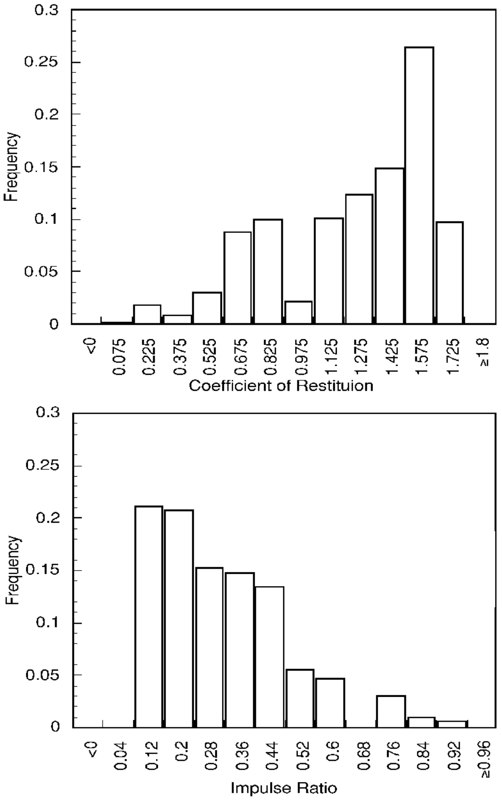

FIGURE 9. Frequency distribution of Monte Carlo results at apparent incident angle of 10°.

Thus, by considering variations in the microparticle diameter and the local slope of the surface, the Monte Carlo method can successfully predict the impact results of a rough surface. This also shows that the departure of

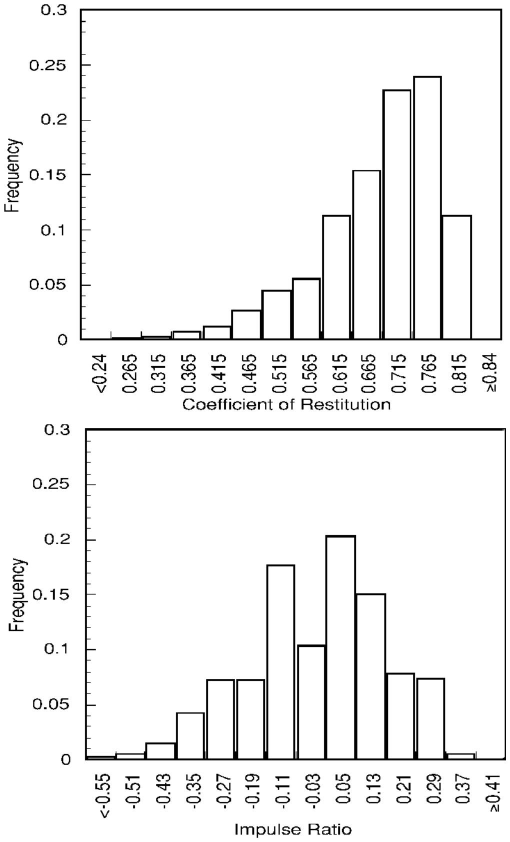

FIGURE 10. Frequency distribution of Monte Carlo results at apparent incident angle of 85°.

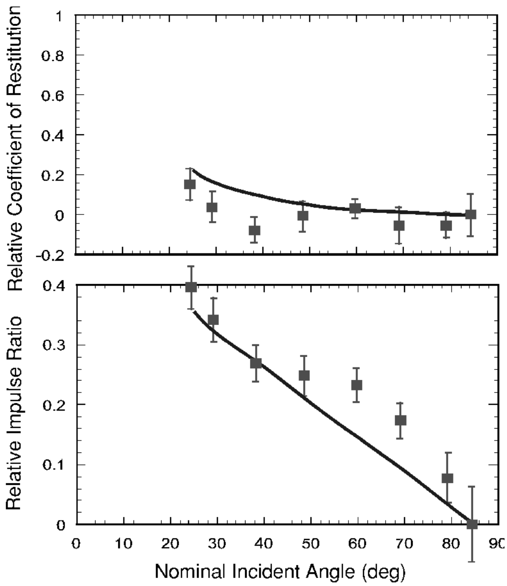

FIGURE 11. Monte Carlo simulations (solid line) and experimental results (solid squares).

experimental data from the ideal rigid body model can be attributed to surface roughness effects.

The Monte Carlo approach also can be applied to study more complex impact conditions. One example is the impact of *Lycopodium* spores on a *Formica* surface. In this case, both the surfaces of the microparticle and the substrate are rough. Scanning electron micrography of a *Lycopodium* spore (Li 1999) revealed its surface to be irregular and full of cavities and small peaks, hence making it virtually impossible to perform a surface roughness profile using conventional techniques. Because of this, for convenience only, the distribution of the spore surface roughness angle was assumed to be the same as that of the *Formica* surface and the size distribution of the *Lycopodium* spores was assumed to be normal with a mean diameter of 30 μm and a standard deviation of 1.7 μm.

The relative coefficient of restitution and the relative impulse ratio, $\mu_{\text{relative}} = \mu - \mu_{85°}$, from the Monte Carlo simulation are shown in Figure 11. Experimental data are represented by solid squares with 95% confidence level error bars. It can be seen that the trends of the simulation results follow the experimental results rather well, given the arbitrarily assumed distribution the spores' surface roughness angle. This simple approach does not fully model the microparticle's impact response. But it does suggest that this type of approach may be very suitable to model such complex impact situations, especially considering its ease in implementation.

CONCLUSIONS

The Monte Carlo approach was applied successfully to simulate both the normal and the oblique impact of microparticles onto substrate surfaces. For normal impacts, the Monte Carlo method was used to determine the percentage of microparticle capture by the substrate surface and the average capture velocity. The results showed that for a polydisperse microsphere normal impact with a molecularly-smooth surface, transition to capture occurs over a relatively narrow normal impact velocity range. Also, the capture velocity decreased with increasing microsphere diameter.

For oblique impacts, the Monte Carlo method was used to examine the effect of surface roughness. The simulation results for the impact of microspheres onto a rough *Formica* surface showed very good agreement with experimental results. Results verified that surface irregularities cause apparent, unrealistically high measured values of the coefficient of restitution and of the impulse ratio. This implies that attempts to measure impact coefficients at low angles of incidence using rough surfaces will be confounded. Further, asymmetry in the local surface roughness angle distribution led to asymmetries in the distributions of the apparent coefficient of restitution and the apparent impulse ratio. Extending the Monte Carlo approach to model the impact of *Lycopodium* spores with a *Formica* surface also proved to be reasonably successful.

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