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Granular Attrition as a Diffusion Phenomenon

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Introduction

Attrition of solid particles is a commonly encountered but usually undesirable occurrence in processes involving granular material. For example, attrition of particles in fluidization and pneumatic transport systems is an issue of considerable industrial concern and research efforts have been devoted to the understanding and quantification of this phenomenon. However, granular attrition is also a complex and poorly understood process for which no general theory currently exists. The most popular approach taken by a number of research workers in deriving theoretical models for granular attrition processes has been through the application of a chemical kinetics analogy. The success of this approach has been limited so far. Paramanathan and Bridgwater[1] reported that a simple first order kinetics model where the rate of disappearance of particles in a given size interval due to breakage is proportional to the weight of particles present gives limited agreement with experimental results. This was largely due to anomalously high initial attrition rates which cannot be satisfactorily accounted for by the model. They proposed a modified first order kinetics model with three parameters where the rate of attrition depends on the deviation from attrition at infinite strain. However, it was found that this three-parameter model was not suitable for describing attrition of some of the materials tested in their annular shear cell experiments and no significant benefits in terms of modeling accuracy could be obtained even at the expense of having an additional parameter in the model. They suggested that this might be due to inherent inaccuracies in the theory used. Ayazi Shamlou et al.[2] carried out experiments on attrition of soda glass beads in a gas-fluidized bed and proposed a model which states that the rate of attrition is first order with respect to the total initial mass of intact particles and about 0.8th order with respect to time. Cook et al.[3] performed attrition tests in a circulating fluidized bed and selected a second-order kinetics model as one which best fit their experimental data. The model may be interpreted to describe attrition as a process whose driving force is the deviation of the weight of solids remaining in a bed raised to the second power from the corresponding squared minimum weight required for attrition to become negligible. This minimum weight is generally a strong function of gas velocity and may also be dependent on material properties and other operating conditions and so has to be determined experimentally before the model may be used for making any theoretical predictions. Furthermore, the authors mentioned that the second-order kinetics model may only be applicable where elutriation of fines takes place, as in the experiments they conducted. The most successful and versatile model for describing granular attrition so far has been the empirical formulation due to Gwyn[4] which states that the weight fraction of particles attrited is proportional to the shear strain (or equivalently, time, under constant strain rate conditions) raised to a certain power. Bridgwater[5] found the formulation to be more satisfactory for describing attrition of high density polyethylene in an annular shear cell than a first-order kinetics model. Neil and Bridgwater[6, 7] also found the same formulation to describe well their experimental data for attrition of molecular sieve beads, heavy soda ash and tetra-acetyl-ethylene-diamine particles in various systems such as the annular shear cell, fluidized bed and screw pugmill. However, though mostly successful, the Gwyn formulation is not without limitations. Bridgwater[5] commented that Gwyn's formulation is incomplete in the sense that it implies an infinite initial attrition rate at zero shear strain and also allows the amount of attrited material to increase without bound at large strains. Ghadiri et al.[8] carried out annular shear cell experiments with porous silica catalyst beads and observed deviations of their experimental results from the Gwyn formulation under some operating conditions such as at high normal stress loads.

Theoretical models based on chemical kinetics analogies or their variants may be limited in their capabilities to describe granular attrition processes quantitatively. We have also verified during the initial phase of this study that models derived based on more complex kinetics than those mentioned to be inadequate as well. A general and coherent theory of granular attrition capable of unifying all experimental data collected to date using various types of material, systems and operating conditions is still lacking in the literature. Here, we propose a novel approach to the modeling of granular attrition by treating such processes as analogs to mass diffusion. The model derived is adequate for correlating with experimental data reported in the literature and numerical simulation results obtained in the present study. This may suggest similarities in statistical characteristics between granular attrition and diffusion of material. Further, we show that the present model exhibits correct asymptotic behaviors in contrast to the Gwyn formulation and may be a generalization of this empirical correlation.

Description of Model

During granular attrition, the weight fraction of large particles decreases while that of small particles increases. Weight fraction of particles shifts from large sizes towards smaller sizes and never in the opposite direction, much like the diffusion of material down a concentration gradient in the continuum sense. As such, we propose to treat the process of bulk granular attrition as the diffusion of weight fraction of granular materials in particle-size space:

$$\frac{\partial W}{\partial t} = D\frac{\partial^2 W}{\partial x^2} \tag{1}$$

where W(x, t) is the weight fraction of particles, t is attrition time, x is a dimensionless particle size defined as $\frac{d}{d_o}$, d_o and d are parameters characterizing the size of intact and attrited particles respectively and may be taken to be their diameters, D would be referred to as attrition diffusivity and may be interpreted to be a measure of the attritability of particles. The boundary conditions to be applied are W(0, t) = 0, W(1, t) = 1 and W(x, 0) = 0. The essential features include the requirements that no particle achieves zero size as a result of attrition at any point in time, a constant availability of intact particles and the absence of any attrited particles at the start of the attrition process. The corresponding solution to Eq. (1) may then be written as:

$$W = \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\left\{\exp\left[-(n\pi)^2 Dt\right]-1\right\}\sin(n\pi x) \tag{2}$$

The weight fraction of particles which has undergone attrition at time t, denoted W', is then the integral of W in the interval x = 0 to 1:

$$W' = \frac{4}{\pi^2} \sum_{\substack{n=1 \\ (n \text{ odd})}}^{\infty} \frac{1}{n^2} \left\{1 - \exp\left[-(n\pi)^2 Dt\right]\right\} \qquad (3)$$

Eq. (3) is correlated with experimental data reported in the literature for various types of systems, operating conditions and granular material using the attrition diffusivity as the fitting parameter. A physical interpretation of this parameter will then be proposed.

Numerical Simulation

In order to further substantiate the validity of the model proposed in this study, we have carried out computer simulations of granular attrition during pneumatic conveying around a sharp bend using the Discrete Element Method (DEM) originally developed by Cundall and Strack[9]. The computational model used combines DEM with Computational Fluid Dynamics (CFD) for modeling the fluid phase and Ghadiri's attrition model for simulating particle fragmentation or chipping based on inter-particle or particle-wall impact velocities. The equations in DEM governing the translational and rotational motions of individual solid particles are Newton's laws of motion:

$$m_i \frac{dv_i}{dt} = \sum_{j=1}^{N} \left(f_{c,ij} + f_{d,ij}\right) + m_i g + f_{f,i} \qquad (4)$$

$$I_i \frac{d\omega_i}{dt} = \sum_{j=1}^{N} T_{ij} \qquad (5)$$

where m_i and v_i are the mass and velocity of particle i, N is the number of particles in contact with this particle, $f_{c,ij}$ and $f_{d,ij}$ are the contact and viscous contact damping forces respectively, $f_{f,i}$ is the fluid drag force due to an interstitial fluid, I_i is the moment of inertia of particle i, ω_i is its angular velocity and T_{ij} is the torque arising from contact forces which will cause the particle to rotate. The normal ($f_{cn,ij}$, $f_{dn,ij}$) and tangential ($f_{ct,ij}$, $f_{dt,ij}$) components of the contact and damping forces are calculated according to a linear force-displacement model:

$$f_{cn,ij} = -\left(\kappa_{n,i}\delta_{n,ij}\right)n_i \qquad (6)$$

$$f_{ct,ij} = -\left(\kappa_{t,i}\delta_{t,ij}\right)t_i \qquad (7)$$

$$f_{dn,ij} = -\eta_{n,i}\left(v_r \cdot n_i\right)n_i \qquad (8)$$

$$f_{dt,ij} = -\eta_{t,i}\left[\left(v_r \cdot t_i\right)t_i + \left(\omega_i \times R_i - \omega_j \times R_j\right)\right] \qquad (9)$$

where $\kappa_{n,i}$, $\delta_{n,ij}$, n_i, $\eta_{n,i}$ and $\kappa_{t,i}$, $\delta_{t,ij}$, t_i, $\eta_{t,i}$ are the spring constants, displacements between particles, unit vectors and viscous contact damping coefficients in the normal and tangential directions respectively, v_r is the relative velocity between particles and R_i and R_j are the radii of particles i and j respectively. If $\left|f_{ct,ij}\right| > \left|f_{cn,ij}\right| \tan\phi + c$ then 'slippage' between the two contacting surfaces is simulated by a Coulomb-type friction law, $\left|f_{ct,ij}\right| = \left|f_{cn,ij}\right| \tan\phi + c$ where $\tan\phi$ is analogous to the coefficient of friction and c is a measure of cohesion between the two contacting surfaces.

The fluid drag force model due to Di Felice[10] which is applicable over a wide range of particle Reynolds numbers was used for evaluating the fluid drag force. The equations in this model include:

$$f_{f,i} = f_{f0,i}\varepsilon_i^{-\chi} \tag{10}$$

$$f_{f0,i} = 0.5c_{d0,i}\rho_f \pi R_i^2 |u_i - v_i|(u_i - v_i) \tag{11}$$

$$\chi = 3.7 - 0.65\exp\left[-\frac{(1.5 - \log_{10} Re_{p,i})^2}{2}\right] \tag{12}$$

$$c_{d0,i} = \left(0.63 + \frac{4.8}{Re_{p,i}^{0.5}}\right)^2 \tag{13}$$

$$Re_{p,i} = \frac{2\rho_f R_i |u_i - v_i|}{\mu_f} \tag{14}$$

where $f_{f0,i}$ is the fluid drag force on particle i in the absence of other particles, χ is an empirical parameter, ε_i is the local average porosity in the vicinity of particle i, $c_{d0,i}$ is the drag coefficient, $Re_{p,i}$ is the Reynolds number based on particle diameter, ρ_f is the fluid density, μ_f is the fluid viscosity and u_i is the fluid velocity.

The motion of the continuum gas phase is governed by the Navier-Stokes equations with interphase interactions taken into account as an additional source term in the momentum equation:

$$\frac{\partial \varepsilon}{\partial t} + \nabla \cdot (\varepsilon u) = 0 \tag{15}$$

$$\frac{\partial(\rho_f \varepsilon u)}{\partial t} + \nabla \cdot (\rho_f \varepsilon uu) = -\varepsilon \nabla P + \nabla \cdot (\mu_f \varepsilon \nabla u) + \rho_f \varepsilon g - F \tag{16}$$

where u is the velocity vector, ε is the local average porosity, P is the fluid pressure and F is the source term due to fluid-particle interaction.

The Ghadiri's attrition model accounts for two different mechanisms of attrition, namely chipping and fragmentation with the former occurring at impact velocities between 4 m s^{-1} and 13 m s^{-1} and the latter above 13 m s^{-1}. The respective equations for calculating particle sizes produced by the two mechanisms are:

$$d_s = \left(\alpha_f \frac{\rho_s H v_s^2 d_{so}^4}{K_c^2}\right)^{\frac{1}{3}} \tag{17}$$

$$(3 - \zeta')\ln\left(\frac{d_s}{d_{so}}\right) = \ln\lambda' + \zeta'\ln\left(\frac{\rho_s H v_s^2 d_{so}}{K_c^2}\right) \tag{18}$$

where α_f is a proportionality factor, d_s is the diameter of the smaller part of a particle after impact, d_{so} is the diameter of the mother particle before impact, H is the material hardness, v_s is the particle impact velocity, λ' and ζ' are parameters that are determined experimentally and K_c is the critical stress intensity factor. The various empirical parameters found in the model determine the sizes of particle fragments upon attrition while the occurrence of the attrition process itself depends only on the impact velocity. In the absence of experimental values for these parameters, arbitrary but reasonable values have been selected to simplify the equations to the following form[11]:

$$d_s = \left(2\times10^{-4}\rho_s v_s^2 d_{so}^4\right)^{\frac{1}{3}} \tag{19}$$

$$2\ln\left(\frac{d_s}{d_{so}}\right) = \ln\left(2\times10^{-4}\rho_s v_s^2 d_{so}\right) \tag{20}$$

The system geometry simulated consists of a 1.0 m vertical conveying pipe of diameter 0.04 m containing 1000 spherical particles with initial diameters of 2.8 mm. Periodic boundary conditions were applied to simulate an open flow system such that particles which were carried out of the conveying pipe by the flowing air were simulated to re-enter from the inlet of the pipe with the same velocities and radial positions. The flow of air and particles with application of periodic boundary conditions was carried out for 5 s of physical time during which the solid particles cycled through the pipe segment numerous times and reached a fully developed flow state. A sharp bend in the system was then simulated by the imposition of a wall at the upper end of the vertical pipe and the number of particle fragments formed upon collision and attrition at the wall was then recorded.

Results and Discussion

Figure 1(a) shows attrition data obtained by Paramanathan and Bridgwater[1, 12] using granular NaCl and molecular sieve beads as the granular material in an annular shear cell while 1(b) shows those reported by Ghadiri et al.[8] for porous silica catalyst particles in the same type of equipment. It may be seen that the present model has been successful in reproducing the attrition behavior in terms of the weight fraction of particles attrited at various times for these different types of granular material in an annular shear cell.

Attrition data obtained using gas-fluidized beds[2, 3] are compared with the model in Figures 2(a) and (b) respectively and good agreements are also observed. As mentioned previously, the attrition diffusivity D may be interpreted to be the propensity of particles to undergo attrition under the specific conditions applied. It shows larger magnitudes with increasing severity of the operating conditions used and may be functions of various system parameters. For example, continuing with the analogy between granular attrition and mass diffusion, D may be a function of granular temperature in a similar way that the mass diffusivity is a strong function of thermodynamic temperature. It may also be functions of other system parameters such as solid volume fraction, average particle velocity or material properties. The verification of this may be the subject of a subsequent study.

Similarly, attrition data obtained from the numerical simulations are compared with the model. Figure 3 shows the variation of the weight fraction of particles attrited with respect to time and the corresponding values calculated using Eq. (3). It may be observed that the time scale of the attrition process is different from those seen previously. In most physical experiments, attrition may be allowed to occur over long time intervals and to large extents while in the present DEM simulations, attrition due to the flow of granular materials around a sharp bend occurs over a very short time interval and results in smaller extents of breakage. However in all cases, good agreements are obtained between the experimental or simulation results and the proposed model.

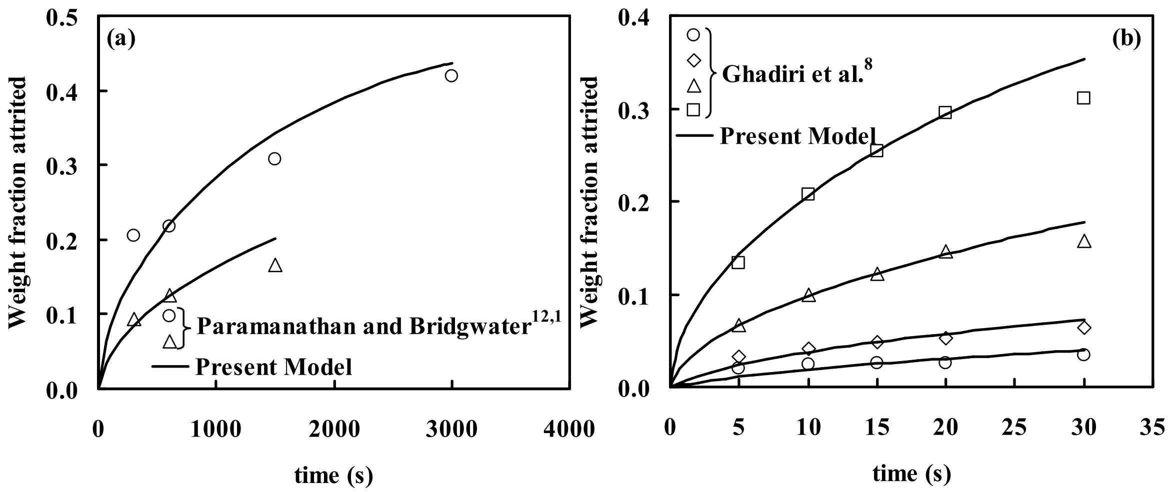

Figure 1. Comparisons of model with attrition data reported for experiments conducted using annular shear cells. The granular material used were (a) 1.7 – 2.0 mm sodium chloride granules[12] (D = 6.82×10^{-5} s^{-1}) and molecular sieve beads[1] (D = 2.36×10^{-5} s^{-1}) with a constant applied normal stress of 41 kPa and (b) 2.0 – 2.36 mm porous silica catalyst carrier beads[8] with varying applied normal stresses of 25 (○), 50 (◊), 100 (Δ) and 200 (□) kPa (D = 6.39×10^{-5}, 1.77×10^{-4}, 9.20×10^{-4}, 3.67×10^{-3} s^{-1} respectively).

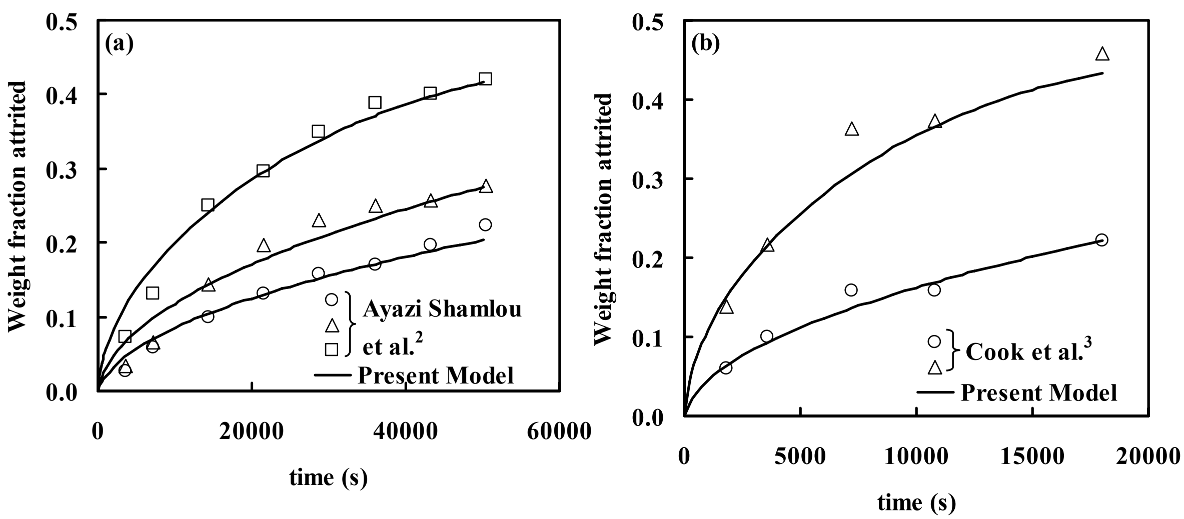

Figure 2. Comparisons of model with attrition data reported for experiments conducted using fluidized beds. The granular material used were (a) 2 mm agglomerate particles made up of 63 – 90 μm soda glass beads[2] with varying superficial gas velocities of 1.1 (○), 1.2 (Δ) and 1.3 (□) times the minimum fluidization velocity (D = 7.16×10^{-7}, 1.28×10^{-6}, 3.46×10^{-6} s^{-1}) and (b) 1764 μm lime sorbents in a circulating fluidized bed[3] with fluidizing velocities of 2 (○) and 4 (Δ) m s^{-1} (D = 2.33×10^{-6}, 1.11×10^{-5} s^{-1}).

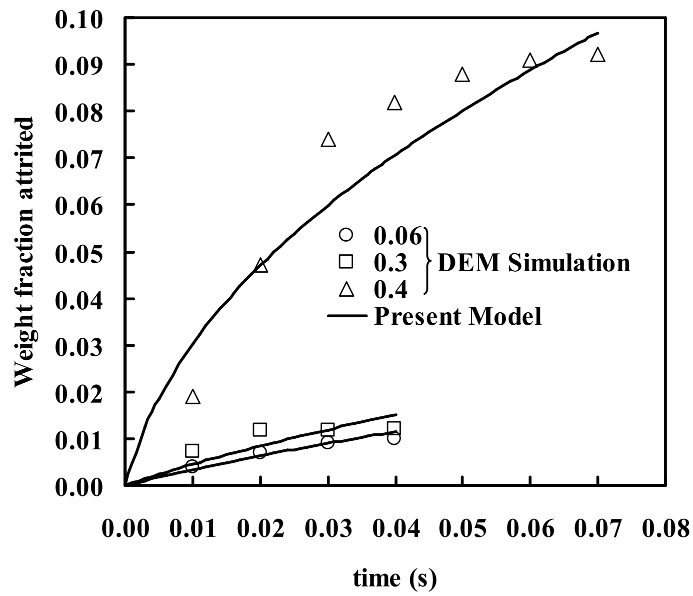

Figure 3. Comparisons of model with attrition data obtained from DEM simulations of pneumatic conveying around a sharp bend. The particles were simulated to have coefficients of restitution 0.06, 0.3 and 0.4 as indicated for the three cases studied respectively. The attrition diffusivities are 8.74×10^{-3}, 1.22×10^{-2} and 0.128 s^{-1} respectively.

A further analysis of the model presented in Eq. (3) will now be made to show a possible correspondence with the Gwyn formulation. We express the exponential term as a Taylor series and after some rearrangements, the resulting equation is written as:

$$W' = \sum_{\substack{n=1 \\ (n\ \text{odd})}}^{\infty} \sum_{m=1}^{\infty} K_{n,m} t^m \qquad (21)$$

where $K_{n,m} = \dfrac{4(-1)^{m+1}\left(n^2\pi^2\right)^{m-1} D^m}{m!}$. In comparison with the Gwyn formulation given by $W' = Kt^m$, it seems that the latter is one term from the infinite series in Eq. (21) or an averaged representation of it. As such, the present model may be a generalization of this empirical formulation. Eq. (3) also shows correct asymptotic behaviors with W' approaching the physically realistic value of 1.0 at large times. The Gwyn formulation, on the other hand, allows weight fraction to become larger than one and thereafter increase without bound as time approaches infinity.

Conclusions

In this paper, we have introduced a simple phenomenological model for bulk granular attrition derived based on a diffusion analogy to the process. We treat granular attrition as a process involving diffusion of the weight fraction of granular materials in a particle-size space. The behavior of the model compares well with experimental data reported in the literature for a wide variety of systems as well as DEM simulation results for attrition in pneumatic conveying about a sharp bend carried out in the present study. Attrition in the latter occurs over a much smaller time scale than those observed in physical experiments. Nevertheless, the model was found to be capable of reproducing the various attrition profiles observed. In addition, it exhibits correct asymptotic behaviors at large times and so is considered more sound than other empirical correlations. From the comparison with the well-established Gwyn correlation, it seems likely that the general success of such power-law type correlation may have arisen from the diffusion-like nature of attrition processes occurring in particle-size space. This suggests that a diffusion analogy for granular attrition may be a good starting point for further theoretical studies of such processes.

Acknowledgements
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