2010

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Quadrature-Based Moment Model for Moderately Dense Polydisperse Gas–Particle Flows

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A quadrature-based moment model is derived for moderately dense polydisperse gas–particle flows starting from the inelastic Boltzmann–Enskog kinetic equation including terms for particle acceleration (e.g., gravity and fluid drag). The derivation is carried out for the joint number density function, f(t,x,u), of particle mass and velocity, and thus, the model can describe the transport of polydisperse particles with size and density differences. The transport equations for the integer moments of the velocity distribution function are derived in exact form for all values of the coefficient of restitution for particle–particle collisions. For particular limiting cases, the moment model is shown to be consistent with hydrodynamic models for gas–particle flows. However, the moment model is more general than the hydrodynamic models because its derivation does not require that the particle Knudsen number (and Mach number) be small.

Introduction

The numerical simulation of gas–particle flows has been a long-time interest of Prof. Gidaspow’s research group.1–3 The transport models used to describe such flows are derived from a kinetic equation for the velocity distribution function. With a few exceptions,4–8 the vast majority of such models9–25 use the Chapman–Enskog26 expansion to derive hydrodynamic equations for the low-order moments of the velocity distribution and gradient-based closures for the stresses and heat flux.1 By the nature of the expansion, hydrodynamic models are accurate for near-equilibrium flows wherein the particle–particle collisions occur on a much shorter time scale than other processes,25 (e.g., spatial transport). In other words, hydrodynamic models are valid for small particle Knudsen numbers, Kn ≪ 1, where Kn is inversely proportional to the collision frequency.

For molecular gases, hydrodynamic models apply over a wide range of practical systems. However, because of inelasticity and fluid drag, the granular temperature in many gas–particle flows of industrial interest (e.g., riser flows) is relatively low compared to the mean particle velocity (i.e., the particle Mach number is large27). For this reason, many practical gas–particle flows behave as nonequilibrium granular gases for which hydrodynamic descriptions miss important physics.9 Borrowing from the theory of rarefied gas dynamics,28 nonequilibrium transport models can be derived starting from a kinetic equation. In moment methods, transport equations for the higher-order velocity moments are formulated and solved.28 Because the moment equations are derived without assuming Kn ≪ 1, they are (in principle) valid for arbitrary Knudsen numbers.7,29 Nevertheless, regardless of the value of the Knudsen number, it is important to note that, for granular flows, it is not entirely obvious that a closed kinetic equation (see Appendix A) can adequately capture the underlying dynamics because of a lack of clear separation of scales.25 However, this is an entirely separate issue from the question of whether a moment method is adequate for capturing the nonequilibrium behavior of solutions to a particular closed kinetic equation. Thus, here, we take the position that the Boltzmann–Enskog kinetic equation (with the “classical” closure described in Appendix A) adequately captures the important physics for moderately dense gas–particle flows and focus on deriving a reduced description based on moments. The validity of the moment method can be tested by comparing its predictions to direct simulations of the closed kinetic equation30 [as opposed to direct comparisons with experiments or molecular dynamics (MD) simulations]. In turn, the validity of the closed kinetic equation can be demonstrated by comparing its solution to MD simulations. Ultimately, one would hope that agreement might be achieved between all levels of comparison, but this is not guaranteed in advance.

Our previous works6,7,27,29,31,32 have focused on developing moment methods for dilute gas–particle flows where the solids volume fraction is small enough (ν < 1%) that the Boltzmann kinetic equation with binary hard-sphere collisions is applicable. Moreover, because Kn ≈ 1/ν, the Knudsen number in dilute gas–particle flows is large enough to make nonequilibrium effects dominant throughout the entire flow domain. In this work, we extend our modeling approach to moderately dilute gas–particle flows by using the inelastic Boltzmann–Enskog kinetic equation for binary hard-sphere collisions as our starting point. (Note that, by eliminating the fluid drag term, our model can also be applied to granular gases.) In principle, the model can be used for particle volume fractions near the close-packed limit (i.e., dense flows) as long as the particle interactions are well described by binary collisions. In comparison to the Boltzmann kinetic equation, the Boltzmann–Enskog collision term contains finite-size particle effects instead of considering the collisions to occur between point particles. Furthermore, in addition to accounting for finite-size effects, we also include polydispersity effects such as a distribution of particle diameters and/or particle densities. The resulting gas–particle flow model is therefore applicable to moderately dense polydisperse gas–particle flows with an arbitrary degree of inelasticity. (As noted earlier, a moment method should only be compared to solutions to the kinetic equation from which it was derived. Thus, the inelasticity of interest is that contained in the kinetic equation, which is a model for the physical system.)
To close the moment transport equations, we use a quadrature-based method of moments (Q MOM). This approach has several advantages over classical moment methods, and its numerical implementation is reasonably well understood for dilute fluids. Here, Q MOM is first applied to represent the polydispersity of the particles, resulting in a multicomponent Boltzmann–Enskog kinetic equation for each representative particle size. Then, Q MOM is applied to the Boltzmann–Enskog collision term to derive the velocity moments of the collision term for arbitrary non-negative-integer orders. This step, which requires Taylor-series expansions to account for finite-size effects and analytical integration over the hard-sphere collision angles, is the technically most challenging part of the derivation. The resulting expressions are exact for hard-sphere collisions for any value of the coefficient of restitution. The second step is to apply the quadrature formulas to close the integrals over the velocity distribution functions for each term in the Taylor-series expansion. Here, because of the complexity of the expressions, we consider terms to first order in the Taylor series. However, the extension to higher-order terms would follow the same procedure. Once the derivation of the moment transport equations is complete, we compare the resulting equations to the classical hydrodynamic models for monodisperse and polydisperse particles. Finally, conclusions are drawn concerning the implementation of the moment equations. Further details on the mathematical manipulations used in the derivation are given in the appendices.

Inelastic Boltzmann–Enskog Kinetic Equation

In this work, we consider collisions between smooth (i.e., frictionless) spherical particles with different densities and/or diameters. The latter enter into the dynamics through the particle mass $m$ and diameter $d$. We consider only collisions during which the particle mass and diameter are conserved and exclude other processes that might change these properties (e.g., surface condensation or aggregation). Likewise, by assuming smooth spherical particles, we ensure that the particle angular momentum does not change during a collision, and hence, only the particle velocity needs to be taken into account in the kinetic equation. In this work, we limit ourselves to hard-sphere collisions, which implies that the particle velocities after a collision can be written as explicit functions of the particle velocities before the collision, the coefficient of restitution, and the particle masses. This assumption, which corresponds to most molecular dynamic (MD) simulations of particle systems, allows for the derivation of exact expressions for the collision integrals. More details on hard-sphere collisions can be found in the book by Cercignani.

The starting point for our model derivation is the kinetic equation governing the joint mass, velocity number density function $f(t, x, m, u)$

$$\partial_t f + u \cdot \nabla_x f + \partial_u (A f) = C$$

where $t$ is time, $x$ is spatial location, $m$ is particle mass, $u$ is particle velocity, and $A$ is an external force per unit mass (acceleration). Note that a specific form for the external force is not required for our derivation, but it could include fluid drag and gravity for gas–particle flows. $C$ represents binary inelastic hard-sphere collisions and is modeled here using the generalized hard-sphere Boltzmann–Enskog collision operator. Because the form of the collision term is rather complicated (see Appendix A), we first define a new function $B$ by enumerating all of the collision partners with mass $m^*$

$$B(m, m^*, u) = \int_0^\infty \beta(m, m^*) B(m, m^*, u) \, dm^*$$

where $\beta(m, m^*) = \beta(m^*, m) = \pi a^2$ is the collision cross section, $s$ is the center-to-center distance at collision, $\sigma(m, m^*) = r(m) + r(m^*)$, the particle radii are $r = \{(m/4\pi\rho)^{1/3}\}$ and $r^* = \{(m^*/4\pi\rho^*)^{1/3}\}$, and the particle densities are $\rho$ and $\rho^*$.

For hard-sphere collisions, the Boltzmann–Enskog collision term for fixed values of $m$ and $m^*$ is given by

$$B(m, m^*, u) = \frac{1}{\pi} \int_0^\infty \int_{S^2} |f^{(t)}(t, x, m, u; x - \nu, m^*, u'^*)|\nu \cdot |\nu| \, d\nu$$

where the function $f^{(t)}$ denotes the pair distribution function, which can further be expressed (see Appendix A) in terms of the single-particle distribution function and a radial distribution function $g_0(m, \nu, m^*, \nu')$ depending on the solids volume fractions $\nu$ and $\nu^*$. For example, for a binary system, an example expression for $g_0$ is

$$g_0 = \frac{1}{1 - \nu} + \frac{3d_1d_2}{d_1 + d_2} \times (1 - \nu)^2 + \left(\frac{2}{d_1 + d_2}\right)^3 \times \frac{\nu^2}{(1 - \nu)^2}$$

where $d_1$ and $d_2$ are the particle diameters, $n_1$ and $n_2$ are the number densities, and $\xi = 4\pi n_1 d_1^2 + 4\pi n_2 d_2^2$. In eq 3, $n = -(x - x^*)/x - x^*$ is the unit vector in the direction between the particle centers, $\nu = u - u^*$ (with magnitude $g$) is the velocity difference before a direct collision, and $\gamma$ is a factor relating the precollision velocities for direct collisions ($u, u^*$) to those for inverse collisions ($u'', u'^*$$\gamma')$. These velocities are related by

$$u = u'' - m^*[1 + e(m, m^*, g')](g'' \cdot n)$$

$$u^* = u'^* + m^*[1 + e(m, m^*, g')](g' \cdot n)$$

where $0 \leq e \leq 1$ is the coefficient of restitution with the property $e(m, m^*, g) = e(m^*, m, g)$ and $g'' = u'' - u'^*$ (with magnitude $g''$) is the velocity difference before an inverse collision. The surface $S^*$ is the unit half-sphere on which $g \cdot n > 0$ (i.e., velocity differences that result in collisions), and $R$ denotes the real line.

As noted above, we assume in eqs 2 and 4 that the particle physical properties do not change during a collision event (e.g., $m'' = m' = m$ and $m''^* = m''^* = m^*$). The Boltzmann collision term results from eq 3 by setting $g_0 = 1$ and $\gamma = 0$. For elastic rebounds, $e = 1$, and for more physically realistic inelastic rebounds, we include a possible dependence on $g$ in order to model the experimentally observed increase in elasticity for small $g$ [i.e., $e(m, m^*, 0) = 1$]. The factor $\gamma$ can be defined in terms of the underlying Jacobian $\partial(u'', u'^*)/\partial(u, u^*)$ as

$$\gamma = \frac{|\nu'|}{|\nu|} \frac{\partial(u'', u'^*)}{\partial(u, u^*)} = \frac{1}{e(m, m^*, g)}$$

For cases where the coefficient of restitution $e$ is independent of the relative velocity $g$, the underlying Jacobian reduces to $\partial(u'', u'^*)/\partial(u, u^*) = 1/e(m, m^*)$, and the factor $\gamma$ reduces to $\gamma = 1/e^2(m, m^*)$.

Quadrature-Based Moment Method

The direct solution of the kinetic equation is expensive because of the need to describe the high-dimensional phase space for mass and velocity. To reduce the computational expense, moment methods are attractive alternative because
the phase-space variables are integrated out of the governing equations, leaving only the dependence on physical space and time. However, the moment transport equations do not appear in closed form, and approximation methods are needed for closure. For gas–particle flows that do not dominated by collisions, a quadrature-based moment method can be effectively used to close the moment equations. (Note that QMOM also applies in the low-Knudsen-number limit, but will not be as efficient as a hydrodynamic model because the collision term applies in the low-Knudsen-number limit, but will not be as efficient as a hydrodynamic model because the collision term appears explicitly in the transport equations, making them very stiff.) In this section, we describe how such a method can be applied to eq 1.

**Quadrature Representation of Moments.** In a quadrature-based moment method, the density function is represented by weighted delta functions in mass–velocity phase space

\[ f(m, u) = \sum_{a=1}^{N} n_{a}(m - m_{a}) \delta(u - u_{a}) \]  

(6)

where \( \delta(u - u_{a}) \equiv \delta(u_{1} - u_{a1}) \delta(u_{2} - u_{2a}) \delta(u_{3} - u_{3a}) \). In this formulation, the weights \( n_{a} \) and abscissas \( (m_{a}, u_{a}) \) are time-dependent Eulerian fields (which are not necessarily smooth).

The quadrature approximation for the moments of the number density function as over velocity phase space, we find the quadrature representation of the mass probability density function as

\[ \langle m^{k}m^{l}m^{3} \rangle = \int R^{3} \int_{0}^{\pi} m_{a}^{k}m_{b}^{l}m_{c}^{3} f(m) \, dm \, du = \sum_{a=1}^{N} n_{a}m_{a}^{k}u_{a}^{l}u_{a}^{3} \]  

(7)

where \( k \) and \( l \) are assumed to be non-negative integers in the following derivation. The fundamental idea behind quadrature-based moment methods is that the weights and abscissas should be chosen such that as many moments as possible are determined by the moment transport equations found from eq 1.

To represent the density function using quadrature, we construct a tensor product in mass–velocity phase space

\[ f(m, u) = \sum_{a=1}^{N_{m}} \sum_{a=1}^{N_{u}} n_{a}(m - m_{a}) \delta(u - u_{a}) \]  

(8)

with \( N_{m} \) nodes in mass space located at \( m_{a} \) and, for each mass node, \( N_{u} \) nodes in velocity space located at \( u_{a} \). By integrating over velocity phase space, we find the quadrature representation of the mass probability density function as

\[ f_{a}(m) = \sum_{a=1}^{N_{m}} n_{a} \delta(m - m_{a}) \]  

(9)

where \( p_{a} \) is the fraction of particles with mass \( m_{a} \). The number density of particles with mass \( m_{a} \) is

\[ n_{a} = \sum_{i=1}^{N_{a}} n_{a} \]  

(10)

and \( p_{a} = n_{a}/\sum_{i=1}^{N_{a}} n_{i} \). Note that \( N = N_{m}N_{u} \) and that eq 8 differs from eq 6 only by how the \( N \) nodes are numbered.

The assumptions underlying eq 1 imply that the mass abscissas \( m_{a} \) are constants. However, in more general flows (e.g., aggregating particles), this need not be the case. When the mass abscissas are constant, they can be computed from the initial particle size distribution using the quadrature algorithm described below (i.e., they will be input parameters to the simulation). Cases where the mass abscissas change can also be treated using QMOM, but the moment-inversion algorithm must be modified to account for such changes.\(^{33}\)

**Quadrature Algorithm for Mass Abscissas.** A key step in the solution algorithm is the definition of a moment-inversion algorithm to find the weights and the mass abscissas given a specific set of moments. To find the \( N_{m} \) mass abscissas \( m_{a} \), one can employ mass moments \( (m^{k}) \) with \( k = 0, ..., 2N_{m} - 1 \). The zero-order moment \( (k = 0) \) is given by \( \langle 1 \rangle = \sum_{a=1}^{N} n_{a} \) and represents the average number density of particles. The higher-order mass moments have the form

\[ \langle m^{k} \rangle = \sum_{a=1}^{N} n_{a}m_{a}^{k} \]  

(11)

Given the moments \( \langle m^{k} \rangle \), which can be computed from a given mass distribution function \( f_{m} \), the product–difference (PD) algorithm\(^{37}\) or the Wheeler algorithm\(^{38}\) can be used to efficiently compute \( m_{a} \). Because these masses are constant, they need only be computed at the beginning of the simulation, and one can solve \( N_{m} \) inelastic multicomponent Boltzmann–Enskog equations for the velocity distribution functions as discussed next.

**Multicomponent Boltzmann–Enskog Equation.** Polydisperse particles with constant mass can be described by a multicomponent Boltzmann–Enskog equation. Assuming that each particle size has a unique mass \( m_{a} \), one can relate the generalized Boltzmann–Enskog equation given in eq 1 to the multicomponent Boltzmann–Enskog equation. For simplicity, we consider here the Boltzmann equation with elastic collisions.\(^{32}\) However, the derivation using the generalized Boltzmann–Enskog binary collision operator is completely analogous.

Formally, for constant masses, one can write the joint mass–velocity distribution function as

\[ f(m, u) = \sum_{a=1}^{N_{m}} f_{a}(u) \delta(m - m_{a}) \]  

(12)

where \( f_{a} \) is the velocity distribution function for particles with mass \( m_{a} \). The Boltzmann equation reads

\[ \partial_{t} f + u \cdot \partial_{x} f + \partial_{\epsilon} f = \int_{0}^{\infty} \frac{\beta(m, \epsilon)}{\pi} \int_{R^{3}} f(m, u') \{ f(m, u) - f_{a}(u_{a}^{*}) \} |g_{a} \cdot n| \, dn \, du \]  

(13)

Writing

\[ f(m, u^{*}) = \sum_{b=1}^{N_{m}} f_{b}(u_{b}) \delta(m^{*} - m_{b}) \]  

(14)

one can re-express the integral with respect to \( m^{*} \) in eq 13 as

\[ \partial_{t} f + u \cdot \partial_{x} f + \partial_{\epsilon} f = \sum_{b=1}^{N_{m}} \frac{\beta(m, m_{b})}{\pi} \int_{R^{3}} \int_{S^{2}} \{ f(m, u) f_{b}(u_{b}^{*}) \} |g_{b} \cdot n| \, dn \, du \]  

(15)

where \( g_{b} = u - u_{b} \).

The next step is to integrate eq 15 over a small finite interval surrounding \( m_{a} \) for each \( a \in (1, ..., N_{m}) \) and to use the identity

\[ \int_{m_{a} - \epsilon}^{m_{a} + \epsilon} f(m, u_{a}) \, dm = f_{a}(u_{a}) \]  

(16)

Note that this is the only step that requires \( m_{a} \) to be constant. This procedure yields
\[ \partial_t f_a + u_a \cdot \nabla f_a + \partial_u^\star (A_a f_a) = \]
\[ \sum_{b=1}^{N_a} \sigma_{ab}^\star \int_{R^3} \int_{R^3} [f_b(u') f_b(u'')] \cdot [g_{ab} \cdot n] \, dn \, du' \]
\[ \quad \text{for} \quad a \neq \star \]
\[ \text{and} \quad \int_{R^3} \int_{R^3} m C(m, u) \, dm \, du = 0 \quad (21) \]
\[ \text{and} \quad \int_{R^3} \int_{R^3} m u C(m, u) \, dm \, du = 0 \quad (22) \]

These conservation properties must be retained in numerical approximations used to treat eq 1. Note that eqs 21 and 22 correspond to particular moments of the velocity density function. For other moments, the contribution due to collisions is non-zero. For the moment-inversion algorithm, one needs the transport equations for integer moments of arbitrary non-negative order.

**Derivation of Moment Transport Equations.** To apply the quadrature method of moments, we must derive transport equations for the moments defined in eq 7. In previous work, the moment transport equations were derived for all terms in eq 1 except C. We thus derive the contribution due to the inelastic Boltzmann–Enskog collision term here.

**Collision Term.** Define first a velocity integral, corresponding to the source term for velocity moments due to inelastic hard-sphere Boltzmann–Enskog collisions for given values of \( m \) and \( m^\star \) (see eq 2), by
\[ B_{i, i, j} (m, m^\star) = \int_{R^3} u_i u_j u_i^b B \, du = C_{i, i, j} - \frac{1}{2} \mathbf{V} \cdot \mathbf{G}_{i, i, j} + O(\sigma^2) \]
(23)
where we have retained terms to first order in \( \sigma \). In this expression, the gradient vector with respect to position \( \mathbf{x} \) is denoted by \( \mathbf{V} \). In the Boltzmann limit (\( \sigma \to 0 \)), \( \mathbf{G}_{i, i, j} \) makes no contribution to the collision term. The first term on the right-hand side of eq 23 is referred to as the collision contribution, and the second term as the collisional-flux contribution.

Using the properties of the inelastic Boltzmann–Enskog collision integral, the collision contribution in eq 23 can be written as
\[ C_{i, i, j} = g_0 \int_{R^3} \int_{R^3} g_{i, j, j} (\omega, u, g) f(m, u) f(m^\star, u^\star) \, du \, du^\star \]
(24)
where, to first order in \( \sigma \), \( g_{i, j, j} \) is defined by
\[ g_{i, j, j} = \frac{1}{4\pi} \int_{S^2} [(u_i^b)^2 (u_j^b)^2 - u_i^b u_j^b] |g \cdot n| (1 + \frac{\sigma}{2} n \cdot \nabla D) \, dn \]
(25)
and \( D \), defined as
\[ D \equiv \ln \left( \frac{f(m^\star, u^\star)}{f(m, u)} \right) = \ln \left( \frac{E^\star}{E} \right) \]
(26)
do not depend on \( n \). The primed velocity components (which depend on \( n \)) are defined by
\[ u^\prime = u - n (g \cdot n) n \]
\[ u^\star = u + \omega (g \cdot n) n \]
(27)
with \( \omega \) and \( \omega^\star \) defined by
\[ \omega = \frac{m^* (1 + e(m, m^*, g))}{(m + m^*)} \quad \text{and} \quad \omega^* = \frac{m (1 + e(m, m^*, g))}{(m + m^*)} \]  
(28)

As noted earlier, we have assumed that the coefficient of restitution \(e\) can depend on the masses of the two particles involved in the collision, as well as their relative velocity. As a consequence of the conservation of momentum, \(m\omega = m^*\omega^*\).

The collisional-flux contribution in eq \(23\) is defined by

\[ G_{l,\ell\ell'} = \sigma g_0 \int_{0}^{2\pi} \int_{\theta}^{\theta'} g F_{l,\ell\ell'}(\omega, u, d)(m, u) f(m^*, u^*) d\omega^* d\omega \]  
(29)

where, to first order in \(\sigma\)

\[ F_{l,\ell\ell'} = \frac{1}{\pi g} \int_{0}^{2\pi} \int_{\theta}^{\theta'} g \left[n u_{1l}^* u_{1l}^* (u_{1l}^* u_{1l})^t \right] g \cdot n \left(1 + \frac{1}{2} n \cdot \nabla D\right) d\omega \]  
(30)

The distribution-function integrals in eqs \(24\) and \(29\) will be treated using quadrature (eq \(6\)). [As described elsewhere, \(9\) by making a small simplification to the integrand, it is possible to express the distribution-function integrals in closed form (i.e., as functions of the moments). For inelastic cases, this can be done when \(e\) is independent of \(g\), and the simplification retains the exact dependence on \(e\).] Therefore, as a preliminary step, we are interested in finding analytical expressions for \(I_{l,\ell\ell'}\) and \(F_{l,\ell\ell'}\) by explicitly evaluating the integrals in eqs \(25\) and \(30\) over the collision angles for given values of \(u\) and \(g\).

**Integrals over Collision Angles.** Following the method presented elsewhere, \(31\) the integrals in eqs \(25\) and \(30\) can be written for non-negative integer values of \(l_1, l_2, l_3\), and \(l\) as multinomial expansions without introducing any approximations.

We first define a linear transformation, \(L(g)\), from the laboratory frame of reference into the collision frame of reference. (See Appendix B for the definition of the transformation matrix.) In the collision frame of reference, using the transformation matrix \(L\), the unit vector \(n\) transforms to \(n' = L n\) where

\[ n^+ = [n_1, n_{21}^*, n_{31}^*] = [\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta] \]  
(31)

and \(d n^+ = \sin \theta \, d\theta \, d\phi\), where \(0 \leq \theta \leq \pi/2\) and \(0 \leq \phi \leq 2\pi\) are the collision angles. Using \(n g \cdot n = g \cos \theta\), the integrals in eqs \(25\) and \(30\) become

\[ I_{l,\ell\ell'} = \frac{1}{\pi} \int_{0}^{2\pi} \int_{\theta}^{\theta'} \left[(u_1^*)^l (u_2^*)^\ell (u_3^*)^\ell' \right] D^j \cos \theta \, \sin \theta \, d\theta \, d\phi \]  
(32)

and

\[ F_{l,\ell\ell'} = \frac{1}{\pi} \int_{0}^{2\pi} \int_{\theta}^{\theta'} \left[(u_1^*)^l (u_2^*)^\ell (u_3^*)^\ell' \right] D^j \cos \theta \, \sin \theta \, d\theta \, d\phi \]  
(33)

where, using the identity \(n = L^T n^+\), the primed velocity components can now be expressed as

\[ u_1^* = u_1 - \omega g \cos \theta (L_{11} n_1^* + L_{12} n_{12}^* + L_{13} n_{13}^*) \]  
\[ u_2^* = u_2 - \omega g \cos \theta (L_{21} n_1^* + L_{22} n_{12}^* + L_{23} n_{13}^*) \]  
\[ u_3^* = u_3 - \omega g \cos \theta (L_{31} n_1^* + L_{32} n_{12}^* + L_{33} n_{13}^*) \]  
(34)

and the terms in the expansion of \(D^j\) to first order in \(\sigma\) become

\[ D^j = 1 + (L_{11} n_1^* + L_{12} n_{12}^* + L_{13} n_{13}^*) \frac{\partial D}{\partial x_1} + (L_{21} n_1^* + L_{22} n_{12}^* + L_{23} n_{13}^*) \frac{\partial D}{\partial x_2} + (L_{31} n_1^* + L_{32} n_{12}^* + L_{33} n_{13}^*) \frac{\partial D}{\partial x_3} + O(\sigma^2) \]  
(35)

Note that the components of \(L\) depend on \(g\), but not on the collision angles (see Appendix B).

To simplify the notation, we note that, given the form of eq \(35\), the right-hand sides of eqs \(32\) and \(33\) can be written as

\[ I_{l,\ell\ell'} = I_{l,\ell\ell'}^{(0)} + I_{l,\ell\ell'}^{(1)} \frac{\partial D}{\partial x_1} + I_{l,\ell\ell'}^{(2)} \frac{\partial D}{\partial x_2} + I_{l,\ell\ell'}^{(3)} \frac{\partial D}{\partial x_3} + O(\sigma^2) \]  
(36)

and the components of the vector \(F_{l,\ell\ell'}\) can be written as

\[ F_{l,\ell\ell'} = F_{l,\ell\ell'}^{(0)} + F_{l,\ell\ell'}^{(1)} \frac{\partial D}{\partial x_1} + F_{l,\ell\ell'}^{(2)} \frac{\partial D}{\partial x_2} + F_{l,\ell\ell'}^{(3)} \frac{\partial D}{\partial x_3} + O(\sigma^2) \]  
(37)

The coefficients \(I_{l,\ell\ell'}^{(0)}, I_{l,\ell\ell'}^{(0)}, F_{l,\ell\ell'}^{(0)}\) are determined by integrating over the collision angles \(\theta\) and \(\phi\).

The next step is to use multinomial expansions to express the non-negative integer powers of the primed velocity components appearing in eqs \(32\) and \(33\) in terms of finite sums. For example

\[ (u_1^*)^l = \sum_{i=0}^{l} \sum_{j=0}^{l} \sum_{k=0}^{l} (-\omega g)^i u_1^j u_2^k L_{11} L_{22} L_{33} \times \cos \theta)^i (\sin \theta)^j (\cos \phi)^k (\sin \phi)^l \]  
(38)

The first term in the expansion \((i_l = 0)\) is \(u_1^0\). Analogous expansions result for \((u_2^0)^l\) and \((u_3^0)^l\). Taking the product of these three expansions, the coefficients in eqs \(36\) and \(37\) can be expressed as finite sums of the product of two integrals involving sines and cosines of \(\theta\) and \(\phi\), respectively. (See Appendix C.)

The final results for \(I_{l,\ell\ell'}^{(0)}\) and \(F_{l,\ell\ell'}^{(0)}\) read

\[ I_{l,\ell\ell'}^{(0)} = \sum_{i=0}^{l} \sum_{j=0}^{l} \sum_{k=0}^{l} (-\omega g)^i u_1^j u_2^k \times \cos \theta)^i (\sin \theta)^j (\cos \phi)^k (\sin \phi)^l \]  
(39)

and

\[ F_{l,\ell\ell'}^{(0)} = -\sum_{i=0}^{l} \sum_{j=0}^{l} \sum_{k=0}^{l} (-\omega g)^i u_1^j u_2^k \times \cos \theta)^i (\sin \theta)^j (\cos \phi)^k (\sin \phi)^l \]  
(40)

where (by definition) \(S_{000}^{(0)} = 0\) and the other \(S_{n00}^{(0)}\) coefficients are given in Appendix C. The coefficients \(S_{n00}^{(0)}\) depend only on the components of \(g\) through the components of \(L\) (see Appendix B). Note that

\[ F_{l,\ell\ell'}^{(0)} = -\rho_{l,\ell\ell'} \]  
(41)

Thus, to first order in \(\sigma\), we need only compute \(\rho_{l,\ell\ell'}\) for \(n = 0, 1, 2, 3\). Equations \(39\) and \(40\) provide exact computable expressions for the integrals over the collision angles given the particle masses and velocities before collision for any set of non-negative integers \(l_1, l_2, l_3\). (The expressions are exact for inelastic hard-sphere collisions because they follow directly by integration over the collision angles without introducing any
The moment source term due to collisions can then be written as

\[ C_{\text{ijkl}}^{(0)} + \frac{1}{2} \int m^2 \beta g_{\text{ijkl}} \, g^{(0)} D(f, f^*) \, dm \, du \, \, du^* \]  

and, for \( i = 1 \sim 3 \)

\[ C_{\text{ijkl}}^{(0)} = \frac{1}{2} \int m^2 \beta g_{\text{ijkl}} \, g^{(0)} D(f, f^*) \, dm \, du \, \, du^* \]  

Note that the above expressions are exact for hard-sphere collisions and, thus, contain the exact dependence on the coefficient of restitution \( e \) through the definition of \( \omega \).

Collison Source Terms. The final step is to write the source terms due to the moment \( \{m^2 u_i^l u_j^j u_k^l u_l^j\} \), starting from eq 2 and using eq 23, it is straightforward to show that this source term is given by

\[ I_{\text{ijkl}}^{(0)} = \int_0^\infty \int_0^\infty m^2 \beta C_{\text{ijkl}}^{(0)} \, dm \, du \, \, du^* - \frac{1}{2} \left( \int_0^\infty \int_0^\infty m^2 \beta G_{\text{ijkl}}^{(0)} \, dm \, du \, \, du^* \right) + O(\sigma^2) \]  

Using the expressions in eqs 36 and 37. the integrals on the right-hand side of eq 42 can be rewritten in terms of the coefficients \( F_{\text{ijkl}}^{(0)} \) and \( F_{\text{ijkl}}^{(0)} \), which depend on \( u, g, m, m^*, \) and spatial gradients of \( D \). The latter can be rewritten in terms of \( f \) and \( f^* \) using the identity

\[ D(f, f^*) = f^* \frac{\partial D}{\partial x_i} f = \frac{\partial f^*}{\partial x_i} f - f^* \frac{\partial f}{\partial x_i} \]  

The moment source term due to collisions can then be written as

\[ I_{\text{ijkl}}^{(0)} = \sum_{i=1}^3 \left( C_{\text{ijkl}}^{(0)} - \frac{1}{2} \left( \int_0^\infty \int_0^\infty m^2 \beta G_{\text{ijkl}}^{(0)} \, dm \, du \, \, du^* \right) + O(\sigma^2) \right) \]  

and, for \( i = 1 \sim 3 \)

\[ C_{\text{ijkl}}^{(0)} = \frac{1}{2} \int m^2 \beta g_{\text{ijkl}} \, g^{(0)} D(f, f^*) \, dm \, du \, \, du^* \]  

where

\[ C_{\text{ijkl}}^{(0)} = \int m^2 \beta g_{\text{ijkl}} \, g^{(0)} D(f, f^*) \, dm \, du \, \, du^* \]  

The other terms in the expansion in eq 44 can also be handled using quadrature as discussed in Appendix D. However, for simplicity, we will hereinafter truncate the expansion at order \( \sigma \) and write \( C_{\text{ijkl}}^{(0)} \) as

\[ C_{\text{ijkl}}^{(0)} = \frac{1}{2} \sum_{a=1}^N \sum_{b=1}^N m_n \frac{\partial U_{\text{ijkl}}^{(a)}}{\partial x_i} \frac{\partial U_{\text{ijkl}}^{(b)}}{\partial x_j} \]  

where \( D_{\text{ijkl}}^{(a)} \) represents the partial derivative terms described in Appendix D. [Here, \( h(m, u, m^*, u^*) = \int m^2 \beta g_{\text{ijkl}} \, g^{(0)} D(f, f^*) \, dm \, du \, \, du^* \).] The final expression for \( I_{\text{ijkl}}^{(0)} \) can now be added to the contributions from the other terms in eq 1.

**Moment Transport Equations: General Form.** In previous work,\(^{33}\) the source terms in the moment transport equation were computed for all processes except collisions. By including the Boltzmann–Enskog collision term, the moment transport equation becomes

\[ \frac{\partial \{m^2 u_i^l u_j^j u_k^l u_l^j\}}{\partial t} + \sum_{a=1}^N \left( \frac{\partial}{\partial x_i} m_n \frac{\partial U_{\text{ijkl}}^{(a)}}{\partial x_j} \right) + \frac{\partial}{\partial x_j} m_n \frac{\partial U_{\text{ijkl}}^{(a)}}{\partial x_i} + \frac{\partial}{\partial x_l} m_n \frac{\partial U_{\text{ijkl}}^{(a)}}{\partial x_j} = P_{\text{ijkl}}^{(a)} + O(\sigma^2) \]  

where the node fluxes on the left-hand side are defined by kinetic and collisional contributions

| Table 1. \( P^{(a)}_{\text{ijkl}}(x, u, g) \) Terms for Moments up to Second Order |
|------------------|------------------|------------------|
| \( P_{0000}^{(0)} = 0 \) | \( P_{0010}^{(0)} = -2 \) \( g \) \( v \) \( u \) |
| \( P_{1000}^{(0)} = -4 \) \( g \) \( v \) \( u \) | \( \frac{1}{2} m^2 \beta g_{\text{ijkl}}^{(0)} D(f, f^*) \, dm \, du \, \, du^* \) |
| \( P_{0100}^{(0)} = -4 \) \( g \) \( v \) \( u \) | \( \frac{1}{2} m^2 \beta g_{\text{ijkl}}^{(0)} D(f, f^*) \, dm \, du \, \, du^* \) |

It is significant to note that the above expressions are exact for hard-sphere collisions and, thus, contain the exact dependence on the coefficient of restitution \( e \) through the definition of \( \omega \).
and the first-order collisional-flux terms are

\[ \langle K_{ij,\alpha}^{(n)} \rangle_a = \frac{1}{2} \sum_{\beta=1}^{N} n_{\beta} \rho_{\beta} g_{\beta} \rho_{\alpha} g_{\alpha} \langle \omega_{\alpha \beta} \rangle_{\alpha} \langle \omega_{\alpha \beta} \rangle_{\beta} \] (54)

The source terms on the right hand side of eq 52 are defined by

\[ P_{ij,l,\alpha} = \sum_{a=1}^{N} \sum_{i=1}^{N} n_{a} \rho_{a} g_{a} \rho_{ij,\alpha} (l_{ij,\alpha} A_{3,\beta} + l_{ij,\beta} A_{3,\alpha}) \]

\[ l_{ij,\alpha} A_{3,\alpha} = \sum_{a=1}^{N} \sum_{\beta=1}^{N} n_{a} \rho_{a} g_{a} \rho_{ij,\alpha} \langle \omega_{\alpha \beta} \rangle_{\alpha} \langle \omega_{\alpha \beta} \rangle_{\beta} + \sum_{i=1}^{3} C_{ij,\alpha}^{(i)} (55) \]

The terms on the right-hand side of eq 55 have the following physical significance. The first term corresponds to acceleration due to the external forces (e.g., gravity, drag, etc.). The remaining two terms result from inelastic hard-sphere collisions, namely, the zero-order and first-order collision terms, respectively.

### Moment Transport Equations: Monodisperse Particles.

For the special case of a monodisperse system, the moment equations in eq 52 reduce to

\[ \frac{\partial (u_{ij}^{(1)} \rho_{ij}^{(1)})}{\partial t} + \sum_{a=1}^{N} \left( \frac{\partial}{\partial x_1} \rho_{ij,a} u_{ij,a}^{(1)} + \frac{\partial}{\partial x_2} \rho_{ij,a} u_{ij,a}^{(2)} \right) = P_{ij,a} + O(\sigma^2) \] (56)

with

\[ U_{ij,a}^{(1)} = u_{ij,a}^{(1)} + u_{ij,a}^{(2)} - \langle K_{ij,a}^{(1)} \rangle_a \] (57)

\[ U_{ij,a}^{(2)} = u_{ij,a}^{(1)} + u_{ij,a}^{(2)} - \langle K_{ij,a}^{(2)} \rangle_a \]

\[ U_{ij,a}^{(3)} = u_{ij,a}^{(1)} + u_{ij,a}^{(2)} - \langle K_{ij,a}^{(3)} \rangle_a \]

\[ \langle K_{ij,a}^{(n)} \rangle_a = 3 \sum_{i=1}^{N} v_{i} g_{i} \rho_{ji,a} \langle \omega_{\alpha \beta} \rangle_{\alpha} \langle \omega_{\alpha \beta} \rangle_{\beta} \] (58)

and (with summations over the \( \alpha \) velocity abscessas)

<table>
<thead>
<tr>
<th>Table 4. ( f_{ij,\alpha}^{(n)}(\omega_{\alpha},u_{\alpha},g) ) Terms for Second-Order Moments</th>
</tr>
</thead>
<tbody>
<tr>
<td>( f_{ij,\alpha}^{(1)} = \langle (u_{ij}^{(1)} g_{i}) (u_{ij}^{(1)} g_{j}) \rangle - \langle u_{ij}^{(1)} g_{i} \rangle \langle u_{ij}^{(1)} g_{j} \rangle )</td>
</tr>
<tr>
<td>( f_{ij,\alpha}^{(2)} = \langle (u_{ij}^{(2)} g_{i}) (u_{ij}^{(2)} g_{j}) \rangle - \langle u_{ij}^{(2)} g_{i} \rangle \langle u_{ij}^{(2)} g_{j} \rangle )</td>
</tr>
<tr>
<td>( f_{ij,\alpha}^{(3)} = \langle (u_{ij}^{(3)} g_{i}) (u_{ij}^{(3)} g_{j}) \rangle - \langle u_{ij}^{(3)} g_{i} \rangle \langle u_{ij}^{(3)} g_{j} \rangle )</td>
</tr>
</tbody>
</table>

where \( P_{ij,a} \) are given by

\[ P_{ij,a} = \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} v_{\alpha} v_{\beta} g_{\alpha} \rho_{\alpha} g_{\alpha} \rho_{\beta} g_{\beta} \] (59)

and \( \sigma \) is a fixed number.

The mean particle momentum equation resulting from eq 56 can be written in the “standard” form as

\[ \frac{\partial \rho_{ij}^{(1)}}{\partial t} + \frac{\partial}{\partial x_1} (\rho_{ij}^{(1)} u_{ij}^{(1)}) + \frac{\partial}{\partial x_2} (\rho_{ij}^{(1)} u_{ij}^{(2)}) = Q_{ij} \] (61)

where \( Q_{ij} \) has kinetic and collisional contributions

\[ Q_{ij} = \rho_{ij}^{(1)} + \frac{2}{5} \sum_{a=1}^{N} \sum_{\beta=1}^{N} (1 + \epsilon_{\alpha \beta}) v_{\alpha} v_{\beta} \left[ \frac{1}{2} g_{\alpha} g_{\beta} \delta_{ij} - g_{i} g_{j} \rho_{\alpha \beta} \right] \] (62)

and \( \epsilon_{\alpha \beta} = \epsilon(\sigma, g_{\beta}) \) is the restitution coefficient, which can depend on the relative velocity of the two abscessas. The velocity covariance tensor is defined by \( \sigma_{ij} = \langle (u_{ij} - U_{ij})(u_{ij} - U_{ij}) \rangle / \rho \). The higher acceleration is defined by \( A_{ij} = \sum_{a=1}^{N} \rho_{ij,a} A_{3,\alpha} \). The higher-order collision term is

\[ P_{ij,a} = -\frac{2}{5} \sum_{a=1}^{N} \sum_{\beta=1}^{N} (1 + \epsilon_{\alpha \beta}) v_{\alpha} v_{\beta} \left[ \frac{1}{2} g_{\alpha} g_{\beta} \delta_{ij} + g_{i} g_{j} \rho_{\alpha \beta} \right] \] (63)

and as shown in Appendix D, \( D_{ij}^{(n)} = -D_{ij}^{(n)} \), which implies that \( P_{ij} = 0 \) (i.e., the higher-order collision term conserves momentum).
Note that \( \mathbf{Q} \) is a symmetric second-order tensor. Defining the granular temperature as
\[
T = \frac{1}{3} (\sigma_{11} + \sigma_{22} + \sigma_{33})
\] (65)
the granular pressure can be defined from the trace of \( \mathbf{Q} \) as
\[
p = \nu T + \frac{g_0}{3} \sum_{\alpha=1}^{N_x} \sum_{\beta=1}^{N_x} (1 + e_{\alpha\beta}) \nu_{\alpha \beta} \sigma_{\alpha \beta}
\] (66)
(Note that, for clarity, we do not introduce the solids density \( \rho_s \) in the definition of granular pressure. Likewise, the mean solids momentum will be defined by \( \rho_s \nu \). Because \( \rho_s \) is constant, we can take \( \rho = 1 \).) The granular stress tensor \( \tau \), found from the decomposition \( \mathbf{Q} = \tau + p \mathbf{I} \), is then given by
\[
\tau_{ij} = \nu (\sigma_{ij} - T \delta_{ij}) + \frac{2g_0}{5} \sum_{\alpha=1}^{N_x} \sum_{\beta=1}^{N_x} (1 + e_{\alpha\beta}) \nu_{\alpha \beta} \left(g_{\alpha \beta} \sigma_{\alpha \beta} - \frac{1}{3} \delta_{\alpha \beta} \right)
\] (67)
In hydrodynamic models, the granular pressure and stress tensor must be closed in terms of the hydrodynamic variables \( \nu \) and \( T \) (i.e., an equation of state and a constitutive relation must be derived).

In the special case where \( e_{\alpha\beta} \) is independent of collision velocity (\( e_{\alpha\beta} = e \)), the granular pressure and stress tensor reduce to
\[
p = \nu T [1 + 2\nu (1 + e) g_0]
\] (68)
which is the same as the expression found elsewhere,\(^{15}\) and
\[
\tau_{ij} = \left( 1 + \frac{4g_0 e (1 + e)}{5} \right) \nu (\sigma_{ij} - T \delta_{ij})
\] (69)
respectively. In the context of hydrodynamic models, \( p \) in eq 68 is closed, but \( \sigma_{ij} \) must be closed by introducing a Chapman–Enskog expansion about the equilibrium distribution function, which is valid only for small Knudsen numbers. In contrast, quadrature-based moment methods solve the transport equation for the second-order moments, so \( \tau \) from eq 69 will be in closed form for arbitrary Knudsen number. In the limit \( Kn \ll 1 \), it can be shown using a Chapman–Enskog expansion of the moment equations\(^{20}\) that the two expressions found for the stress tensor agree to first order in \( Kn \).

Finally, we should note that, even though eq 68 is the same in both theories, the actual values of \( p \) are different because the transport equations for \( T \) are not the same. For example, the expression for the “heat” flux in the moment method involves third-order moments and (except for \( Kn \ll 1 \)) cannot be written in terms of the gradient of the \( T \). Thus, for a given application, the granular temperature field predicted by the moment method will not be the same as the one predicted by a hydrodynamic model. Then, because of the coupled nature of the transport equations, the solids volume fraction and mean particle velocity fields predicted by the two models will also be different.

**Moment Transport Equations: Polydisperse Particles.** Because the masses \( m_a \) are constant, it is possible to decompose eq 52 into transport equations for the velocity moments \( \langle u_i u_j u_k \rangle_a \). The first step is to replace the summations over the abscissas as follows
\[
\sum_{a=1}^{N_a} \sum_{i=1}^{N_x} \sum_{j=1}^{N_x} (n_{a_i}, \mathbf{u}_a) \rightarrow \sum_{a=1}^{N_a} \sum_{i=1}^{N_x} \sum_{j=1}^{N_x} (n_{a_i}, \mathbf{u}_a)
\] (70)

Then, to write the equation using the particle density \( \rho_a \) and solids volume fraction \( \nu_a \), we use the identity \( m_a \nu_a = \rho_a \nu_a \) and rescale the moments such that the zero-order moment is \( \langle 1 \rangle_a = \rho_a \nu_a \). It then follows from the definition of the velocity moments that
\[
\frac{\partial \langle u_i^l u_j^l u_k^l \rangle_a}{\partial t} + \frac{\partial}{\partial x_k} (\rho_a \nu_a U_k^{(l)} u_i^l u_j^l u_k^l) + \frac{\partial}{\partial x_j} (\rho_a \nu_a U_j^{(l)} u_i^l u_j^l u_k^l) + \frac{\partial}{\partial x_i} (\rho_a \nu_a U_i^{(l)} u_i^l u_j^l u_k^l) = \langle P_{i, j, l} \rangle_a + O(d_a^2)
\] (71)
wherein spatial fluxes are defined using
\[
U_i^{(1)} = u_i^{(1)} + d_i + \langle \nu_{\alpha} \rangle_a
\]
\[
U_i^{(2)} = u_i^{(2)} + d_i + \langle \nu_{\alpha} \rangle_a
\]
\[
U_i^{(3)} = u_i^{(3)} + d_i + \langle \nu_{\alpha} \rangle_a
\]
and the source terms on the right-hand side are defined by
\[
\langle K_{i, j, l} \rangle_a = \sum_{\nu=1}^{N_a} \nu \sum_{i=1}^{N_x} \sum_{j=1}^{N_x} \sum_{l=1}^{N_x} \nu_i^l g_{\nu_i^l} \langle \nu_{\alpha} \rangle_a \langle \nu_{\alpha} \rangle_a \langle \nu_{\alpha} \rangle_a
\]
(72)
with \( d_a \) equal to the particle diameter and
\[
\lambda = \frac{d_a + d_r}{2d_r}
\] (75)
At the end of eq 74, \( \langle D_{i, j, l} \rangle_a \) represents the partial derivative terms described in Appendix D, calculated for the case of constant \( m_a \).

For comparison with multifluid models for polydisperse gas–particle flows, we can derive explicit equations for the solids volume fraction \( \nu_a \) and average particle velocity \( U_a \) of \( \alpha \)-type particles, defined by
\[
\nu_a = \sum_{i=1}^{N_a} \nu_i
\] (76)
and
\[
U_a = \frac{1}{\nu_a} \sum_{i=1}^{N_a} \nu_i \mathbf{u}_i
\] (77)
respectively, starting from eq 71. From their definitions, we have \( \partial \nu_a / \partial t = 0 \) and \( \partial \rho_a / \partial t = 0 \). Thus, the continuity equation for each \( \alpha \) reduces to the usual expression
\[
\frac{\partial \rho_a \nu_a}{\partial t} + \nabla \cdot (\rho_a \nu_a \mathbf{U}_a) = 0
\] (78)
Note that we retain a separate mean velocity for each “phase.”
α, instead of using the mass-average velocity of all \( N_m \) phases. (Using 1 = \( \sum \rho A \), the phase-average density is defined by \( \rho = \sum \rho A \) and the mass-average velocity \( \bar{U} \) is defined by \( \bar{U} = \sum \rho A \bar{v} A \)). For this reason, the continuity equation does not contain a “diffusion” term because of the mean relative velocity between phases.24,25

The mean momentum equation for \( \alpha \)-type particles resulting from eq 71 can be written as

\[
\frac{d \rho A v^a U^a}{d t} + \nabla \cdot (\rho A v^a U U^a + \rho A Q^a) = \rho A (A)_a + \rho A (P)_a
\]

(79)

where \( \langle Q \rangle_a \) has kinetic and collisional contributions

\[
\langle Q \rangle_a = v_\alpha \sigma^\alpha + 2 \sum_{\beta=1}^{N} g_{0,0} \mu^\alpha \zeta^\beta \sum_{i=1}^{N_a} \sum_{j=1}^{N} [1 + e_{\alpha \beta}(g_{ij}^\beta)] v_i v_j \times \left( \frac{1}{2} \delta_{ij}^\beta I + g_{ij}^\beta g_{ij}^\beta \right)
\]

(80)

\( e_{\alpha \beta} \) is the restitution coefficient for collisions between \( \alpha \)-type and \( \beta \)-type particles, and

\[
\mu_{\alpha \beta} = \frac{2 m_\beta}{m_\alpha + m_\beta} = \frac{2 \rho \beta \sigma_\beta^3}{\rho_\alpha \sigma_\alpha^3 + \rho_\beta \sigma_\beta^3}
\]

(81)

The velocity-covariance tensor for an \( \alpha \)-type particle is defined by

\[
\sigma_a = \frac{1}{v^a} \sum_{i=1}^{N_a} v^a_i (u^a_i - U^a)(u^a_i - U^a)
\]

(82)

The average acceleration is defined by

\[
\langle A \rangle_a = \sum_{i=1}^{N_a} v^a_i A^a
\]

(83)

The collision term is

\[
\langle P \rangle_a = 3 \sum_{\beta=1}^{N} \frac{g_{0,0} \mu^\alpha \zeta^\beta}{\sigma_\beta^3} \times \sum_{i=1}^{N_a} \sum_{j=1}^{N} [1 + e_{\alpha \beta}(g_{ij}^\beta)] v_i v_j g_{ij}^\beta (u_i - u_j) - \frac{4}{5} \sum_{\beta=1}^{N} \frac{g_{0,0} \mu^\alpha \zeta^\beta}{\sigma_\beta^3} \sum_{i=1}^{N_a} \sum_{j=1}^{N} [1 + e_{\alpha \beta}(g_{ij}^\beta)] v_i v_j D_{ij}^\beta
\]

(84)

In this expression, \( D_{ij}^\beta \) is a first-order tensor involving the derivatives of the weights and abscissas, found as described in Appendix D. As a consequence of the conservation of total momentum, it can be shown that \( \sum \rho A (P)_a = 0 \).

For the case where \( e_{\alpha \beta} \) does not depend on the relative velocity, the components of \( D_{ij}^\beta \) can be written as

\[
D_{ij}^\beta = \sum_{j=1}^{N} \left( \frac{1}{2} \delta_{ij}^\beta \right) \frac{\partial \ln v_j}{\partial x_j} + \frac{\partial \ln v_i}{\partial x_j}
\]

and

\[
\sum_{j=1}^{N} \sum_{k=1}^{N} (g_{ij} \delta_{jk} + g_{jk} \delta_{ik} + g_{ki} \delta_{ij}) \frac{\partial}{\partial x_j} (u_{ki} + u_{ik})
\]

(85)

From this expression, it is easily shown that \( D_{ij}^\beta = - D_{ji}^\beta \), which is true in general. This property is useful for demonstrating that the total momentum is conserved (see Appendix D).

Finally, we note that, for the case where \( e_{\alpha \beta} \) depends on the relative velocity, \( D_{ij}^\beta \) has the same form as in eq 85 but with additional partial derivatives involving \( e_{\alpha \beta} \).

As was done in the monodisperse case, we can define a granular temperature for each \( \alpha \) as

\[
T_\alpha = \frac{1}{3} (\sigma_{11} + \sigma_{22} + \sigma_{33})
\]

(86)

Likewise, a granular pressure can be defined from the trace of \( \langle Q \rangle_a \) as

\[
p_a = v_a T_a + \frac{1}{3} \sum_{\beta=1}^{N_a} \sum_{i=1}^{N_a} \sum_{j=1}^{N_a} [1 + e_{\alpha \beta}(g_{ij}^\beta)] v_i v_j g_{ij}^\beta
\]

(87)

The particle stress tensor \( \tau_a \) is found from the decomposition \( \langle Q \rangle_a = \tau_a + p_a I \). For the special case where \( e_{\alpha \beta} \) is independent of collision velocity, the granular pressure reduces to

\[
p_a = v_a T_a + \frac{1}{3} \sum_{\beta=1}^{N_a} \sum_{i=1}^{N_a} \sum_{j=1}^{N_a} [1 + e_{\alpha \beta}(g_{ij}^\beta)] v_i v_j g_{ij}^\beta
\]

(88)

Note that the granular pressure for each phase depends on the granular temperatures in all phases and on the differences in the mean velocities. The latter is a direct result of using the phase-average velocity in eqs 78 and 79 and will be true for any kinetic theory that uses phase-average velocities. (This follows from the fact that \( p_a \) can be expressed in closed form in terms of velocity moments to second order.) The granular stress tensor will also be a complicated function of the granular temperatures and mean velocities. In most multifluid models for polydisperse particles, simplified versions of eq 88 and of \( T_a \) are used that do not depend on the mean velocity differences.26 Likewise, a simplified version of eq 84 is used where \( D_{ij}^\beta \) is neglected and the remaining terms (which are usually called the solid—solid drag terms and which, because they involve the magnitude of the velocity difference, cannot be closed in terms of the lower-order moments) are closed in terms of the mean velocities (i.e., it is customary to neglect contributions due to second- and higher-order moments). In the quadrature-based moment method developed in this work, such simplifications are avoided.

Discussion and Conclusions

The principal result reported in this work is the moment transport (eq 52) for polydisperse gas—particle flows. Starting from the Boltzmann—Enskog gas—particle flows. Starting from the Boltzmann—Enskog kinetic equation for moderately dense binary collisions, the moment transport equations were derived without ad hoc assumptions or other simplifications by directly evaluating the integrals over the collision angles in closed form. In this manner, the exact dependence on the degree of elasticity is retained in the moment transport equations. The moment model is therefore a valid representation of the closed kinetic equation (where “closed” in this context refers to the truncation of the Taylor series and closure of the pair correlation function as described in Appendix A) for any value of \( e \), including cases where \( e \) depends on the relative velocity. A quadrature-based moment method, valid for arbitrary Knudsen numbers, was used to evaluate the integrals with the velocity distribution.
function. Consistent with the Taylor-series expansion in powers of particle diameter, the Boltzmann–Enskog collision integral was determined to first order. The moment model is thus valid for cases where the particle diameter is small compared to the system size. To verify the model, the transport equations for the solids volume fraction and mean particle momentum were compared to the expressions derived using the Chapman–Enskog expansion and, for special cases, were found to yield identical results for the granular pressure (as well as any other quantity that can be computed in closed form).

The next step needed to implement the moment model for gas–particle flow simulations is to develop a numerical algorithm for treating the moment transport equations. In the Boltzmann limit, such an algorithm already exists,\textsuperscript{7,27,29} so the next step will be to implement the existing kinetic-based method discussed in Appendix E to handle the first-order collisional-flux term in eq 52. Because the flux term resembles classical hyperbolic fluxes found in compressible gas flows, it should be relatively straightforward to implement a finite-volume solver\textsuperscript{30} for the moment transport equations that is valid in the limit where the collision-flux term is dominant (i.e., the hydrodynamic limit). Depending on the relative importance of finite-size effects, it might also be possible to neglect the higher-order collision term in eq 59, which introduces gradients in the weights and abscissas. For example, convection-dominated gas–particle flows should be adequately described by the Boltzmann collision term in eq 59. It is important to note that such a simplification is possible for polydisperse flows when the model includes a separate mean momentum equation for each particle type, as opposed to using the average velocity of all types. Models of the latter type require “species” diffusion coefficients\textsuperscript{24,25} to model the relative velocity between different types of particles. As described elsewhere,\textsuperscript{8} it might be possible to reduce the computational cost of evaluating the collision terms by utilizing a kinetic model\textsuperscript{40} for hard-sphere collisions in place of the exact collision integrals developed in this work. The coupling with the gas-phase continuity and momentum equations will also be an important consideration for moderately dense gas–particle flows.\textsuperscript{27} In particular, it will be necessary to handle dense cases where \( g_0 \) approaches infinity near close packing. However, knowledge on how to treat such difficulties is already available based on previous work with hydrodynamic models.\textsuperscript{41}

**Acknowledgment**

We gratefully acknowledge support from National Energy Technology Laboratory of the U.S. Department of Energy.

**Appendix A: Derivation of the Moment Integral**

As discussed in the main text, the multidimensional integral in eq 23 corresponding to the source term for the velocity moments due to Boltzmann–Enskog collisions can be expressed in a more convenient form using the properties of the hard-sphere collision integral.\textsuperscript{31,34} In this appendix, we describe the derivation of eq 23.

For the sake of generality, we consider the change in property \( \psi \equiv \psi(u,m) \) due to the collision term for fixed values of \( m \) and \( m^* \) in eq 3. The corresponding collision term is given by

\[
B[\psi(u,m)] = \int_{R^n} \psi(u,m) B(m,m^*,u) \, du
\]

where

\[
B(m,m^*,u) = \frac{1}{\pi} \int_{R^n} \int_{S^n} \left[ g(t,x,m,u''x - on,m^*,u'') - f(t,x,m,u;x + on,m^*,u) \right] |g \cdot n| \, dn \, du
\]

The right-hand side of eq 89 can be rewritten, using the definition for \( \psi \), as

\[
B[\psi(u,m)] = \frac{1}{\pi} \int_{R^n} \int_{R^n} \int_{S^n} \psi(u,m) f(t,x,m,u'';x - on,m^*,u'') |g \cdot n| \, dn \, du
\]

Adding the pair distribution function \( f^{(2)}(t,x,m,u;x - on,m^*,u) \) to \( f^{(2)}(t,x,m,u;x + on,m^*,u) \) in the above equation and then subtracting it gives

\[
B[\psi(u,m)] = \frac{1}{2\pi} \int_{R^n} \int_{R^n} \int_{S^n} \psi(u',m) - \psi(u,m) \left[ f^{(2)}(t,x,m,u;x - on,m^*,u) + f^{(2)}(t,x,m,u;x + on,m^*,u) \right] |g \cdot n| \, dn \, du
\]

which can be re-expressed using Taylor-series approximations about \( f^{(2)}(t,x - 1/2on,m,u;x + 1/2on,m^*,u) \) as

\[
B[\psi(u,m)] = C[\psi(u,m)] - \frac{1}{2} \nabla \cdot G[\psi(u,m)]
\]

where the collisional source term is given by

\[
C[\psi(u,m)] = \frac{1}{\pi} \int_{R^n} \int_{R^n} \int_{S^n} \left[ \psi(u',m) - \psi(u,m) \right] \left[ \frac{1}{2} \frac{\nabla}{(2k)^{1/2}} \right] f^{(2)}(t,x - 1/2on,m,u;x + 1/2on,m^*,u) |g \cdot n| \, dn \, du
\]

and the collisional-flux term is given by

\[
B[\psi(u,m)] = \int_{R^n} \psi(u,m) B(m,m^*,u) \, du
\]
$G[\psi(u, m)] = -\frac{\sigma}{\pi} \int_{4\pi} \int_{S^2} n[\psi(u', m) - \psi(u, m)] \times 
abla^2 f(t, x - \frac{1}{2}\sigma n, m, u, x + \frac{1}{2}\sigma n, m^*, u^*) \cdot \nabla n \, dn \, du^* \, du(96)$

In the main text, a first-order approximation is used wherein the summation terms for $k = 1, ..., \infty$ are neglected.

The pair correlation function appearing in the collisional source and flux terms can be expressed in terms of the product of two single-particle velocity distribution functions and a radial distribution function as

$$f^{(2)}(t, x - \frac{1}{2}\sigma n, m, u, x + \frac{1}{2}\sigma n, m^*, u^*) = g_0(x - \frac{1}{2}\sigma n, m, x + \frac{1}{2}\sigma n, m^*, u^*) \times f(t, x - \frac{1}{2}\sigma n, m, u) \times f(t, x + \frac{1}{2}\sigma n, m^*, u^*) \tag{97}$$

The radial distribution function can be modeled as a function of the particle volume fractions and diameters. Neglecting the spatial gradients of $g_0$ and using Taylor-series approximations of the single-particle distribution functions about $f(t, x, m, u)$ then yields

$$f^{(2)}(t, x - \frac{1}{2}\sigma n, m, u, x + \frac{1}{2}\sigma n, m^*, u^*) = g_0(x - \frac{1}{2}\sigma n, m, x + \frac{1}{2}\sigma n, m^*, u^*) \times \left(1 + \frac{1}{2}\sigma n \cdot \nabla \ln \left[ \frac{f(t, x, m^*, u^*)}{f(t, x, m, u)} \right] + O(\sigma^2) \right) \tag{98}$$

With this expression, the collision source term in eq 94 in now closed in terms of the single-particle distribution function. Specifically for $\psi = u_i^i u_i^j u_i^k u_i^l$, the expressions for $C_i^2 j^2 j^3 j^3$ and $G_i^2 j^2 j^3 j^3$ in eq 23 follow from the approximations (to first order) for $C(\psi)$ and $G(\psi)$ appearing in eq 95 and 96, combined with eq 98 and neglecting second-order terms.

**Appendix B: Transformation Matrix**

The transformation matrix from the laboratory frame ($x$) to the collision frame of reference ($\hat{x}$) depends only on the relative velocity vector $g = u - u^*$. By convention, $g$ is aligned with the $x_1$ axis. Thus, the orthonormal transformation matrix defined such that $x^* = L x$ can be written as

$$L = \begin{bmatrix} \sin \phi_1 & -\cos \phi_1 & 0 \\ \cos \theta_1 \cos \phi_1 & \cos \theta_1 \sin \phi_1 & -\sin \theta_1 \\ \sin \theta_1 \cos \phi_1 & \sin \theta_1 \sin \phi_1 & \cos \theta_1 \end{bmatrix} \tag{99}$$

where the spherical angles $0 \leq \theta_1 \leq \pi$ and $0 \leq \phi_1 \leq 2\pi$ are related to $g$ by

$$g_1 = g \sin \theta_1 \cos \phi_1$$
$$g_2 = g \sin \theta_1 \sin \phi_1$$
$$g_3 = g \cos \theta_1 \tag{100}$$

Note that the ordering of the first and second rows of $L$ is not important and that $L$ is defined only for $g > 0$. In the main text, the components of $L$ are denoted as $L_{ij}(g/g)$, but they could equally well be denoted by $L_{ij}(\theta_i, \phi_i)$.

The following code illustrates how the spherical angles can be computed from $g/g$:

```plaintext
if norm(g) == 0 return
gn = g/norm(g);
theta1 = acos(gn(3));
sth = sin(theta1);
phi1 = 0;
if sth ~= 0
  if gn(2) > 0
    phi1 = acos(gn(1)/sth);
  elseif gn(2) < 0
    phi1 = pi + acos(-gn(1)/sth);
  elseif gn(1) < 0
    phi1 = pi;
end
end
```

Finally, note that the reader should not confuse the spherical angles $(\theta_1, \phi_1)$ (which parametrize $g/g$) with the collision angles $(\theta, \phi)$ (which parametrize $n$). Indeed, the integrals over the collision angles are done with fixed values of the spherical angles (i.e., fixed values of $g$).

**Appendix C: Integrals over the Collision Angles**

The coefficients $S_{ij}^{(n)}$ appearing in the main text that result from integrating over the collisions angles are defined for $i_1 + i_2 + i_3 > 0$ by

$$S_{ij}^{(n)} = \sum_{i_1 i_2} L_{r_{i_1}} L_{r_{i_2}} L_{i_1} L_{i_2} K_{i_1 j_1} K_{i_2} K_{j_2} K_{j_3} K_{j_4} \tag{101}$$

and for $n = 1-3$ by

$$S_{ij}^{(1)} = \sum_{i_1 i_2} L_{r_{i_1}} L_{r_{i_2}} L_{i_1} L_{i_2} K_{i_1 j_1} K_{i_2} K_{j_2} K_{j_3} K_{j_4} K_{i_1} K_{i_2} K_{j_3} K_{j_4} \tag{102}$$

$$S_{ij}^{(2)} = \sum_{i_1 i_2} L_{r_{i_1}} L_{r_{i_2}} L_{i_1} L_{i_2} K_{i_1 j_1} K_{i_2} K_{j_2} K_{j_3} K_{j_4} K_{i_1} K_{i_2} K_{j_3} K_{j_4} \tag{103}$$

$$S_{ij}^{(3)} = \sum_{i_1 i_2} L_{r_{i_1}} L_{r_{i_2}} L_{i_1} L_{i_2} K_{i_1 j_1} K_{i_2} K_{j_2} K_{j_3} K_{j_4} K_{i_1} K_{i_2} K_{j_3} K_{j_4} \tag{104}$$

$$S_{ij}^{(4)} = \sum_{i_1 i_2} L_{r_{i_1}} L_{r_{i_2}} L_{i_1} L_{i_2} K_{i_1 j_1} K_{i_2} K_{j_2} K_{j_3} K_{j_4} K_{i_1} K_{i_2} K_{j_3} K_{j_4} \tag{105}$$

where the summation operator is defined by

$$S_{ij}^{(k)} = \sum_{i_1 i_2} L_{r_{i_1}} L_{r_{i_2}} L_{i_1} L_{i_2} K_{i_1 j_1} K_{i_2} K_{j_2} K_{j_3} K_{j_4} K_{i_1} K_{i_2} K_{j_3} K_{j_4} \tag{106}$$
\[
\sum_{j_1,j_2,j_3} = \sum_{i_1}^{i_1} \sum_{i_2}^{i_2} \sum_{j_4}^{j_4} \sum_{j_5}^{j_5} \sum_{j_6}^{j_6} \sum_{j_7}^{j_7} \sum_{j_8}^{j_8} (i_1(i_2)(i_3)(j_4)(j_5)(j_6)(j_7)(j_8))
\]

(106)

and \(i = i_1 + i_2 + i_3, j = j_4 + j_5 + j_6, k = k_1 + k_2 + k_3\). As described in Appendix B, the components of \(L\) can be parametrized in terms of two spherical angles \(\theta_i\) and \(\phi_i\), which are found from \(\mathbf{g}\). Thus, each coefficient \(S_{ijk}^{(ij)}\) (for fixed values of its indices) depends on \(0 \leq \theta_i \leq \pi\) and \(0 \leq \phi_i \leq 2\pi\) and can therefore be stored in a two-dimensional look-up table for efficient computations.

The constants \(K_{ijk}\) are defined by 10 integrals over the collision angles

\[
K_{ijk}^{(0)} = A_{i-j-k} B_{i-k-j} \quad K_{ijk}^{(1)} = A_{i-j-k} B_{i-k-j+1} \quad K_{ijk}^{(2)} = A_{i-j-k} B_{i-k-j+1} \quad K_{ijk}^{(3)} = A_{i-j-k} B_{i-k-j+1}
\]

(107)

where the functions \(A\) and \(B\) can be written in terms of the beta function \(B(x,y)\) as

\[
A_{a,b} = \frac{1}{\pi} \int_0^{\pi} (\sin \phi)^a (\cos \phi)^b d\phi = [1 + (-1)^a][1 + (-1)^b] \frac{1}{2a+1} \times B\left(\frac{a+1}{2}, \frac{b+1}{2}\right)
\]

(108)

and

\[
B_{a,b} = \int_0^{2\pi} (\cos \theta)^a (\sin \theta)^b d\theta = \frac{1}{2} B\left(\frac{a+2}{2}, \frac{b+2}{2}\right)
\]

(109)

The beta function is related to the gamma function \(\Gamma(x)\) by

\[
B(x,y) = \frac{\Gamma(x) \Gamma(y)}{\Gamma(x+y)}
\]

Some useful identities for evaluating \(A\) and \(B\) are \(\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}\) and \(\Gamma(1+x) = x!\).

Appendix D: Quadrature Closure of Higher-Order Collision Terms

In Appendix A and the main text, we showed that the Boltzmann–Enskog collision term generates for each moment an expansion in powers of \(\sigma\) with coefficients \(C_{ijk}^{(ij)}\) and \(G_{ijk}^{(ij)}\). The zero-order terms (\(i = 0\)) are treated in the main text using quadrature. Here, we describe how the higher-order terms can be represented using quadrature.

The principal technical difficulty in treating the higher-order terms is the presence of the expression

\[
D(f,f^*) = f \frac{\partial f^*}{\partial x_i} - f^* \frac{\partial f}{\partial x_i}
\]

(110)

which involves partial derivatives of the density function. For clarity, let us consider a closely related problem defined by

\[
H^{(i)} = \int h(m, u, m^*, u^*) D(f, f^*) \, dm \, du \, dm^* \, du^*
\]

(111)

where \(h\) is an arbitrary function of its arguments. Note that the coefficients defined in eqs 47 and 48 have the same form as eq 111, differing only by how \(h\) is defined for each case.

In the quadrature method of moments, the density functions are represented by sums of delta functions

\[
f = \sum_{\alpha=1}^{N} n_{\alpha} \delta(m - m_{\alpha}) \delta(u - u_{\alpha})
\]

and

\[
f^* = \sum_{\beta=1}^{N} n_{\beta} \delta(m^* - m_{\beta}) \delta(u^* - u_{\beta})
\]

(112)

where \(\delta(x) = \delta(x_1) \delta(x_2) \delta(x_3)\). Thus, by denoting the first derivative of a delta function as \(\delta^{(1)}(x)\) with the property

\[
\int_{x}^{x+\delta} \delta^{(1)}(x - y) \, g(y) \, dx = -\frac{dg}{dx}(y)
\]

we can write the partial derivative of the density function as

\[
\frac{\partial f}{\partial x_j} = \sum_{\alpha=1}^{N} n_{\alpha} \delta(m - m_{\alpha}) \delta(u - u_{\alpha}) \times
\]

\[
\left[ \frac{1}{n_{\alpha}} \frac{\partial n_{\alpha}}{\partial x_j} \delta^{(1)}(m - m_{\alpha}) \frac{\partial u_{\alpha}}{\partial x_j} \delta^{(1)}(u - u_{\alpha}) - \frac{\partial m_{\alpha}}{\partial x_j} \delta^{(1)}(m - m_{\alpha}) \frac{\partial u_{\alpha}}{\partial x_j} \delta^{(1)}(u - u_{\alpha}) - \frac{\partial u_{\alpha}}{\partial x_j} \delta^{(1)}(u - u_{\alpha}) \right]
\]

(113)

with an analogous expression for the partial derivative of \(f^*\). Using these results, it is straightforward to construct the quadrature representation of \(D(f,f^*)\) defined in eq 110 as

\[
D(f,f^*) = \sum_{a=1}^{N} \sum_{b=1}^{N} n_{a} n_{b} \delta(m - m_{a}) \delta(u - u_{a}) \delta(m^* - m_{b}) \delta(u^* - u_{b}) \times
\]

\[
\left[ \frac{1}{n_{a}} \frac{\partial n_{a}}{\partial x_j} - \frac{1}{n_{b}} \frac{\partial n_{b}}{\partial x_j} + \frac{\partial m_{a}}{\partial x_j} \delta^{(1)}(m - m_{a}) \frac{\partial u_{a}}{\partial x_j} \delta^{(1)}(u - u_{a}) - \frac{\partial m_{b}}{\partial x_j} \delta^{(1)}(m - m_{b}) \frac{\partial u_{b}}{\partial x_j} \delta^{(1)}(u - u_{b}) - \frac{\partial u_{a}}{\partial x_j} \delta^{(1)}(u - u_{a}) - \frac{\partial u_{b}}{\partial x_j} \delta^{(1)}(u - u_{b}) - \frac{\partial u_{a}}{\partial x_j} \delta^{(1)}(u - u_{a}) \right]
\]

(114)

There are 10 terms inside the square brackets on the right-hand side of eq 114, each of which will generate a separate term from eq 111.

The first two terms in \(H^{(i)}\) yield

\[
H_1 = \sum_{a=1}^{N} \sum_{b=1}^{N} \left( n_{a} \frac{\partial n_{a}}{\partial x_j} - n_{b} \frac{\partial n_{b}}{\partial x_j} \right) h_{a\beta}
\]

(115)

where \(h_{a\beta} = h(m_{a}, u_{a}, m_{b}, u_{b})\). The remaining terms involve partial derivatives of \(h\)

\[
H_2 = \sum_{a=1}^{N} \sum_{b=1}^{N} n_{a} n_{b} \left( \frac{\partial h_{a\beta} \partial m_{a}}{\partial x_j} \delta^{(1)}(m^* - m_{b}) - \frac{\partial h_{a\beta} \partial m_{a}}{\partial x_j} \delta^{(1)}(u^* - u_{b}) \right)
\]

(116)
Collecting the terms, we can express $H^{(i)}$ as

$$H^{(i)} = \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} n_{\alpha} n_{\beta} h_{\alpha \beta} D^{(i)}_{\alpha \beta}$$

(120)

where

$$D^{(i)}_{\alpha \beta} = \frac{\partial}{\partial x_{\alpha}} \ln n_{\beta} + \frac{\partial}{\partial x_{\beta}} \ln n_{\alpha} + \frac{\partial u_{\alpha}^{*}}{\partial x_{\beta}} \frac{\partial}{\partial x_{\alpha}} \ln h_{\alpha \beta} + \frac{\partial u_{\beta}^{*}}{\partial x_{\alpha}} \frac{\partial}{\partial x_{\beta}} \ln h_{\alpha \beta} + \frac{\partial}{\partial x_{\alpha}} \ln h_{\alpha \beta} + \frac{\partial}{\partial x_{\beta}} \ln h_{\alpha \beta}$$

(121)

When applying these formulas to construct the higher-order coefficients defined in the main text, the most arduous task is the evaluation of the eight partial derivatives appearing in eq 121 of the term representing $h$ for each coefficient.

As an example, we first demonstrate for the case where $m_{\alpha} = m$ is constant (i.e., monodisperse particles) that the higher-order terms in the mean momentum equation are zero. The moments corresponding to the mean momentum are zero. The moment equation then has the form

$$\frac{\partial}{\partial x_{i}} \sum_{\alpha=1}^{N} n_{\alpha} \frac{\partial}{\partial x_{i}} \ln n_{\alpha} + \frac{\partial}{\partial x_{i}} \sum_{\alpha=1}^{N} n_{\alpha} \frac{\partial}{\partial x_{i}} \ln u_{\alpha}^{*} + \sum_{\alpha=1}^{N} n_{\alpha} \frac{\partial}{\partial x_{i}} \ln h_{\alpha \beta} = 0$$

(122)

where $n_{\alpha}$ is the solids volume fraction of abscissa $\alpha$, $h_{\alpha \beta}$ is given by

$$h_{\alpha \beta} = [1 + e(g_{\alpha \beta})] \frac{1}{2} g_{\alpha \beta}^{2} \delta_{\alpha \beta} + g_{\alpha \beta} g_{\alpha \beta}$$

(123)

and (with no summation implied over $\beta$)

$$D^{(i)}_{\alpha \beta} = \frac{\partial}{\partial x_{\alpha}} \ln v_{\beta} + \frac{\partial}{\partial x_{\beta}} \ln v_{\alpha} + \frac{\partial u_{\alpha}^{*}}{\partial x_{\beta}} \frac{\partial}{\partial x_{\alpha}} \ln h_{\alpha \beta} + \frac{\partial u_{\beta}^{*}}{\partial x_{\alpha}} \frac{\partial}{\partial x_{\beta}} \ln h_{\alpha \beta} + \frac{\partial}{\partial x_{\alpha}} \ln h_{\alpha \beta} + \frac{\partial}{\partial x_{\beta}} \ln h_{\alpha \beta}$$

(124)

Note that $h^{(i)}_{\alpha \beta}$ depends only on $g_{\alpha \beta} = u_{\alpha} - u_{\beta}$ and that $h^{(i)}_{\alpha \beta} = h^{(i)}_{\alpha \beta}$. Thus, the summation inside the parentheses in eq 122 can be rewritten as

$$\sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} V_{\alpha} V_{\beta} h^{(i)}_{\alpha \beta} D^{(i)}_{\alpha \beta} = \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} V_{\alpha} V_{\beta} h^{(i)}_{\alpha \beta} (D^{(i)}_{\alpha \beta} + D^{(i)}_{\beta \alpha})$$

(125)

However, from eq 124 it can easily be shown that $D^{(i)}_{\alpha \beta} = -D^{(i)}_{\beta \alpha}$, and thus, $P_{i} = 0$. This result is a direct consequence of the fact that, for first-order moments, $F^{(i)}_{n\alpha\beta\iota\lambda\rho\sigma}$ does not depend explicitly on $u_{\alpha}$. This is not the case for second- and higher-order moments (see Table 4).

In comparison to the monodisperse case discussed above, a slightly more complicated situation occurs for the polydisperse case where the coefficient of restitution is independent of relative velocity. The first-order moments for this case involve derivatives of

$$h_{\alpha \beta}(g) = \left(1 - \frac{1}{2} g^{2} \delta_{\alpha \beta} + g_{\alpha \beta} \right)$$

(126)

with respect to $u$ and $u^{*}$. However, because $h_{\alpha \beta}$ depends only on $g$, we can apply the chain rule to compute these derivatives

$$\frac{\partial h_{\alpha \beta}}{\partial u_{\alpha}} = \frac{\partial h_{\alpha \beta}}{\partial g_{\alpha}} \frac{\partial g_{\alpha}}{\partial u_{\alpha}} = \frac{\partial h_{\alpha \beta}}{\partial g_{\alpha}}$$

(127)

$$\frac{\partial h_{\alpha \beta}}{\partial u^{*}_{\alpha \beta}} = \frac{\partial h_{\alpha \beta}}{\partial g_{\alpha}}$$

(128)

where we have used the definition $g = u - u^{*}$ and the repeated index $n$ implies summation. The derivative with respect to $g_{\alpha}$ is straightforward to compute

$$\frac{\partial h_{\alpha \beta}}{\partial g_{\alpha}} = g_{\alpha} \delta_{\alpha \beta} + g_{\alpha \beta}$$

(129)

and the gradient term then has the form

$$\frac{\partial u_{\alpha}^{*}}{\partial x_{\alpha}} - \frac{\partial u_{\alpha}^{*}}{\partial x_{\alpha}} \frac{\partial h_{\alpha \beta}}{\partial u_{\alpha}^{*}} = (g_{\alpha} \delta_{\alpha \beta} + g_{\alpha \beta} \delta_{\alpha \beta}) \frac{\partial u_{\alpha}^{*}}{\partial x_{\alpha}} + \frac{\partial u_{\alpha}^{*}}{\partial x_{\alpha}}$$

(130)

Applying the quadrature formulas, the higher-order collision term becomes

$$H^{(jk)} = \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} \left(1 - \frac{1}{2} g_{\alpha \beta}^{2} \delta_{\alpha \beta} + g_{\alpha \beta} g_{\alpha \beta} \right) \left( \frac{\partial n_{\alpha}}{\partial x_{\alpha}} - \frac{\partial n_{\alpha}}{\partial x_{\alpha}} \frac{\partial h_{\alpha \beta}}{\partial u_{\alpha}^{*}} + \sum_{\alpha=1}^{N} n_{\alpha} \frac{\partial}{\partial x_{\alpha}} \frac{\partial h_{\alpha \beta}}{\partial u_{\alpha}^{*}} \right) \left( \frac{\partial u_{\alpha}^{*}}{\partial x_{\alpha}} + \frac{\partial u_{\alpha}^{*}}{\partial x_{\alpha}} \right)$$

(131)

This relation is used in the main text to find the components of $D_{\alpha \beta \iota \lambda \rho \sigma}$ given in eq 85.

**Appendix E: Kinetic-Based Spatial Fluxes**

The moment transport equation appears in conservative form and can be efficiently solved using kinetic-based finite-volume methods.6,7,29 In the dilute regime, the use of kinetic-based spatial fluxes is very important for capturing particle trajectory crossing effects and other large-Knudsen-number effects. Here, we extend the kinetic-based fluxes to the moderately dense regime where the collisional-flux contribution becomes significant.

In conservative form, eq 52 can be rewritten as

$$\frac{\partial (m_{\alpha} u_{\alpha}^{*} u_{\beta}^{*} u_{\gamma}^{*} u_{\delta}^{*})}{\partial t} + \nabla \cdot \mathbf{Q}_{\alpha \beta \gamma \delta} = P_{\alpha \beta \gamma \delta}$$

(132)

where $Q_{\alpha \beta \gamma \delta}$ and $Q_{\alpha \beta \gamma \delta}^{k}$ are the kinetic-based fluxes for moment $(m_{\alpha} u_{\beta}^{*} u_{\gamma}^{*} u_{\delta}^{*})$. The $i$th component of these fluxes are defined by
\[ Q_{ij,\alpha d} = \sum_{\alpha=1}^{N} n_{\alpha} m_{\alpha}^d U_{ij,\alpha d} H' (u_{\alpha}) \]
\[ Q_{ij,\alpha d}^+ = \sum_{\alpha=1}^{N} n_{\alpha} m_{\alpha}^d U_{ij,\alpha d}^0 H^+ (u_{\alpha}) \]

where the kinetic flux-splitting functions \( H' (x) \) and \( H^+ (x) \) are given by
\[ H' (x) = \begin{cases} 
1 & x < 0 \\
0.5 & x = 0 \\
1 - H^-(x) & x > 0
\end{cases} \]

As discussed elsewhere, physically, the kinetic-based fluxes represent the contributions due to the negative (positive) velocities in the moment integrals. For example, in the \( x_1 \) direction, the flux splitting is defined by
\[ \int_{R_c} Q_{i1} (u) f (u) \, du = \int_{-\infty}^{0} \left[ \int_{R_c} Q_{i1} (u) f (u) \, du \right] \, du_1 + \int_{0}^{\infty} \left[ \int_{R_c} Q_{i1} (u) f (u) \, du \right] \, du_1 \]

Introducing the quadrature representation of \( f (u) \) then leads to eq 133.

The numerical flux function in the finite-volume representation uses information at the boundary between neighboring cells. For example, in the \( x_1 \) direction, the numerical flux function is given by
\[ G_{i1,j1,i2,j2} (W_i, W_j) = Q_{i1,j1,i2,j2}^+ (W_i) + Q_{i1,j1,i2,j2}^- (W_j) \]

where \( W_i (W_j) \) represents the weights and abscissas in the cell on the left (right) of the boundary. Because they are exactly consistent with the underlying kinetic equation, the kinetic-based fluxes are guaranteed to yield realizable moments. This fact makes the overall numerical algorithm robust for any value of the particle Knudsen number. In comparison, non-kinetic-based fluxes (e.g., using finite differences) would fail when the Knudsen number is outside the hydrodynamic regime.

**Literature Cited**