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The Particle-Particle Drag Term in a Multiparticle Model of Fluidization

Topical Report

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1.0 EXECUTIVE SUMMARY

The multiparticle model being developed at the U.S. Department of Energy's Morgantown Energy Technology Center (DOE/METC) simulates fluidization phenomena such as segregation, elutriation, and solids mixing by describing the different types of solid particles as distinct particulate phases. To account for the momentum transfer between the particulate phases due to collisions, the model requires constitutive relations known as particle-particle drag terms. In dilute systems, such as pneumatic conveyors, the particle-particle drag has been measured and empirical correlations have been developed. But similar measurements are not possible in dense systems, such as fluidized beds. Hence, an expression for the particle-particle drag term was derived based on the kinetic theory of dense gases. To test the accuracy of that expression, the predictions of the model were compared to experimental data. Yang and Keairns (1982) fluidized uniform mixtures of dolomite and acrylic particles for various times and measured the rate of separation of the dolomite particles. The dolomite particles, being heavier and larger than the acrylic particles, were found to settle rapidly. The experimental data suggest that the rate of settling is strongly dependent upon the particle-particle drag and, hence, the simulation of these experiments is useful for determining the accuracy of the particle-particle drag term. Computer simulations have shown that the model predicts the initial rate of separation reasonably well. The predicted equilibrium concentrations of dolomite particles in the upper layer of acrylic particles, however, do not agree with the experimental data. This is thought to be because of the absence of granular stress from the model. Further refinement of the particle-particle drag term will be sought only after including granular stress in the model.

2.0 INTRODUCTION

The multiparticle model of fluidization being developed at METC uses multiphase flow equations to describe the fluid and the particulates in a fluidized bed. The model can describe the flow of several different particulate phases, each particulate phase being composed of particles of identical densities and sizes. Because of this ability, the model can be used to study fluidization phenomena of practical importance, such as segregation, elutriation, and solids mixing.

The multiparticle model evolved from a single particulate phase model of Gidaspow and Ettehadieh (1983). Their equations can be generalized for more than one particulate phase to obtain the set of continuity and momentum equations presented in Table 1. In these equations, the subscript 'k' denotes the kth phase and ranges from 1 to N, N being the total number of phases. In addition to these equations, several constitutive relations are required to complete the model: The fluid-particle drag term, F_{1k} (subscript 1 denoting the fluid) in Equation 2, describes the momentum transfer between the fluid and the kth particulate phase. It has been the subject of many investigations (for example: Syamlal and O'Brien, 1987). Fortunately, in this case, accurate experiments can be conducted to determine the drag on a single spherical particle moving in a fluid, and these data can be generalized to obtain the drag on a cloud of particles. Alternatively, the drag can be calculated from empirical correlations, such as the Ergun (1952) equation, which give the pressure drop in a fluid flowing through a packed bed of particles.

Like the fluid-particle drag terms, particle-particle drag (PPD) terms need to be included in a multiparticle model. The term F_{kj} describes the

Table 1. Governing Equations of the Multiparticle Model

Continuity Equations:

$$\frac{\partial}{\partial t}(\varepsilon_k \rho_k) + \nabla \cdot (\varepsilon_k \rho_k v_k) = 0 \qquad (1)$$

Momentum Equations:

$$\frac{\partial}{\partial t}(\varepsilon_k \rho_k v_k) + \nabla \cdot (\varepsilon_k \rho_k v_k v_k) = -\varepsilon_k \nabla P - \varepsilon_k \nabla P_s + \varepsilon_k \rho_k g + \sum_{j=1}^{N} [F_{kj}(v_j - v_k)] \qquad (2)$$

momentum exchange between the kth and j^{th} particulate phases. Nakamura and Capes (1976) and Arastoopour, Lin, and Gidaspow (1980) found that it was necessary to introduce such a term to model the segregation in a pneumatic conveyor transporting a mixture of particles. Such a term will be even more important in dense systems, such as fluidized beds.

Arastoopour, Wang, and Weil (1982) attempted to measure PPD in a dilute system in which the void fraction was greater than 0.99. They measured the velocity of an isolated coarse particle flowing countercurrent to pneumatically-conveyed fine particles. The force exerted by the fine particles on the coarse particle was deduced from a steady-state momentum balance and correlated with the velocity difference between the fines and the coarse particles. From these experiments, they developed the correlation

$$F_{kj} = C_f \varepsilon_j \rho_j |v_k - v_j| / d_k$$

where the dimensionless constant $C_f = 0.7 d_k^{-0.146}$ (d_k in meters), subscript k denotes the coarse particles and subscript j denotes the fine particles. Arastoopour and Cutchin (1985) studied the cocurrent flow of coarse particles in a pneumatic conveyor of fine particles and reported another correlation for the

PPD. But similar measurements are not possible in dense systems, such as the fluidized beds.

Several theoretical expressions for the PPD term in a dilute system, which were derived using simple models of collision between two representative particles, are available in the literature (for example: Soo, 1967; Nakamura and Capes, 1976; Doss, Srinivasan, and Raptis, 1986). They differ from one another only by a numerical factor. Syamlal (1985) attempted a similar derivation of the PPD term for a dense bed. This resulted in an expression similar to that of Nakamura and Capes (1976), except for a multiplicative factor. Later in this report we will derive an expression for the PPD based on the kinetic theory of dense gases.

To gain confidence in such theoretical expressions, it is necessary to test their accuracy. This can be done by comparing the solutions of the multiparticle model to experimental data that are sensitive to the PPD. Settling experiments in fluidized beds are, in general, sensitive to the PPD. When a binary mixture of particles is fluidized, under certain conditions the denser and larger particles will settle. While settling, these particles continually interact with the upward-moving fine particles and, hence, the rate of settling strongly depends upon the PPD. Such data can be compared to the numerical solutions of the multiparticle model to determine the accuracy of the theoretical expressions for the PPD.

3.0 THE PARTICLE-PARTICLE DRAG TERM

The theoretical expressions for the PPD term have been derived by assuming that the momentum transfer occurs primarily because of binary collisions between the particles. Simple physical models of the collision of two representative particles are used in such derivations (for example: Syamlal, 1985). Using such an approach, Nakamura and Capes (1976) derived the expression

$$F_{kj} = \frac{3g(1+e)\varepsilon_k\rho_k\varepsilon_j\rho_j(d_k+d_j)^2}{2(\rho_k d_k^3 + \rho_j d_j^3)} |v_{kj}| \tag{3}$$

in the limit of very small particulate concentrations. They included g as an adjustable parameter and found by fitting experimental data that its value was in the range of 1.0-5.0. They argued that the adjustable parameter is greater than 1.0, because multiple collisions, which were not accounted for in the derivation, tend to increase the PPD. Syamlal (1985) derived a similar expression for a dense system and found that g is given by

$$g = \frac{(\varepsilon_k+\varepsilon_j)^{1/3} + 3\varepsilon_{kj}^{1/3}}{3[\varepsilon_{kj}^{1/3} - (\varepsilon_k+\varepsilon_j)^{1/3}]} \tag{4}$$

The factor ε_{kj}, which represents the maximum possible packing of the binary mixture, can be obtained from an empirical formula, such as the one given by Fedors and Landel (1979):

$$\varepsilon_{kj} = \begin{cases} [(\Phi_k-\Phi_j) + (1-a)(1-\Phi_k)\Phi_j]\ [\Phi_k + (1-\Phi_j)\Phi_k]\ X_k/\Phi_k + \Phi_j \\ \qquad \text{for } X_k \le \Phi_k/[\Phi_k + (1-\Phi_k)\Phi_j] \\ (1-a)\ [\Phi_k + (1-\Phi_k)\Phi_j]\ (1-X_k) + \Phi_k \\ \qquad \text{for } X_k \ge \Phi_k/[\Phi_k + (1-\Phi_k)\Phi_j] \end{cases} \tag{5}$$

Here $a = \sqrt{(d_j/d_k)}$, k and j being assigned such that $d_k \geq d_j$. Φ_k is the maximum volume fraction of the kth single-particle system, and $X_k = \varepsilon_k/(\varepsilon_k + \varepsilon_j)$.

The factor g, given by Equation (4), acts as a correction term for increased particle concentration. Similar correction terms are often used in the kinetic theory of dense gases. For example, the factor g bears a formal resemblance to the factor χ (which came to be known as the radial distribution function at contact) introduced by Chapman and Cowling (1970, p.298). They state that χ is determined by two opposing mechanisms. First, in a dense system, because the particle volume is comparable with the volume occupied by the particulate phase, the volume in which the center of a colliding particle can lie is reduced. This effect increases the probability of collisions. Equation (4) accounts for this effect. Second, in a dense system the particles shield one another, reducing the probability of collisions. This effect is not accounted for in Equation (4). It is difficult to include this effect in the simple derivation used to get Equations (3) and (4); it is even more difficult to include such an effect in derivations for systems consisting of more than two particulate phases.

These difficulties can be overcome by using the formal methods of the kinetic theory of dense gases to derive an expression for the PPD. Later, we will see that the factor g given by Equation (4) is, indeed, the radial distribution function at contact of a mixture of hard spheres. The form of the radial distribution function has been well studied, and based on the kinetic theory of dense gases, several analytical expressions are available in the literature. Also in this approach the assumptions are more precisely stated and it is easier to visualize the generalizations to systems consisting of more than two

particulate phases. Hence we will derive the PPD term using the methods of the kinetic theory of dense gases.

In the following derivation we follow the steps used by Lun, et al. (1984). Refer to Figure 1 for a diagram of the collisions. At the instant of a typical collision, a "j" particle is located at **r** and a "k" particle is located at $\mathbf{r}-\sigma\mathbf{b}$, where **b** is the unit vector in the direction of the line connecting the centers of the particles and $\sigma = (d_k+d_j)/2$. The probable number of collisions, such that the center of the "j" particle is in the volume $d\mathbf{r}$ and the particle velocities $\mathbf{c}_k$ and $\mathbf{c}_j$ and **b** lie within ranges $d\mathbf{c}_k$, $d\mathbf{c}_j$, and $d\mathbf{b}$, is

$$\sigma^2(\mathbf{c}_{kj}\cdot\mathbf{b})f^{(2)}(\mathbf{r}-\sigma\mathbf{b},\mathbf{c}_k;\ \mathbf{r},\mathbf{c}_j;\ t)\ d\mathbf{b}\ d\mathbf{c}_k\ d\mathbf{c}_j\ d\mathbf{r}\ dt \tag{6}$$

where $\mathbf{c}_{kj} = \mathbf{c}_k - \mathbf{c}_j$.

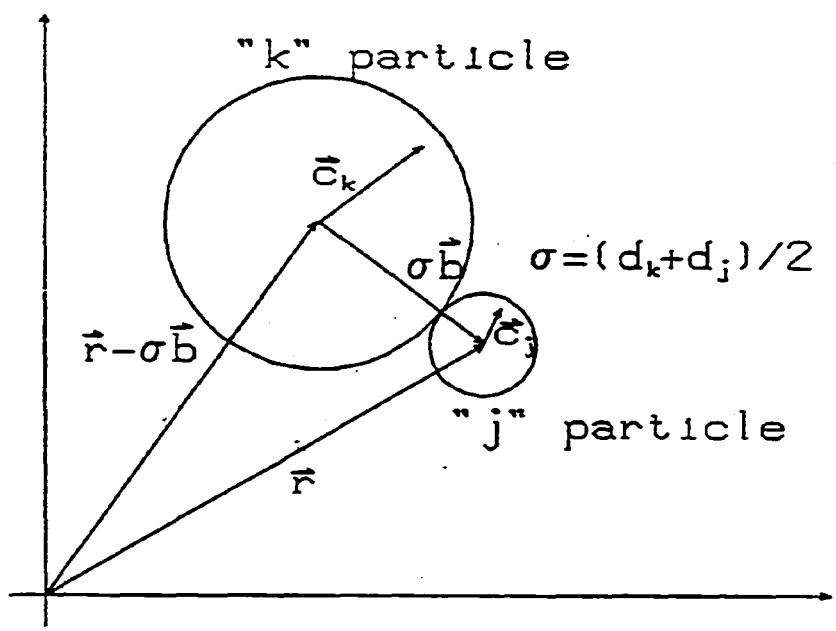

FIGURE 1. COLLISION OF TWO PARTICLES

The collisional pair-distribution function, $f^{(2)}$, is such that $f^{(2)} dr_k dr_j dc_k dc_j$ gives the probability of finding a "k" particle in a volume dr_k around r_k with its velocity in the range of c_k and c_k+dc_k and a "j" particle in a volume dr_j around r_j with its velocity in the range of c_j and c_j+dc_j. During a collision, Δm is the momentum transferred between particles "k" and "j". Considering only particles that are about to collide (ie. taking $c_{kj}.b > 0$), we find that the collisional rate of momentum transfer per unit volume is given by

$$I_{kj} = \sigma^2 \int_{c_{kj}.b>0} \Delta m \; (c_{kj}.b) \; f_{kj}^{(2)}(r-\sigma b, c_k; r, c_j \; ; t) \; db \; dc_k dc_j \tag{7}$$

Following Savage and Jeffrey (1981), we assume that $f^{(2)}$ can be expressed as a product of the radial distribution function g_{kj} and the singlet velocity distribution functions, $f^{(1)}$, for each particle:

$$f^{(2)} = g_{kj} f_k^{(1)} f_j^{(1)} . \tag{8}$$

Assuming that all the particles of each type have identical velocities, the singlet velocity distribution functions may be expressed, using Dirac delta functions, as

$$f_k^{(1)} = 6\varepsilon_k \delta(c_k - v_k)/\pi d_k^3 \tag{9}$$

and

$$f_j^{(1)} = 6\varepsilon_j \delta(c_j - v_j)/\pi d_j^3, \tag{10}$$

where v_k and v_j are the velocities of the particulate phases. To use more realistic singlet velocity distribution functions, it will be necessary to solve "granular temperature" equations as done by Lun, et al. (1984). Note that as required by its definition, $f^{(1)}$ has been formulated such that the number

density of the particles is obtained when $f^{(1)}$ is integrated over the entire range of velocities. Also note that we assume that $f_k^{(1)}$ determined at $\mathbf{r}$ is approximately equal to the required $f_k^{(1)}$ at $\mathbf{r}-\sigma\mathbf{b}$. A discussion of the form of g_{kj} will be deferred until the completion of the derivation; we do not need to know its form to perform the necessary integrations.

For a collision between two smooth, inelastic, spherical particles of diameters d_k and d_j and of masses m_k and m_j the conservation of linear momentum can be written as

$$m_k\mathbf{c}_k' = m_k\mathbf{c}_k - \mathbf{J} \tag{11}$$

and

$$m_j\mathbf{c}_j' = m_j\mathbf{c}_j - \mathbf{J}, \tag{12}$$

where $\mathbf{c}_k$ and $\mathbf{c}_j$ are the velocities before collision, $\mathbf{c}_k'$ and $\mathbf{c}_j'$ are the velocities after collision, and $\mathbf{J}$ is the impulsive force between the particles. For inelastic collisions, we assume that the relative velocity $\mathbf{c}_{kj}$ in the direction of $\mathbf{b}$ is changed during a collision such that

$$\mathbf{b}.\mathbf{c}_{kj}' = -e(\mathbf{b}.\mathbf{c}_{kj}), \tag{13}$$

where e is the coefficient of restitution. Equations (11), (12), and (13) determine the component of $\mathbf{J}$ in the direction of $\mathbf{b}$,

$$\mathbf{b}.\mathbf{J} = -(1+e)\mathbf{b}.\mathbf{c}_{kj} \;/\; (1/m_k + 1/m_j). \tag{14}$$

Assuming that the particles slide during a collision, the component of $\mathbf{J}$ in a direction $\mathbf{t}$ normal to $\mathbf{b}$ (or tangential to the sliding surfaces) can be related to $\mathbf{b}.\mathbf{J}$ by Coulomb's law of friction as

$$J_t = \mu(\mathbf{b}.\mathbf{J}), \tag{15}$$

where μ is the coefficient of friction. Now the impulsive force $\mathbf{J}$ can be written as

$$\mathbf{J} = (\mathbf{b}.\mathbf{J})\mathbf{b} + J_t\,\mathbf{t} = (\mathbf{b}.\mathbf{J})(\mathbf{b} + \mu\mathbf{t}). \tag{16}$$

The direction of t can be obtained by noting that it must be perpendicular to b and also lie in the plane formed by b and c_{kj} (Ahmadi and Shahinpoor, 1983). Thus it can be written as

$$\mathbf{t} = \frac{\mathbf{b} \times (\mathbf{c}_{kj} \times \mathbf{b})}{|\mathbf{b} \times (\mathbf{c}_{kj} \times \mathbf{b})|} = \frac{\mathbf{c}_{kj} - (\mathbf{c}_{kj}.\mathbf{b})\mathbf{b}}{|\mathbf{c}_{kj} - (\mathbf{c}_{kj}.\mathbf{b})\mathbf{b}|}. \tag{17}$$

Using this expression for J in Equation (11), we can get the change in momentum:

$$\Delta\mathbf{m} = m_k(\mathbf{c}_k' - \mathbf{c}_k) = -\mathbf{J} = \frac{-(1+e)m_k m_j(\mathbf{b}.\mathbf{c}_{kj})}{(m_k+m_j)}\left(\mathbf{b} + \mu\,\frac{\mathbf{c}_{kj} - (\mathbf{c}_{kj}.\mathbf{b})\mathbf{b}}{|\mathbf{c}_{kj} - (\mathbf{c}_{kj}.\mathbf{b})\mathbf{b}|}\right) \tag{18}$$

Substituting this in equation (7), we get

$$I_{kj} = -\frac{36\,\sigma^2(1+e)}{\pi^2\,d_k^3 d_j^3(m_k+m_j)}\,m_k m_j \varepsilon_k \varepsilon_j g_{kj} \int_{\mathbf{c}_{kj}.\mathbf{b}>0} (\mathbf{c}_{kj}.\mathbf{b})^2(\mathbf{b}+\mu\mathbf{t})\,\delta(\mathbf{c}_k-\mathbf{v}_k)\,\delta(\mathbf{c}_j-\mathbf{v}_j)\,d\mathbf{b}\,d\mathbf{c}_k d\mathbf{c}_j \tag{19}$$

Integrating over $d\mathbf{c}_k$ and $d\mathbf{c}_j$, $\mathbf{c}_{kj}$ is replaced by $\mathbf{v}_{kj}$ by virtue of the delta functions. The integration over db can be performed (Chapman and Cowling, 1970; p. 319) to get

$$I_{kj} = -36\sigma^2(1+e)(\pi/2+\mu\pi^2/8)m_k m_j \varepsilon_k \varepsilon_j g_{kj}|\mathbf{v}_{kj}|\mathbf{v}_{kj} \;/\; [\pi^2 d_k^3 d_j^3(m_k+m_j)] \tag{20}$$

Since by definition $I_{kj} = -F_{kj}\mathbf{v}_{kj}$, we get

$$F_{kj} = -36\sigma^2(1+e)(\pi/2+\mu\pi^2/8)m_k m_j \varepsilon_k \varepsilon_j g_{kj}|\mathbf{v}_{kj}| \;/\; [\pi^2 d_k^3 d_j^3(m_k+m_j)] \tag{21}$$

and, expressing the mass of the particles in terms of their densities and diameters ($m_k = \pi d_k^3\rho_k/6$ and $m_j = \pi d_j^3\rho_j/6$), we obtain

$$F_{kj} = 3(1+e)(\pi/2+\mu\pi^2/8)\varepsilon_k\rho_k\varepsilon_j\rho_j(d_k+d_j)^2\,g_{kj}|\mathbf{v}_{kj}| \;/\; [2\pi(\rho_k d_k^3 + \rho_j d_j^3)]. \tag{22}$$

Setting μ equal to zero and comparing this to Equation (3), it can be seen that the constant g of Nakamura and Capes (1976) and the factor g of Syamlal (1985),

defined by Equation (4), are equivalent to half the radial distribution function at contact (i.e., $g_{kj}/2$).

Although this derivation has required several simplifying assumptions, it has allowed the association of g with the radial distribution function at contact. This function is more rigorously derived in the literature on the kinetic theory of dense gases and can be adopted from there for use in Equation (22). For a mixture of hard spheres, Lebowitz(1964) solved a generalized Percus-Yevick equation to obtain the formula

$$g_{kj} = 1/\varepsilon + [3(\Sigma^N_{i=2}\varepsilon_i/d_i)d_k d_j]/\varepsilon^2(d_k+d_j), \tag{23}$$

where ε is the void fraction given by

$$\varepsilon = \varepsilon_1 = 1 - (\Sigma^N_{i=2}\varepsilon_i). \tag{24}$$

Note that in Equations (23) and (24) we exclude i=1, since, by convention, i=1 denotes the fluid. In Figure 2, the radial distribution function g_{kj} for a binary mixture of particles of diameters 0.127cm and 0.057cm as given by Equation (23) is compared to the function g of Syamlal (1985), given by Equation (4). As expected, both of the functions increase monotonically with increasing solids volume fraction. The function g is in general greater than g_{kj} and, for a densely packed system consisting mainly of one of the components, it is an order of magnitude larger than g_{kj}. To determine which of these magnitudes is more realistic, it is necessary to compare numerical results to relevant experimental data as we do in the next section. Meanwhile, however, some of the mathematical features of g_{kj} can be found to be more physically realistic.

First, the function g has the same form for the conditions of an excess of fine particles as for an excess of coarse particles. The function g_{kj}, on the other hand, increases with increasing fines concentration. This implies that the

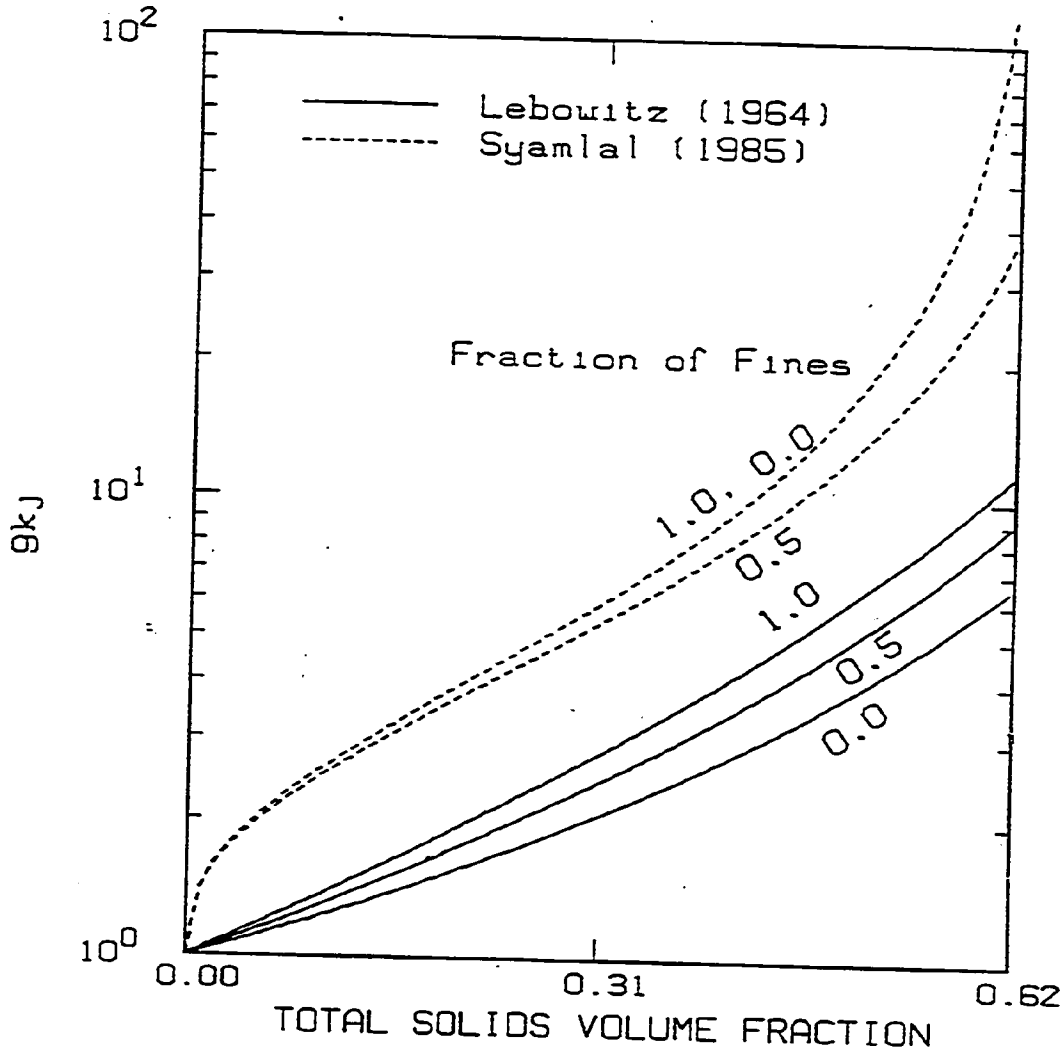

FIGURE 2. A COMPARISON OF THE RADIAL DISTRIBUTION FUNCTIONS

resistance offered by an excess of fines on a small amount of coarse particles is larger than that by an excess of coarse particles on a small amount of fines. This is reasonable, since fines can flow more easily through the void space between densely-packed coarse particles while the converse is not true.

Second, the function g_{kj} has a mathematical form that satisfies a necessary additivity condition. Using a multiparticle model, a binary mixture of particles A and B can be described in terms of particulate phases in several ways. For example, consider two cases, one in which the particles are described as Phase-A and Phase-B and another in which they are described as Phase-A, Phase-B1, and Phase-B2. Regardless of how we choose to represent the B particles, their effect on the A particles should remain unchanged. This implies that, in our example, the sum of the F_{kj}'s of Phase-B1 and Phase-B2 must be equal to the F_{kj} of Phase-B. It can be easily verified that this is the case when F_{kj} is given by Equations (22) and (23) and that it is not the case when F_{kj} is given by Equations (3) and (4).

Finally, it can be seen from Equation (23) that g_{kj} correctly accounts for the effect of particles other than the kth and the jth particles in a multiparticle mixture on the collisions between the kth and the jth particles, whereas the expression for g does not include the properties of particles other than the kth and the jth. Because of the above-mentioned reasons, we can conclude that the factor g obtained from a simple derivation lacks the physically realistic mathematical features of g_{kj} derived using the more rigorous methods of the kinetic theory of dense gases.

4.0 SIMULATION OF YANG AND KEAIRNS'S EXPERIMENT

To determine the accuracy of the PPD term derived in the previous section, computer simulations based on the settling experiments of Yang and Keairns (1982) were conducted. Yang and Keairns (1982) studied the rate of separation of dolomite particles in a fluidized bed containing a mixture of acrylic particles and dolomite particles. The dolomite particles were larger and heavier than the acrylic particles; hence, they settled very rapidly when the fluidization velocity was smaller than their minimum fluidization velocity. As the dolomite particles settle, they continually collide with the upward moving acrylic particles. Thus, the rate of settling is strongly dependent upon the PPD between the acrylic and dolomite particles. Also, the monotonicity of the experimental rate of settling curves for small fluidization velocities suggests that the mixing caused by bubbles or solids circulation in the bed are probably of lesser importance than the mixing caused by particle-particle collisions. For these reasons, the simulation of Yang and Keairns's (1982) experiments is useful for determining the accuracy of the PPD term.

The experimental procedure of Yang and Keairns (1982) consisted of fluidizing a uniform mixture of dolomite and acrylic particles for a short time, then defluidizing the bed and measuring the particle concentrations at various axial locations to obtain dolomite-concentration profiles. By repeating the experiments for various durations, they obtained the dolomite-concentration profiles as a function of time.

The equations presented in Table 1 were used to develop a multiparticle computer code. The details of the numerical technique used in the code can be found

elsewhere (Syamlal, 1985; Syamlal, 1987). The computer simulation conditions are summarized in Table 2. In the experiments, it was found that the fluidized

Table 2. Computer Simulation Conditions

Particles:	dk (cm)	ρk (g/cm3)	Weight Fraction
Dolomite	0.1272	2.61	0.6
Acrylic	0.0571	1.11	0.4
Fluid	Air		
Superficial Fluid Velocities	40, 50 cm/s		
Bed Dimensions	Diameter = 7 cm Height = 11 cm		
Cell Sizes	Radial: 0.5 cm, Axial: 1.0 cm		
Time Step	0.0005 s		

bed reached a steady state in 5-10 seconds. Hence the computer simulations were carried out for a duration of 10 seconds.

All the computer simulations were performed by setting the coefficient of friction, μ, equal to zero. It can be seen from Equation (22) that this approximation will change the magnitude of PPD at most by a factor of 2, since the value of μ is close to 1.0. The conclusions of this preliminary study will not be affected by such a change in the PPD. Some initial computer simulations were carried out using Syamlal's (1985) PPD term. These simulations indicated that the rate of separation is very small and that the two particulate phases remained well mixed; at the end of 3 seconds of simulation with 40 cm/s superficial air velocity, the predicted weight fraction of dolomite at the top of the bed was found to be around 0.5 (see Figure 3). This is contrary to the experimental observation of very rapid settling. Because of this, and

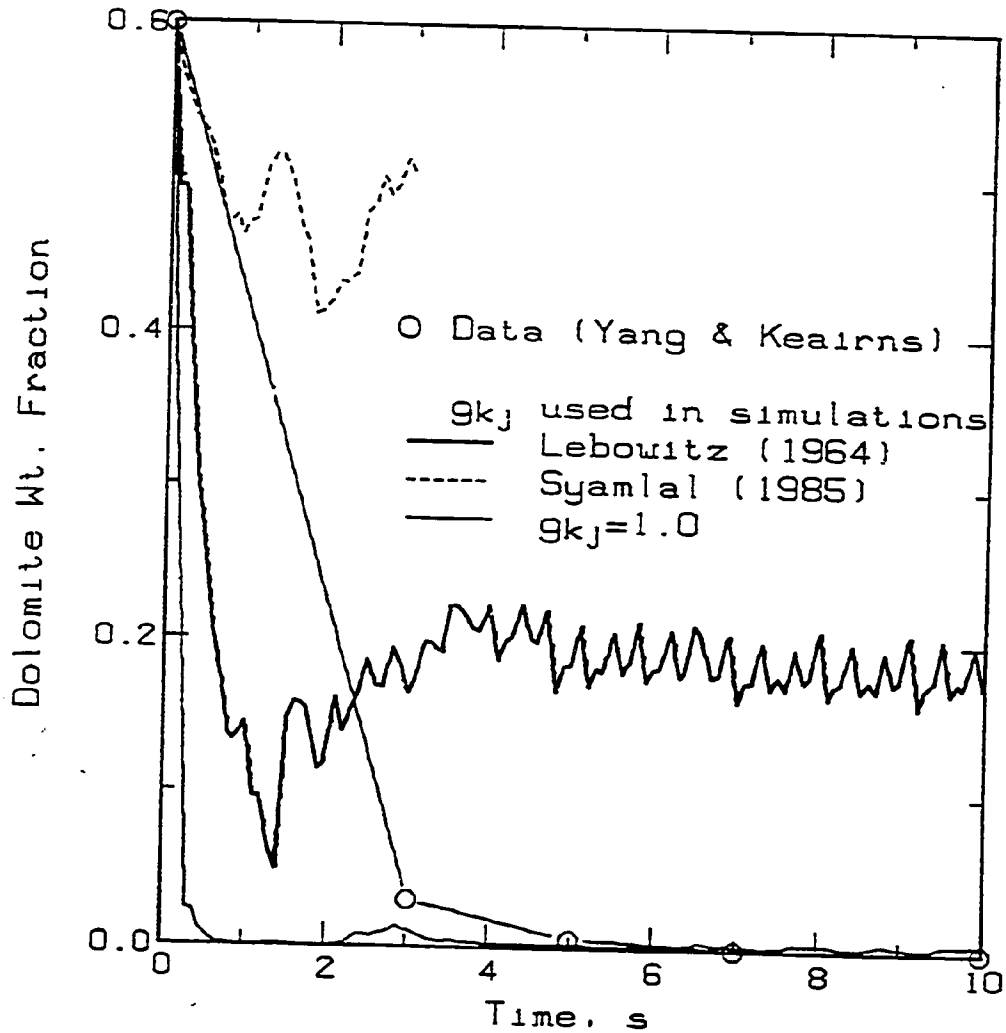

FIGURE 3. RATE OF DOLOMITE SEPARATION AT A FLUIDIZATION VELOCITY OF 40 cm/s

considering the more realistic mathematical properties of the function g_{kj} discussed in the previous section, subsequent simulations were carried out using g_{kj} as derived by Lebowitz (1964). For comparison, simulations were also carried out by setting $g_{kj}=1$.

In Figure 3, experimentally observed (Yang and Keairns, 1982) and numerically-simulated dolomite concentrations at the top of the bed are plotted as a function of time for a period of 10 seconds when the superficial air velocity is 40 cm/s. The rate of initial separation is strongly influenced by the magnitude of the PPD. For the present set of experimental data, the extent of resolution possible for the initial rate of separation is given by the line connecting the data points at t=0 and t=3 seconds. If the numerically-simulated separation curves are below this line, the predicted initial rate of separation is possibly comparable to the experimental data. The simulation results using the g_{kj} of Lebowitz (1964) indicate a very rapid initial separation phase (~1.5 sec.) that satisfies this condition. Thus, the predicted initial rate of separation, using g_{kj}, is comparable to the experimental data. However, the equilibrium weight fraction of dolomite in this case does not agree with the experimental data which indicate a monotonic reduction in the dolomite weight fraction that ultimately leaves a top layer free of dolomite particles. An examination of the predicted velocity fields of the two particulate phases indicates that the excessive mixing of the particles is caused by the solids circulation in the bed. This may be because of the absence of particulate-phase viscous stresses in the present model. Thus, we conjecture that the inclusion of viscous stresses may lead to the correct prediction of the equilibrium dolomite weight fractions.

Also shown in Figure 3 is the predicted settling curve when g_{kj} is set equal to 1. In this case, an even more rapid initial rate of settling is predicted, but the equilibrium dolomite concentration at the top of the bed is comparable to the experimental data. This, of course, only illustrates the effect of a weaker PPD and is not a demonstration that g_{kj} should be equal to 1. That condition would imply (as in the case of ideal gases in the kinetic theory) that the presence of one particle at some location in the bed does not affect the probability of finding another particle close to it. This is certainly not true in a dense bed.

Another reason for our objections to the condition $g_{kj} = 1$ can be found in Figure 4, in which the simulation results for a fluidization velocity of 50 cm/s are given. The data of Yang and Keairns (1982) indicate that the settling behavior has not changed significantly from the previous case (fluidization velocity = 40 cm/s). However, the simulation results for $g_{kj}=1$ indicate that the equilibrium dolomite concentration at the top of the bed is not comparable to the experimental data. Thus, even with $g_{kj}=1$, the increased fluidization velocity increases the solids circulation and, hence, the mixing. The simulation results, using the g_{kj} of Lebowitz (1964), indicate that the equilibrium dolomite concentration at the top of the bed has increased to 0.4, which is again because of the increased solids circulation. Note, however, that the initial rate of separation is still comparable to the experimental data in the sense discussed previously. Hence it can be concluded that the PPD term models the initial rate of separation reasonably well, but the predicted equilibrium weight fraction of dolomite does not compare with experimental data because of the overprediction of the intensity of solids circulation. Hence, further

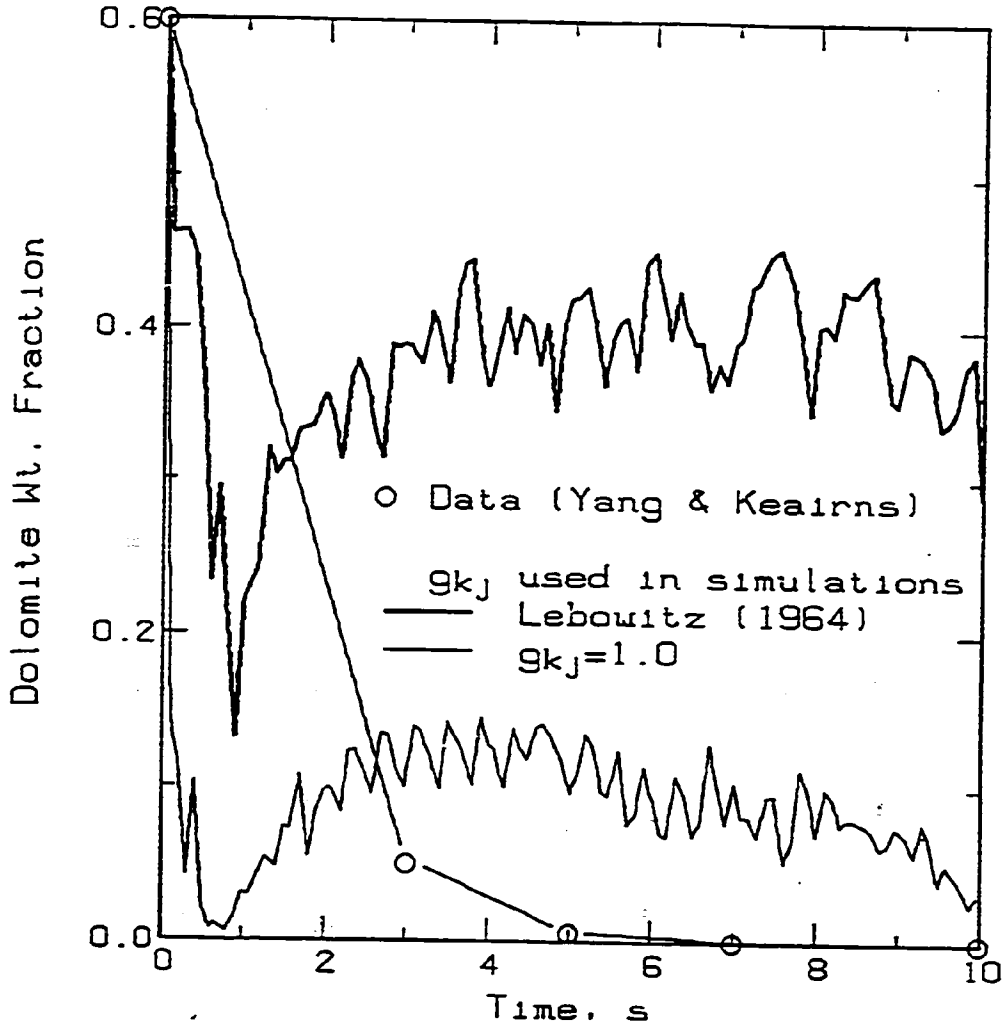

FIGURE 4. RATE OF DOLOMITE SEPARATION AT A FLUIDIZATION VELOCITY OF 50 cm/s

refinement of the PPD term can be sought only after including realistic granular stress terms in the multiparticle model.

5.0 CONCLUSIONS

A derivation using the methods of the kinetic theory of dense gases has shown that a factor appearing in the particle-particle drag term is the radial distribution function for hard spheres at contact, g_{kj}. The major assumption made in the derivation is that all the particles at a spatial location move at the continuum velocity. When an expression for g_{kj} given by Syamlal (1985) is used for simulations, the predicted initial rate of separation in a fluidized bed is found to be not acceptable compared to a set of experimental data of Yang and Keairns (1982). When an expression for g_{kj} given by Lebowitz (1964) is used, an initial rate of settling comparable to the experimental data is obtained. Also, since Lebowitz's (1964) expression has mathematical features that are more physically realistic it is recommended as the appropriate radial distribution function. The equilibrium weight fractions predicted when this radial distribution function is used, however, do not agree well with the experimental data. The reason for this is thought to be the excessive solids circulation within the bed. Simulations carried out by setting the radial distribution function equal to 1 reinforce this conclusion. It is conjectured that the absence of the viscous stress terms in the present model leads to the prediction of excessive solids circulation. Hence, further refinement of the particle- particle drag term can be sought only after including realistic granular stress terms in the multiparticle model.

6.0 NOMENCLATURE

$\mathbf{b}$	Impact parameter, or the direction of the line joining the centers of two colliding particles.
$\mathbf{c}_k$	Velocity of k particles in the microscopic sense.
$\mathbf{c}_{kj}$	$= \mathbf{c}_k - \mathbf{c}_j$
d_k	Diameter of kth particle.
e	Coefficient of restitution.
$f^{(1)}$	Singlet velocity distribution function.
$f^{(2)}$	Pair velocity distribution function.
F_{kj}	Coefficient of interphase momentum transfer for phases k and j.
$\mathcal{G}$	Function defined by Equation (4).
$\mathbf{g}$	Body forces such as gravity.
g_{kj}	Radial distribution function at contact for k and j particles.
$\mathbf{J}$	Impulse of the force of collision.
m_k	Mass of a k particle $= \pi d_k^3 \rho_k / 6$.
N	Total number of phases.
p	Pressure.
p_s	Solids Pressure.
$\mathbf{r}$	Position vector.
t	Time.
$\mathbf{t}$	A normal direction to the impact parameter **b**.
$\mathbf{v}_k$	Velocity of the kth phase in the continuum sense.
$\mathbf{v}_{kj}$	$= \mathbf{v}_k - \mathbf{v}_j$

GREEK SYMBOLS

ε	Void fraction.
ε_k	Volume fraction of the kth phase.
ε_{kj}	The maximum particulate volume fraction in a random mixture of particulate phases k and j.

Φ_k The maximum particulate volume fraction of the particulate phase k.

μ Coefficient of friction.

ρ_k Density of the kth phase.

σ Distance between the centers of two colliding particles, eg. $(d_k+d_j)/2$

7.0 REFERENCES

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