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# Review Statistical models for predicting the effect of bidisperse particle collisions on particle velocities and stresses in homogeneous anisotropic turbulent flows

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#### ABSTRACT

The purpose of this paper is to present and compare two statistical models for predicting the effect of collisions on particle velocities and stresses in bidisperse turbulent flows. These models start from a kinetic equation for the probability density function (PDF) of the particle velocity distribution in a homogeneous anisotropic turbulent flow. The kinetic equation describes simultaneously particle-turbulence and particle-particle interactions. The paper is focused on deriving the collision terms in the governing equations of the PDF moments. One of the collision models is based on a Grad-like expansion for the PDF of the velocity distributions of two particles. The other model stems from a Grad-like expansion for the joint fluid-particle PDF. The validity of these models is explored by comparing with Lagrangian simulations of particle tracking in uniformly sheared and isotropic turbulent flows generated by LES. Notwith-standing the fact that the fluid turbulence may be isotropic, the particle velocity fluctuations and the numerical simulations show encouraging agreement.

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## 1. Introduction

In this paper, we consider a binary mixture of particles differing in sizes or material densities. The motion of particles is agitated by fluid turbulence and interparticle collisions. Turbulence is one of the most important mechanisms responsible for interparticle collisions. Because of this, a great body of theoretical studies of the collision rates induced by turbulence has been performed. For the most part these theories relate to the case of isotropic turbulence when the PDF of particle velocities can be described by the equilibrium Gaussian distribution (e.g., Saffman and Turner, 1956; Abrahamson, 1975; Laviéville et al., 1995; Wang et al., 1998; Zaichik et al., 2003). By analogy with modelling the interaction of molecules in the kinetic theory of gases, the statistical models of the transport of colliding particles obey a Boltzmann-type equation for the PDF. However, we must bear in mind that the classical Boltzmann equation relies on the assumption that the motion of molecules is statistically independent (the so-called hypothesis of molecular chaos) and thus the two-particle PDF may be presented as the product of two one-particle PDFs. This assumption is valid only for predicting collisions of high-inertia particles, the response time of which is long with respect to the characteristic eddy-particle interaction time and the motion of which, much like

the motion of molecules, is uncorrelated (statistically independent). When the particles are not of high-inertia, the modelling of collisions should be performed with regard to the correlation of the motion of neighboring particles because of their interaction with the fluid turbulent eddies. Moreover, due to the so-called "crossing trajectory effect" and collisions of different particles, the fluctuating velocities of the particles may be anisotropic even in isotropic turbulence. To account for the impact of the anisotropy of particle velocity fluctuations on collisions, the methods like those used in the kinetic theory of gases can be applied. For this purpose, Laviéville et al. (1997) and Zaichik and Alipchenkov (1997) used the Grad method to model the collision terms in the continuum conservation equations which govern the transport of monodisperse particles in anisotropic turbulent flow.

Modelling binary mixture is of fundamental importance because this is easily extended to the general case of polydisperse particle system. The problem of modelling collisions of different (bidisperse) particles suspended in turbulent flow is far more complicated as compared to the same issue for identical (monodisperse) particles. In the case of bidisperse particles, there are two collision mechanisms, one of which is induced by the fluid turbulence and the other is associated with the mean relative velocity (the relative drift) between the particles of different species. For example, this drift can be caused by gravity. Gourdel et al. (1999) proposed a statistical model for bidisperse particles that took into consideration both of collision mechanisms. This model was based

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on the Maxwell PDF, and consequently it could not predict the effects of the fluctuating velocity anisotropy and the particle motion correlation. By contrast, Fede and Simonin (2005) advanced a model that used the Grad method and hence took account of the turbulent fluctuation anisotropy and the particle velocity correlation, but it could not allow for the relative drift between the particles of different species.

In this paper, we present two statistical collision models, which include the anisotropy of particle fluctuating motion, the correlation of velocities of neighboring particles, and the effect of the relative drift between different particles. The particle volume fraction of both species is assumed to be small enough so that the two-phase system is quite good within the dilute limit and the modification of turbulence by particles may be neglected. An additional point to emphasize is that the collision models presented do not account for the effect of preferential concentration (Squires and Eaton, 1991). This effect is most remarkable when the particle response time is comparable to the Kolmogorov time microscale of turbulence (e.g., see Reade and Collins, 2000; Wang et al., 2000; Zaichik and Alipchenkov, 2003). When the particle response time is much more than the Kolmogorov timescale, the particle concentration fields become defocused because high-inertia particles do not response to fluid vorticity. Thus, the collision models are valid for particles whose response times exceed considerably the Kolmogorov timescale.

The paper is organized as follows. The next section presents the governing equations of the particulate phase which follow from a kinetic equation for the PDF. In Section 3, we deduce the collision terms using a Grad-like expansion of the two-particle PDF. Section 4 constitutes the collision terms using a Grad-like expansion of the joint fluid–particle velocity PDF. Section 5 demonstrates the effect of collisions on the particulate kinetic energy of a binary mixture. In Section 6, we examine the performance of the collision models for the transport of monodisperse particles in a uniformly sheared homogeneous flow. Section 7 examines the validity of the collision models for predicting the sedimentation of bidisperse particles in isotropic turbulence under the action of gravity. A summary of the work is given in Section 8.

#### 2. Governing equations

The theoretical ground of the models being considered is a kinetic equation for the PDF. This kinetic equation describes the interaction of particles with fluid turbulent eddies as well as the interaction of particles due to collisions. The operator providing the particle-turbulence interaction was derived presenting the fluid turbulence by a Gaussian random process with known correlation moments and using the functional formalism (Zaichik, 1999; Zaichik et al., 2004). Modelling the fluid velocity field by a Gaussian process is the key assumption that allows us to express the particle-turbulence interaction in the form of a second-order differential operator. In this paper, we restrict our consideration to homogeneous flows. For such flows, the third-order velocity correlations are strictly equal to zero and the moment set following from the kinetic equation terminates at the second-moment level.

Collisions are treated using the hard-sphere model neglecting the interparticle friction. Then, the particle velocities just after a collision  $\mathbf{v}_{p1}^{\circ}$  and  $\mathbf{v}_{p2}^{\circ}$  are expressed in terms of those before a collision  $\mathbf{v}_{p1}$  and  $\mathbf{v}_{p2}$  by

$$\mathbf{v}_{p1}^{\circ} = \mathbf{v}_{p1} + \frac{m_2}{m_1 + m_2} (1 + e) (\mathbf{w}_p \cdot \mathbf{k}) \mathbf{k},$$
  
$$\mathbf{v}_{p2}^{\circ} = \mathbf{v}_{p2} - \frac{m_1}{m_1 + m_2} (1 + e) (\mathbf{w}_p \cdot \mathbf{k}) \mathbf{k},$$
 (1)

where  $m_1$  and  $m_2$  are the masses of colliding particles, e is the coefficient of restitution,  $\mathbf{w}_p \equiv \mathbf{v}_{p2} - \mathbf{v}_{p1}$  is the relative velocity of parti-

cles before a collision, and  $\mathbf{k}$  is the unit vector directed from the centre of particle 1 to that of particle 2 at contact.

The kinetic equation for the PDF of the particles of species  $\alpha$ ,  $P_{\alpha}(\mathbf{x},\mathbf{v},t) \equiv \langle p_{\alpha} \rangle$ , can be presented in the form

$$\frac{\partial P_{\alpha}}{\partial t} + v_{i} \frac{\partial P_{\alpha}}{\partial x_{i}} + \frac{\partial}{\partial v_{i}} \left[ \left( \frac{U_{i} - v_{i}}{\tau_{\alpha}} + g_{i} \right) P_{\alpha} \right] \\ = -\frac{1}{\tau_{\alpha}} \frac{\partial \langle u_{i}' p_{\alpha} \rangle}{\partial v_{i}} + \left( \frac{\partial P_{\alpha}}{\partial t} \right)_{coll}^{\alpha} + \left( \frac{\partial P_{\alpha}}{\partial t} \right)_{coll}^{\beta}, \quad \beta \neq \alpha,$$
(2)

where  $p_{\alpha}$  is the dynamic probability density of particle velocity,  $\alpha$  and  $\beta$  are 1 or 2, *t* is time,  $x_i$  is the space coordinate,  $v_i$  is the particle velocity,  $\tau_{\alpha}$  is the particle response time,  $U_i$  is the averaged velocity of the carrier fluid, and  $g_i$  is the gravity acceleration.

The first term on the right-hand side of Eq. (2) describes the interaction of particles with fluid turbulent eddies and this is written as (Zaichik, 1999; Zaichik et al., 2004)

$$\frac{1}{\tau_{\alpha}} \frac{\partial \langle u_i' p_{\alpha} \rangle}{\partial v_i} = \lambda_{ij}^{\alpha} \frac{\partial^2 P_{\alpha}}{\partial v_i \partial v_j} + \mu_{ij}^{\alpha} \frac{\partial^2 P_{\alpha}}{\partial x_i \partial v_j}, \tag{3}$$

where the diffusion tensors in phase space,  $\lambda_{ij}^{\alpha}$  and  $\mu_{ij}^{\alpha}$ , are given in the Appendix A.

The two last terms on the right-hand side of (2) represent, respectively, the contribution of collisions with the particles of the species being considered and the other one. The collision operator is written in the form of the Boltzmann integral as applied to the hard-sphere collision model (1)

$$\left(\frac{\partial P_{\alpha}}{\partial t}\right)_{coll}^{\beta} = \sigma^{2} \int_{\mathbf{w}\cdot\mathbf{k}<0} \int \left[ P(\mathbf{x}, \mathbf{v}_{\alpha}^{\circ}, \mathbf{x} + \sigma \mathbf{k}, \mathbf{v}_{\beta}^{\circ}, t) - P(\mathbf{x}, \mathbf{v}_{\alpha}, \mathbf{x} + \sigma \mathbf{k}, \mathbf{v}_{\beta}, t) \right] (\mathbf{w}\cdot\mathbf{k}) d\mathbf{k} d\mathbf{v}_{\beta} \tag{4}$$

with  $\sigma \equiv r_1 + r_2$  being the radius of a collision sphere which is equal to the sum of the radii of colliding particles, and  $P(\mathbf{x}_1, \mathbf{v}_1, \mathbf{x}_2, \mathbf{v}_2, t)$  being the two-particle velocity PDF. The condition  $\mathbf{w} \cdot \mathbf{k} < 0$  indicates that the integration is carried out over the values of  $\mathbf{k}$  and  $\mathbf{v}_{\beta}$  for which particle collisions can be realized.

The kinetic equation completely controls the velocity statistics of the particulate phase. However, for most practical purposes, the kinetic level of modelling is not only computationally too expensive, but is also unnecessary because macroscopic properties are usually all that are needed. Another computationally less expensive way is to solve the conservation equations for several first moments of the PDF. The kinetic Eq. (2) along with (3) and (4) generates a set of governing continuum equation describing the conservation of mass, momentum, and particulate stresses as the appropriate statistical moments of the particle velocity PDF. Since we restrict our consideration to homogeneous flows, the set of the conservation equations for the moments of the PDF can be broken at the second-moment level. Moreover, it is known (e.g., see Jenkins and Richman, 1985) that the collision terms can be decomposed in two contributions that have, respectively, the form of sources and fluxes. The contribution of collisions to fluxes is of importance only in dense particulate flows (at  $\Phi > 0.1$ ). Because the particle volume fraction is assumed to be rather small, the collision terms appear as sources and the contribution of collisions to fluxes is ignored. By this means, the governing equation set for the particles of species  $\alpha$  is given by

$$\frac{\partial \Phi_{\alpha}}{\partial t} + \frac{\partial \Phi_{\alpha} V_{\alpha i}}{\partial x_i} = 0, \tag{5}$$

$$\frac{\partial V_{\alpha i}}{\partial t} + V_{\alpha j}\frac{\partial V_{\alpha i}}{\partial x_j} = -\frac{\partial \Phi_{\alpha} \left\langle v_{\alpha i}' v_{\alpha j}' \right\rangle}{\partial x_j} + \frac{U_i - V_{\alpha i}}{\tau_{\alpha}} + g_i - \mu_{ij}^{\alpha}\frac{\partial \ln \Phi_{\alpha}}{\partial x_j} + \mathbb{C}_i^{\alpha},$$
(6)

$$\frac{\partial \left\langle v_{\alpha i}^{\prime} v_{\alpha j}^{\prime} \right\rangle}{\partial t} + V_{\alpha k} \frac{\partial \left\langle v_{\alpha i}^{\prime} v_{\alpha j}^{\prime} \right\rangle}{\partial x_{k}} \\
= -\left( \left\langle v_{\alpha i}^{\prime} v_{\alpha k}^{\prime} \right\rangle + \mu_{i k}^{\alpha} \right) \frac{\partial V_{\alpha j}}{\partial x_{k}} - \left( \left\langle v_{\alpha j}^{\prime} v_{\alpha k}^{\prime} \right\rangle + \mu_{j k}^{\alpha} \right) \frac{\partial V_{\alpha i}}{\partial x_{k}} + \lambda_{i j}^{\alpha} + \lambda_{j i}^{\alpha} \\
- \frac{2 \left\langle v_{\alpha i}^{\prime} v_{\alpha j}^{\prime} \right\rangle}{\tau_{\alpha}} + \mathbb{C}_{i j}^{\alpha \alpha} + \mathbb{C}_{i j}^{\alpha \beta}, \quad \beta \neq \alpha, \quad (7)$$

$$\begin{split} \Phi_{\alpha} &= \int P_{\alpha} d\mathbf{v}, \quad V_{\alpha i} = \frac{1}{\Phi_{\alpha}} \int v_i P_{\alpha} d\mathbf{v}, \\ \left\langle v_{\alpha i}' v_{\alpha j}' \right\rangle &= \frac{1}{\Phi_{\alpha}} \int (v_i - V_{\alpha i}) (v_j - V_{\alpha j}) P_{\alpha} d\mathbf{v}. \end{split}$$

Here  $\Phi_{\alpha}$ ,  $V_{\alpha i}$ , and  $\langle v'_{\alpha i} v'_{\alpha j} \rangle$  are the particle volume fraction, the average velocity, and the kinetic stresses. It is obvious that, in accordance with (5), collisions do not change the particle fraction. However, as symbolized by  $\mathbb{C}_{i}^{\alpha}$ , the collisions of the particles of the species under consideration with the particles of other species make a contribution to the momentum Eq. (6). Clearly the collisions of identical particles have no effect on their averaged velocity. In (7), the terms  $\mathbb{C}_{ij}^{\alpha \alpha}$  and  $\mathbb{C}_{ij}^{\alpha \beta}$  quantify, respectively, the contributions of collisions of identical and different particles to the balance of the particulate stresses.

The fluid–particle fluctuating velocity covariances are written as (Zaichik, 1999; Zaichik et al., 2004)

$$\left\langle u_{\alpha i}^{\prime} v_{\alpha j}^{\prime} \right\rangle = \frac{1}{\Phi} \left( \int \left\langle u_{i}^{\prime} p_{\alpha} \right\rangle v_{j} d\mathbf{v} - V_{\alpha j} \int \left\langle u_{i}^{\prime} p_{\alpha} \right\rangle d\mathbf{v} \right) = \tau_{\alpha} \left( \lambda_{ij}^{\alpha} - \mu_{ik}^{\alpha} \frac{\partial V_{\alpha j}}{\partial x_{k}} \right),$$
(8)

where  $u_{\alpha i}$  is the fluid velocity viewed by a particle of species  $\alpha$ .

As is seen from (8), collisions do not directly affect the fluidparticle velocity correlations, yet can effect indirectly through changing the response coefficients which appear in  $\lambda_{ii}^{\alpha}$  and  $\mu_{ii}^{\alpha}$ .

To close the equation set (5)–(7) we need only determine the collision terms in (6) and (7). For this purpose we use two statistical models, the simpler of which is based on a Grad-like expansion for the two-particle PDF (hereafter called as the TP model) and the more complicated of which starts from a Grad-like expansion for the joint fluid–particle PDF (hereafter called as the FP model). Grad (1949) proposed to approximate the Boltzmann equation by expanding the single-particle PDF in the Hermite orthogonal polynomials in velocity space. A unique feature in using the Hermite polynomials as the expansion basis rather than any other functions is that the expansion coefficients correspond precisely to the velocity moments of the PDF to the given degree.

#### 3. Collision terms stemming from the two-particle (TP) model

The TP model is based on the presentation of the two-particle PDF as the sum of the zero-order and first-order terms of velocity distribution expansion. This is an expansion in terms of Hermite polynomials. The zero-order term is given by a Gaussian isotropic velocity distribution that allows for correlations between the velocities of two particles due to their response to local fluid turbulence. The first-order term represents a velocity distribution perturbation following from the Grad approach owing to the anisotropy of particle velocities. Notice that the Grad approximation is accurate if the anisotropy tensor of particle fluctuating velocities,  $r_{\alpha ij} \equiv \left\langle v'_{\alpha i} v'_{\alpha k} \right\rangle / \left\langle v'_{\alpha k} v'_{\alpha k} \right\rangle - \delta_{ij}/3$ , can be regarded as a small quantity.

By this means, the two-particle PDF is defined as

$$P(\mathbf{v}_1, \mathbf{v}_2) = P^{(0)}(\mathbf{v}_1, \mathbf{v}_2) + P^{(1)}(\mathbf{v}_1, \mathbf{v}_2)$$
(9)

with the zero-order expansion term being the Gaussian velocity distribution (Fede and Simonin, 2005; Zaichik et al., 2006)

$$P^{(0)}(\mathbf{v}_{1},\mathbf{v}_{2}) = \frac{\Phi_{1}\Phi_{2}}{\left(2\pi\nu_{1}'\nu_{2}'\right)^{3}\left(1-\zeta_{12}^{2}\right)^{3/2}} \times \exp\left[-\frac{1}{2\left(1-\zeta_{12}^{2}\right)}\left(\frac{\nu_{1k}'\nu_{1k}'}{\nu_{1}'^{2}}+\frac{\nu_{2k}'\nu_{2k}'}{\nu_{1}'^{2}}-\frac{2\zeta_{12}'\nu_{1k}'\nu_{2k}'}{\nu_{1}'\nu_{2}'}\right)\right].$$
(10)

Here  $v_{\alpha}^{2} \equiv \langle v_{\alpha k}' v_{\alpha k}' \rangle / 3$  is the particle velocity variance, and  $\zeta_{12}$  is the particle velocity correlation coefficient that is expressed through the particle response coefficient,  $f_{u\alpha} \equiv f_{u \ kk}^{\alpha}/3$ , as

$$C_{12} \equiv (f_{u1}f_{u2})^{1/2}.$$
 (11)

The equilibrium Gaussian PDF (10) properly describes the two-particle velocity distribution in isotropic turbulence, but it does not provide taking account of the particle velocity anisotropy. In order to take this anisotropy into account, the first-order expansion term in (9) is used. According to the Grad approach we take

$$P^{(1)}(\mathbf{v}_{1},\mathbf{v}_{2}) = \left[ \mathcal{R}_{1i}\frac{\partial}{\partial v_{1i}} + \mathcal{R}_{2i}\frac{\partial}{\partial v_{2i}} + \frac{\mathcal{R}_{1ij}}{2}\frac{\partial^{2}}{\partial v_{1i}\partial v_{1j}} + \frac{\mathcal{R}_{2ij}}{2}\frac{\partial^{2}}{\partial v_{2i}\partial v_{2j}} + \frac{\mathcal{Q}_{ij}}{2}\left(\frac{\partial^{2}}{\partial v_{1i}\partial v_{2j}} + \frac{\partial^{2}}{\partial v_{2i}\partial v_{1j}}\right) \right] P^{(0)}(\mathbf{v}_{1},\mathbf{v}_{2}).$$
(12)

The details of determining the coefficients  $\mathcal{R}_{\alpha i}$ ,  $\mathcal{R}_{\alpha ij}$ , and  $\mathcal{Q}_{ij}$  in (12) as well as the collision terms in (6) and (7) are given in the Appendix B.

Using (B7)–(B9), we can derive the mean absolute relative radial velocity between two colliding particles

$$\langle |\boldsymbol{w}_r| \rangle = \langle |\boldsymbol{w}_r| \rangle^{(0)} + \langle |\boldsymbol{w}_r| \rangle^{(1)}, \tag{13}$$

$$\langle |w_r| \rangle^{(0)} = \frac{1}{2\pi\Phi_1\Phi_2} \int \int \int_{\mathbf{w}\cdot\mathbf{k}<0} \int (\mathbf{w}\cdot\mathbf{k}) P^{(0)}(\mathbf{w},\mathbf{q}) d\mathbf{k} d\mathbf{w} d\mathbf{q} = \frac{W}{2} F_0(z),$$
(14)

$$\langle |\mathbf{w}_{r}| \rangle^{(1)} = \frac{1}{2\pi\Phi_{1}\Phi_{2}} \int_{\mathbf{w}\cdot\mathbf{k}<0} \int_{\mathbf{w}\cdot\mathbf{k}<0} (\mathbf{w}\cdot\mathbf{k})P^{(1)}(\mathbf{w},\mathbf{q})d\mathbf{k}d\mathbf{w}d\mathbf{q}$$
$$= -\frac{B_{ij}W_{i}W_{j}W}{8z^{2}}\Psi_{0}(z), \tag{15}$$

$$F_0(z) = \frac{\exp(-z)}{\sqrt{\pi z}} + \operatorname{erf}\sqrt{z}\left(1 + \frac{1}{2z}\right),$$
  
$$\Psi_0(z) = \frac{3\exp(-z)}{\sqrt{\pi z}} + \operatorname{erf}\sqrt{z}\left(1 - \frac{3}{2z}\right),$$

where the drift parameter z measures the ratio between the mean and fluctuating relative velocities of the particles of different species

$$\begin{split} z &= \frac{W^2}{2w'^2}, \quad W_i = V_{2i} - V_{1i}, \quad W = (W_k W_k)^{1/2}, \\ w'^2 &= v'_1^2 + v'_2^2 - 2\zeta_{12} \, v'_1 \, v'_2^2. \end{split}$$

According to (13), the particle collision rate is equal to

$$\beta = 2\pi\sigma^2 \langle |\mathbf{w}_r| \rangle = 2\pi\sigma^2 \left( \langle |\mathbf{w}_r| \rangle^{(0)} + \langle |\mathbf{w}_r| \rangle^{(1)} \right) = \beta^{(0)} + \beta^{(1)}.$$
(16)

Expression (16) represents the collision rate as the sum of two terms, the first of which is valid when the particle fluctuating velocities are isotropic and the second one allows for the contribution of the particle fluctuating velocity anisotropy. The formula of  $\beta^{(0)}$  with (14) was firstly derived by Abrahamson (1975) and later rediscovered by Gourdel et al. (1999); Alipchenkov and Zaichik (2001) and Dodin and Elperin (2002). Eq. (16) can be used for predicting the collision rate of gravity-settling particles in a homogeneous anisotropic turbulent flow field. This is correct for particles

whose response time,  $\tau_{\alpha}$ , is much more than the Kolmogorov timescale,  $\tau_k$ . In order to predict the collision rate of low-inertia particles, it is essential to take into account the contribution of particle interaction with small-scale turbulent eddies to the relative radial velocity as well as to determine the radial distribution function. This problem was recently solved by Ayala et al. (2008) using an analytical parameterization of the relative radial velocity and the radial distribution function in isotopic turbulence. When  $\tau_{\alpha} \gg \tau_k$ ,  $\beta^{(0)}$  in (16) is identical to that proposed by Ayala et al. (2008) and  $\beta^{(1)}$  provides incorporating the effect of velocity fluctuation anisotropy.

In view of  $B_{ii}W_iW_i = O(z)$ , it is easy to obtain

$$\lim_{z \to 0} \frac{\beta^{(1)}}{\beta^{(0)}} = \mathbf{O}(z), \quad \lim_{z \to \infty} \frac{\beta^{(1)}}{\beta^{(0)}} = \mathbf{O}(z^{-1}).$$

Thus, in the limiting cases of small and large drift, the contribution of the anisotropy of particle fluctuating velocities to the collision rate is not of very importance. This effect can be apparently important only when z = O(1).

The collision term involving in the momentum Eq. (6) has the form

$$\mathbb{C}_i^{\alpha} = \mathbb{C}_i^{\alpha(0)} + \mathbb{C}_i^{\alpha(1)},\tag{17}$$

where  $\mathbb{C}_{i}^{\alpha(0)}$  and  $\mathbb{C}_{i}^{\alpha(1)}$  are given by (B10) and (B11).

When the particle velocity correlation coefficient is equal to zero,  $\mathbb{C}_i^{\alpha(0)}$  given by (B10) reduces to the momentum collision term obtained by Gourdel et al. (1999). In the limiting cases of low and large drift, one can obtain from (B10) and (B11) the following evaluations:

$$\lim_{z\to 0} \frac{\mathbb{C}_i^{\alpha(1)}}{\mathbb{C}_i^{\alpha(0)}} = O(1), \quad \lim_{z\to\infty} \frac{\mathbb{C}_i^{\alpha(1)}}{\mathbb{C}_i^{\alpha(0)}} = O(z^{-1}),$$

in line with which the contribution of the anisotropy of particle fluctuating velocities to the collision term of the momentum equation is more important in the case of low drift.

In the balance equation of the particulate stresses (7), the contribution due to collisions of the particles of different species is written as

$$\mathbb{C}_{ij}^{\alpha\beta} = \mathbb{C}_{ij}^{\alpha\beta(0)} + \mathbb{C}_{ij}^{\alpha\beta(1)},\tag{18}$$

where  $\mathbb{C}_{i}^{\alpha(0)}$  and  $\mathbb{C}_{i}^{\alpha(1)}$  are given by (B12) and (B13).

In the case of identical particles, (B12) and (B13) can be reduced to the relations obtained in Zaichik and Alipchenkov (1997)

$$\mathbb{C}_{ij}^{\alpha\alpha(0)} = -\frac{8\Phi_{\alpha}(1-e^{2})\nu_{\alpha}^{3}(1-f_{u\alpha})^{3/2}}{\pi^{1/2}\sigma_{\alpha}}\delta_{ij}, \\
\mathbb{C}_{ij}^{\alpha\alpha(1)} = -\frac{24\Phi_{\alpha}(1+e)(3-e)\nu_{\alpha}^{\prime}(1-f_{u\alpha})^{3/2}}{5\pi^{1/2}\sigma_{\alpha}}\mathcal{R}_{\alpha ij}.$$
(19)

In the limit of large drift, comparing (B12) and (B13) gives

$$\lim_{z\to\infty} \frac{\mathbb{C}_{ij}^{\alpha\beta(1)}}{\mathbb{C}_{ij}^{\alpha\beta(0)}} = O(z^{-1})$$

Thus, it is evident that the contribution of the anisotropy of particle fluctuating velocities to the collision term of the particulate stress equation, like that of the momentum equation, is more important in the case of low drift.

Constricting (18) yields the collision term,  $\mathbb{C}_{k_p}^{\alpha\beta} \equiv \mathbb{C}_{ii}^{\alpha\beta}/2$ , in the balance equation of the particulate kinetic energy,  $k_{p\alpha} \equiv \langle v'_{\alpha i} v'_{\alpha i} \rangle/2$ . Note that (B12) produces the energy collision term,  $\mathbb{C}_{k_p}^{\alpha\beta[0]} \equiv \mathbb{C}_{ii}^{\alpha\beta[0]}/2$ , which coincides with that obtained by Gourdel et al. (1999) when neglecting the particle velocity correlation ( $\zeta_{12} = 0$ ). In the case of no mean particle drift (z = 0),  $\mathbb{C}_{k_p}^{\alpha\beta[0]}$  produced by (B12) is consistent with the energy collision terms obtained in Reade and Collins (1998) and Fede and Simonin (2003).

#### 4. Collision terms stemming from the fluid-particle (FP) model

In evaluating the collision terms by means of the FP model, we make use of the PDF for the particle and fluid velocity viewed by the particle for either species. This PDF is a Grad-like expansion about the zero-order joint PDF which is a Gaussian velocity distribution involving a correlation between a particle and the fluid. The two-particle PDF necessary for the evaluation of the collision integral is derived from a joint fluid-particle velocity PDF for two particles, which was originally approximated by Laviéville (1997) using conditional probability densities for the particle velocity conditioned by the carrier fluid velocity. Then integration over the fluid velocities yields the two-particle PDF represented in terms of Hermite polynomials. It should be noted that, in the framework of the FP model, the Grad approximation is accurate if  $r_{ij}$ ,  $r_{\alpha ij}$ , and  $s_{\alpha ij}$  each are of small quantities (here  $r_{ij} \equiv \langle u'_i u'_i \rangle / \langle u'_k u'_k \rangle - \delta_{ij}/3$ and  $s_{\alpha i j} = \left(\left\langle u_{\alpha i}^{\prime} v_{\alpha j}^{\prime} \right\rangle + \left\langle u_{\alpha j}^{\prime} v_{\alpha i}^{\prime} \right\rangle \right) / 2 \left\langle u_{\alpha k}^{\prime} v_{\alpha k}^{\prime} \right\rangle - \delta_{i j} / 3$  are, respectively, the fluid and fluid-particle anisotropy tensors).

Thus, the collision model being considered in this section starts from the Grad-like expansion of the one-point joint fluid-particle PDF (Laviéville et al., 1997)

$$P(\mathbf{u}_{\alpha}, \mathbf{v}_{\alpha}) = P^{(0)}(\mathbf{u}_{\alpha}, \mathbf{v}_{\alpha}) + P^{(1)}(\mathbf{u}_{\alpha}, \mathbf{v}_{\alpha})$$

$$= \left(1 + \frac{A_{\alpha i j}}{2u'^{4}}u'_{\alpha i}u'_{\alpha j} + \frac{B_{\alpha i j}}{\xi^{2}_{\alpha}u'^{2}}v'^{2}_{\alpha}u'_{\alpha i}v'_{\alpha j} + \frac{\Gamma_{\alpha i j}}{2v'^{4}_{\alpha}}v'_{\alpha i}v'_{\alpha j}\right)P^{(0)}(\mathbf{u}_{\alpha}, \mathbf{v}_{\alpha}),$$
(20)

$$\begin{split} P^{(0)}(\mathbf{u}_{\alpha},\mathbf{v}_{\alpha}) &= \frac{\left(1-\zeta_{\alpha}^{2}\right)^{-3/2} \varPhi_{\alpha}}{\left(2\pi u' \, \upsilon_{\alpha}'\right)^{3}} \\ &\times \exp\left[-\frac{1}{\left(1-\zeta_{\alpha}^{2}\right)} \left(\frac{u_{\alpha k}' u_{\alpha k}'}{2u'^{2}} + \frac{\upsilon_{\alpha k}' \, \upsilon_{\alpha k}'}{2\upsilon_{\alpha}'^{2}} - \frac{\zeta_{\alpha} u_{\alpha k}' \, \upsilon_{\alpha k}'}{u' \, \upsilon_{\alpha}'}\right)\right], \end{split}$$

where  $u'^2$  is the fluid velocity variance, and  $\xi_{\alpha}$  designates the one-point fluid-particle correlation coefficient that is defined as the ratio of the fluid-particle velocity covariance to their variances. The coefficients  $A_{\alpha ij}$ ,  $B_{\alpha ij}$ , and  $\Gamma_{\alpha ij}$  as well as the correlation coefficient  $\xi_{\alpha}$  are given in the Appendix C. In (20),  $P^{(0)}(\mathbf{u}_{\alpha},\mathbf{v}_{\alpha})$  implies that the single fluid (viewed by a particle) and particle velocity distributions are Maxwellian, whereas  $P^{(1)}(\mathbf{u}_{\alpha},\mathbf{v}_{\alpha})$  takes into consideration the effect of the anisotropy of fluid and particle velocity variances and covariances.

When assuming that, in isotropic turbulence, the fluid velocity obeys the Maxwellian distribution, the Grad expansion of the PDF of fluid velocity viewed by a particle has the form

$$P(\mathbf{u}_{\alpha}) = \left(1 + \frac{\mathcal{R}_{ij}}{2u'^4} u'_{\alpha i} u'_{\alpha j}\right) P^{(0)}(\mathbf{u}_{\alpha}),$$
  

$$P^{(0)}(\mathbf{u}_{\alpha}) = \frac{1}{(2\pi u'^2)^{3/2}} \exp\left(-\frac{u'_{\alpha k} u'_{\alpha k}}{2u'^2}\right).$$
(21)

With a view to determine the two-particle PDF, the joint twopair fluid-particle velocity PDF is introduced and modelled as (Laviéville, 1997)

$$P(\mathbf{u}_1, \mathbf{v}_1, \mathbf{u}_2, \mathbf{v}_2) = P(\mathbf{v}_1 | \mathbf{u}_1) P(\mathbf{v}_2 | \mathbf{u}_2) P(\mathbf{u}_1, \mathbf{u}_2).$$
(22)

In (22),  $P(\mathbf{v}_{\alpha}|\mathbf{u}_{\alpha})$  denotes the conditional probability density of particle velocity  $\mathbf{v}_{\alpha}$  conditioned on the fluid velocity  $\mathbf{u}_{\alpha}$ , and it is represented as

$$P(\mathbf{v}_{\alpha}|\mathbf{u}_{\alpha}) = P(\mathbf{u}_{\alpha},\mathbf{v}_{\alpha})/P(\mathbf{u}_{\alpha}).$$
<sup>(23)</sup>

Approximation (22) was obtained using the precise equation that expresses  $P(\mathbf{u}_1, \mathbf{v}_1, \mathbf{u}_2, \mathbf{v}_2)$  in terms of conditional probabilities

$$P(\mathbf{u}_1, \mathbf{v}_1, \mathbf{u}_2, \mathbf{v}_2) = P(\mathbf{v}_1 | \mathbf{u}_1, \mathbf{u}_2, \mathbf{v}_2) P(\mathbf{v}_2 | \mathbf{u}_1, \mathbf{u}_2) P(\mathbf{u}_1, \mathbf{u}_2)$$

and the plausible approximations

 $P(\mathbf{v}_1|\mathbf{u}_1,\mathbf{u}_2,\mathbf{v}_2)\simeq P(\mathbf{v}_1|\mathbf{u}_1), \quad P(\mathbf{v}_2|\mathbf{u}_1,\mathbf{u}_2)\simeq P(\mathbf{v}_2|\mathbf{u}_2).$ 

Integrating  $P(\mathbf{u}_1, \mathbf{v}_1, \mathbf{u}_2, \mathbf{v}_2)$  over the fluid velocity phase subspace, one can derive, from (20)–(23), the following expansion of the velocity PDF of two particles:

$$P(\mathbf{v}_{1}, \mathbf{v}_{2}) = \int \int P(\mathbf{u}_{1}, \mathbf{v}_{1}, \mathbf{u}_{2}, \mathbf{v}_{2}) d\mathbf{u}_{1} d\mathbf{u}_{2}$$
  
= 
$$\int \int \frac{P(\mathbf{u}_{1}, \mathbf{v}_{1}) P(\mathbf{u}_{2}, \mathbf{v}_{2}) P(\mathbf{u}_{1}, \mathbf{u}_{2})}{P(\mathbf{u}_{1}) P(\mathbf{u}_{2})} d\mathbf{u}_{1} d\mathbf{u}_{2}$$
  
= 
$$P^{(0)}(\mathbf{v}_{1}, \mathbf{v}_{2}) + P^{(1)}(\mathbf{v}_{1}, \mathbf{v}_{2}), \qquad (24)$$

where the zero-order expansion term,  $P^{(0)}(\mathbf{v}_1, \mathbf{v}_2)$ , is given by (10) and the first-order one,  $P^{(1)}(\mathbf{v}_1, \mathbf{v}_2)$ , is given by (C1).

As is shown in the Appendix C, the expansion (24) leads to precisely the same relations for the collision rate as well as for the momentum and stress collision terms obtained using the TP model, if we replace the quantities  $B_{ij}$  and  $C_{ij}$  defined in (B9) by the ones  $\tilde{B}_{ij}$ and  $\tilde{C}_{ij}$  defined in (C3).

In the case of identical particles, the stress collision term appearing in (7) is coincident with that obtained by Laviéville et al. (1997)

$$\begin{split} \mathbb{C}_{ij}^{\alpha\alpha(0)} &= -\frac{8\Phi_{\alpha}(1-e^{2})\nu_{\alpha}^{\prime3}(1-\xi_{\alpha}^{2})^{3/2}}{\pi^{1/2}\sigma_{\alpha}}\delta_{ij}, \\ \mathbb{C}_{ij}^{\alpha\alpha(1)} &= -\frac{12\Phi_{\alpha}(1+e)(3-e)\nu_{\alpha}^{\prime}(1-\xi_{\alpha}^{2})^{5/2}}{5\pi^{1/2}\sigma_{\alpha}}\big(\Gamma_{\alpha ij}+\Gamma_{\alpha ji}\big). \end{split}$$
(25)

It should be noted that the collision constitutive relations presented in this section are more general as compared to those obtained in Section 3 using the TP model. The ones based on the FP model provide a direct contribution not only of the anisotropy of particle fluctuating velocities but of that of fluid velocity fluctuations and fluid-particle velocity covariances as well. The conclusions concerning the part of the particle fluctuating velocity anisotropy depending on a value of the drift parameter hold also for the FP model.

#### 5. Collision effect on the particulate kinetic energy

Let us consider the contribution of collisions to macroscopic properties of the binary mixture as a whole. It is clear that the impact of collisions on the momentum of the mixture,  $\rho_1 \Phi_1 V_{1i} + \rho_2 \Phi_2 V_{2i}$ , is absent. The collision term entering into the governing equation of the fluctuating kinetic energy of the mixture,  $k_p \equiv (\rho_1 \Phi_1 k_{p1} + \rho_2 \Phi_2 k_{p2}) / (\rho_1 \Phi_1 + \rho_2 \Phi_2)$ , can be written as

$$\begin{split} \mathbb{C}_{k_p} &= \mathbb{C}_{k_p}^{I} + \mathbb{C}_{k_p}^{II}, \quad \mathbb{C}_{k_p}^{I} = \frac{N_1 m_1 \mathbb{C}_{ii}^{11} + N_2 m_2 \mathbb{C}_{ii}^{22}}{2(N_1 m_1 + N_2 m_2)}, \\ \mathbb{C}_{k_p}^{II} &= \frac{N_1 m_1 \mathbb{C}_{ii}^{12} + N_2 m_2 \mathbb{C}_{ii}^{21}}{2(N_1 m_1 + N_2 m_2)}. \end{split}$$

Here  $\mathbb{C}_{k_p}^l$  and  $\mathbb{C}_{k_p}^{l}$  measure, respectively, the contribution of collisions of identical and different particles. According to (19) or (25),  $\mathbb{C}_{k_p}^l$  is equal to zero if collisions are elastic and it is negative if collisions are inelastic. It means that the collisions of identical particles result in dissipation of the kinetic energy of the particulate phase. For collisions of different particles, the result is ambiguous. To explore the collision effect of different particles, we use the TP model, bearing in mind that using the FP model leads to the same conclusion. The collision term  $\mathbb{C}_{k_p}^{l}$  given by (18) along with (B12) and (B13) has the form

$$\mathbb{C}_{k_{p}}^{II} = \mathbb{C}_{k_{p}}^{II(0)} + \mathbb{C}_{k_{p}}^{II(1)}, \tag{26}$$

$$\mathbb{C}_{k_p}^{II(0)} = \frac{2^{1/2} \pi \sigma^2 N_1 N_2 m_1 m_2 (1+e) w^3}{(m_1 + m_2) (N_1 m_1 + N_2 m_2)} \Pi(z),$$
  
$$\Pi(z) = \frac{(1+e) z^{3/2} F_2(z)}{2} - 2 z^{1/2} F_0(z),$$
(27)

$$\mathbb{C}_{k_{p}}^{II(1)} = \frac{2^{1/2}\pi\sigma^{2}N_{1}N_{2}m_{1}m_{2}(1+e)w^{3}}{8(m_{1}+m_{2})(N_{1}m_{1}+N_{2}m_{2})}W_{k}W_{n}B_{kn} \\ \times \left[\frac{(1+e)(7\Psi_{4}(z)+\Psi_{5}(z))}{2z^{1/2}} + \frac{3\Psi_{2}(z)}{4z^{3/2}} + \frac{(\Psi_{7}(z)-\Psi_{6}(z))}{z^{1/2}}\right].$$
(28)

According to (27) and (28)

$$\lim_{z\to 0} \frac{\mathbb{C}_{k_p}^{II(1)}}{\mathbb{C}_{k_p}^{II(0)}} = O(z), \quad \lim_{z\to\infty} \frac{\mathbb{C}_{k_p}^{II(1)}}{\mathbb{C}_{k_p}^{II(0)}} = O(z^{-1}).$$

Therefore, for the qualitative analysis of (26), we can neglect  $\mathbb{C}_{k_p}^{ll(1)}$  as compared to  $\mathbb{C}_{k_p}^{ll(0)}$ . By this means, the effect of collisions of different particles on the fluctuating kinetic energy of the mixture is determined by the function  $\Pi(z)$  appearing in (27). This function is exhibited in Fig. 1. As is clear, for elastic collisions (e = 1),  $\Pi(z)$  is positive and hence the production of  $k_p$  takes place. This source of the fluctuating energy arises due to the transfer of the average kinetic energy induced by the difference between the mean velocities of the particles of different species towards the fluctuating motion. When collisions are inelastic, they cause the dissipation or production effect depending on a value of drift parameter. Thus, in binary mixture, the collision mechanism can lead to both the dissipation (for low drift) and the generation (for high drift) of the fluctuating kinetic turbulent energy of the particulate phase.

#### 6. Homogeneous shear flow

First, we examine the performance of the collision models for the transport of monodisperse particles in an unsteady homogeneous shear flow with a constant mean velocity gradient. As was mentioned in Section 1, the fraction of particles is assumed to be small enough for the modulation of fluid turbulence to be negligible. Moreover, the gravity force is not taken into consideration. In consequence of homogeneity, it follows from (5) and (6) that the particle fraction does not vary in space, and the mean velocity gradients of the fluid and particulate phases are identical. These gradients are given by

$$\frac{\partial U_i}{\partial x_j} = \frac{\partial V_i}{\partial x_j} = S\delta_{i1}\delta_{j2},\tag{29}$$

where S denotes the imposed mean shear rate.



**Fig. 1.** Effect of the drift parameter on the behavior of the collision term of the fluctuating kinetic energy of the particulate phase  $\mathbb{C}_{k_p}^{I/(0)}$ : 1 - e = 0; 2 - e = 0.5; 3 - e = 1.

To verify the collision models under consideration, we compare predictions with simulations performed previously by Laviéville (1997) and Laviéville et al. (1997) using the Lagrangian tracking method for the particulate phase and LES for the carrier fluid phase. The initial conditions are conformed to an isotropic turbulent state. The mean shear rate is equal to  $S=50 \text{ s}^{-1}$ , the particle diameter is of 656  $\mu$ m, and the particle-to-fluid density ratio is taken as 85.5. The volume particle fraction is equal to  $\Phi$  = 0.0125, and collisions assume to be elastic (e = 1). Because we analyze a uniformly sheared flow with no gravity, the mean velocities of the particulate and fluid phases can be taken as being coincident, and hence the "crossing trajectory effect" is absent. The particulate kinetic stresses are predicted by means of Eq. (7), which is simplified in conformity with (29). The collision terms are determined with the help of (19) or (25). Because this paper is focused on examining the collision models rather than the particle-turbulence interaction models, we define the eddy-particle interaction time by means of the simple isotropic relation,  $T_{l,p,ii} = 0.482k\delta_{ii}/\varepsilon$ (Simonin et al., 1993), where k and  $\varepsilon$  are the turbulence energy of the fluid and its dissipation rate.

In Fig. 2, the time evolution of the particle kinetic stresses from an isotropic state to an equilibrium sheared flow is shown. The particle stresses,  $\langle v'_i v'_j \rangle$ , are normalized with the initial particle kinetic energy,  $k_{p}(0)$ , and time, t, is multiplied by the shear rate, S. Fig. 2 exhibits a strong anisotropy of velocity fluctuations when neglecting interparticle collisions, namely, the value of the streamwise component of velocity fluctuations of high-inertia particles exceeds considerably the respective values in the normal and spanwise directions. This anisotropy is caused by the production of streamwise velocity fluctuations due to the mean shear with lacking small-scale dissipation in the dispersed phase as opposed to the fluid phase. The most remarkable effect of collisions consists in reducing the particle fluctuating velocity anisotropy by decreasing the streamwise stress component and increasing the transverse components. The redistribution of directional velocity fluctuations due to collisions of identical particles resembles a like phenomenon that takes place in fluid turbulence due to pressure fluctuations. It is clear that the predictions given by the TP and FP collision models are quite close, although the FP model leads to a slightly better agreement with the simulations.

To realize why the predictions obtained using the TP and FP models are close, it is significant that the stress collision terms (19) and (25) coincide in the so-called locally equilibrium approximation. In this approximation, the particulate stresses and the



**Fig. 2.** The effect of collisions on the particulate kinetic stresses in a homogeneous shear flow: 1–8 – Laviéville (1997); I – TP model; II – FP model; 1–4, III – without collisions; 5–8 – with collisions.

fluid–particle velocity covariances can be expressed directly in terms of the fluid kinetic stresses from Eqs. (7), (8) and (A1) when neglecting the transport, collision, and velocity gradient contributions

$$\left\langle \boldsymbol{\nu}_{\boldsymbol{x}i}^{\prime}\boldsymbol{\nu}_{\boldsymbol{x}j}^{\prime}\right\rangle = \left\langle \boldsymbol{u}_{\boldsymbol{x}i}^{\prime}\boldsymbol{\nu}_{\boldsymbol{x}j}^{\prime}\right\rangle = f_{\boldsymbol{u}\boldsymbol{x}}\left\langle \boldsymbol{u}_{i}^{\prime}\boldsymbol{u}_{j}^{\prime}\right\rangle, \quad \mathcal{R}_{\boldsymbol{x}ij} = \mathcal{S}_{\boldsymbol{x}ij} = f_{\boldsymbol{u}\boldsymbol{x}}\mathcal{R}_{ij}. \tag{30}$$

Eq. (30) along with  $\xi_{\alpha} = f_{u\alpha}^{1/2}$  yield the relation

$$\Gamma_{\alpha i j} = \frac{\xi_{\alpha}^2 \mathcal{R}_{i j}}{1 - \xi_{\alpha}^2} = \frac{\mathcal{R}_{\alpha i j}}{1 - f_{u \alpha}},$$

which clearly demonstrates the agreement of (19) and (25). Thus, close results given by both collision models testify that the locally equilibrium approximation is capable of describing particle collisions in the flow considered.

#### 7. Particle settling in isotropic turbulence

In this section, we explore the collision models by comparing with numerical simulation of bidisperse particle motion under the action of gravity in an isotropic turbulence generated by LES (Gourdel et al., 1998). Such a flow may be treated as the simplest model of a circulating fluidized bed (Batrak et al., 2005). In conditions under consideration, the momentum Eq. (6) reduces to the force balance in the vertical direction for the particles of each species

$$\frac{V_{\alpha x} - U_x}{\tau_{\alpha}} + g = \mathbb{C}_x^{\alpha}$$
(31)

with g being the gravity acceleration.

Although the fluid turbulence is isotropic, the gravity force leads to the directional dependence of the particle kinetic stresses. Eq. (7) produces the following equations for the particle vertical (x) and horizontal (y) stress components:

$$\frac{2\left(f_{ux}^{\alpha}u^{\prime2}-\left\langle v_{ux}^{\prime2}\right\rangle\right)}{\tau_{\alpha}}+\mathbb{C}_{xx}^{\alpha\alpha}+\mathbb{C}_{xx}^{\alpha\beta}=0, \quad \frac{2\left(f_{uy}^{\alpha}u^{\prime2}-\left\langle v_{xy}^{\prime2}\right\rangle\right)}{\tau_{\alpha}}+\mathbb{C}_{yy}^{\alpha\alpha}+\mathbb{C}_{yy}^{\alpha\beta}=0.$$
(32)

In accordance with (A5), the response coefficients entering into (32) are given by

$$f_{ux}^{\alpha} = \frac{T_{Lpx}^{\alpha}}{\tau_{\alpha} + T_{Lpx}^{\alpha}}, \quad f_{uy}^{\alpha} = \frac{T_{Lpy}^{\alpha}}{\tau_{\alpha} + T_{Lpy}^{\alpha}}, \tag{33}$$

and the response coefficients appearing in the collision terms are defined as  $f_u^{\alpha} = (f_{ux}^{\alpha} + 2f_{uy}^{\alpha})/3$ . Following Csanady (1963), the effect of crossing trajectories on the eddy–particle interaction time is taken into account by means of the following relations:

$$T_{Lpx}^{\alpha} = \frac{T_L}{\left(1 + C_{\gamma} \gamma_{\alpha}^2\right)^{1/2}}, \quad T_{Lpy}^{\alpha} = \frac{T_L}{\left(1 + 4C_{\gamma} \gamma_{\alpha}^2\right)^{1/2}}, \quad \gamma_{\alpha} = \tau_{\alpha} g, \tag{34}$$

where  $T_L$  is the fluid Lagrangian integral timescale, and  $C_{\gamma}$  = 0.45. The particle response time is given by

$$\tau_{\alpha} = \frac{\tau_{\alpha 0}}{\varphi(\operatorname{Re}_{\alpha})}, \quad \tau_{\alpha 0} = \frac{2\rho_{\alpha}r_{\alpha}^{2}}{9\rho\nu}, \quad \varphi(\operatorname{Re}_{\alpha}) = \begin{cases} 1 + 0.15\operatorname{Re}_{\alpha}^{0.687} & \text{for } \operatorname{Re}_{\alpha} \leq 10^{3} \\ 0.11\operatorname{Re}_{\alpha}/6 & \text{for } \operatorname{Re}_{\alpha} > 10^{3} \end{cases}$$

where  $\tau_{\alpha 0}$  is the Stokes particle response time,  $\text{Re}_{\alpha} \equiv 2r_{\alpha}\tau_{\alpha}g/\nu$  is the particle Reynolds number,  $\rho_{\alpha}$  and  $\rho$  are the particle and fluid densities, and  $\nu$  is the fluid kinematic viscosity.

Solutions to Eqs. (31) and (32), where the collision terms are determined using the TP model or the FP model with e = 1, are performed under the conditions corresponding to simulations by Gourdel et al. (1998). The motion of a binary mixture, consisting of the particles of the same size ( $r_{\alpha} = 325 \ \mu\text{m}$ ) but of different

densities ( $\rho_1 = 117.5 \text{ kg/m}^3$ ,  $\rho_2 = 235 \text{ kg/m}^3$ ), is considered. The volume fraction of the light particles is fixed ( $\Phi_1 = 0.013$ ) and that of the heavy particles is varied. The carrier fluid is air, and the fluid flow is assumed to have no average velocity ( $U_x = 0$ ).

Figs. 3 and 4 show comparisons between the model predictions and the numerical simulations of the source terms in the momentum and energy equations for the particles of both species. It is clear that the predictions and the simulations are in quite good agreement, and the results obtained using the TP and FP models are hardly distinguishable.

Fig. 5 displays the average particle velocities of both species,  $V_{\alpha x}$ , as well as the mean velocity of the mixture,  $V_x \equiv (\rho_1 \Phi_1 V_{1x} + \rho_2 \Phi_2 V_{2x})/(\rho_1 \Phi_1 + \rho_2 \Phi_2)$ , versus the volume fraction of the heavy particles,  $\Phi_2$ . In Fig. 5, the free-fall velocities with no collisions,  $V_{\alpha x}^{\infty}$ , are depicted as well. All the velocity examined hold the following inequalities:  $V_{1x}^{\infty} < V_{1x} < V_x < V_{2x} < V_{2x}^{\infty}$ . Due to collisions, momentum transfer takes place from the heavy particles to the light particles and this involves a reduction in the difference between  $V_{2x}$  and  $V_{1x}$  with  $\Phi_2$ . The mean mixture velocity,  $V_x$ , agrees closely with  $V_{1x}^{\infty}$  for small  $\Phi_2$  and approaches  $V_{2x}^{\infty}$  for large  $\Phi_2$ . It is seen a remarkable accord between the predictions and the simulations. The results obtained with the help of both



**Fig. 3.** The source terms in the momentum equations versus the volume fraction of the heavy particles: 1, 3, 5 –  $\mathbb{C}^1_x$ ; 2, 4, 6 –  $\mathbb{C}^2_x$ ; 1, 2 – TP model; 3, 4 – FP model; 5, 6 – Gourdel et al. (1998).



**Fig. 4.** The source terms in the energy equations versus the volume fraction of the heavy particles: 1, 3,  $5 - \mathbb{C}_{ii}^{12}/2$ ; 2, 4,  $6 - \mathbb{C}_{ii}^{21}/2$ ; 1, 2 – TP model; 3, 4 – FP model; 5, 6 – Gourdel et al. (1998).



**Fig. 5.** The average particle velocities:  $1 - V_{1x}^{\infty}$ ; 2,  $6 - V_{1x}$ ;  $3 - V_{2x}^{\infty}$ ; 4,  $7 - V_{2x}$ ; 5,  $8 - V_x$ ; 2, 4, 5 - model predictions; 6, 7, 8 - Gourdel et al. (1998).

the TP model and the FP model for calculating the collision terms are indistinguishable.

Fig. 6 shows the influence of the heavy particle fraction on the particle fluctuating energy of both species. Both the predictions and the simulations exhibit a pronounced maximum of  $k_{p1}$  when  $\Phi_2$  increases. The initial rise in  $k_{p1}$  is attributable to increasing the production of  $k_{p1}$  due to collisions. For large  $\Phi_2$ , collisions lead the mean velocity drift between the species to vanish, rendering their contribution to the particle-turbulence negligible. It is of interest to note that, for small  $\Phi_2$ , the kinetic energy of the heavy particles,  $k_{p2}$ , is more than that of the light particles,  $k_{p1}$ , but, for relatively large  $\Phi_2$ , this inequality becomes opposite. When  $\Phi_2$  is small,  $k_{p2}$  is controlled mainly by the collisions with the light particles, whereas  $k_{p1}$  is governed by involving the light particles to fluid turbulence. When  $\Phi_2$  is relatively large, the contribution of collisions to particle kinetic energy of both species is not important and  $k_{n2}$  is determined by the interaction of particles with fluid turbulent eddies as well. The heavier particles are less responsive to fluid velocity fluctuations, that is the reason why  $k_{p2} < k_{p1}$  at large particle fractions.

In Fig. 7, comparisons between the model predictions and the numerical simulations of the kinetic stresses of the particles of both species are represented. Fig. 7(a) shows the predictions obtained when using only the truncated collision terms  $\mathbb{C}_{\mu}^{\alpha\beta(0)}$ , which are associated with the isotropic Gaussian PDF. Fig. 7(b)



**Fig. 6.** The particle fluctuating kinetic energy: 1, 3,  $5 - k_{p1}$ ; 2, 4,  $6 - k_{p2}$ ; 1, 2 – TP model; 3, 4 – FP model; 5, 6 – Gourdel et al. (1998).



**Fig. 7.** The particle velocity fluctuations: 1, 5, 9 –  $\langle v_{1x}^2 \rangle$ ; 2, 6, 10 –  $\langle v_{1y}^2 \rangle$ ; 3, 7, 11 –  $\langle v_{2x}^2 \rangle$ ; 4, 8, 12 –  $\langle v_{2y}^2 \rangle$ ; 1–4 – TP model; 5–8 – FP model; 9–12 – Gourdel et al. (1998).

demonstrates the results derived when using the full collision terms  $\mathbb{C}_{ij}^{\alpha\beta} \equiv \mathbb{C}_{ij}^{\alpha\beta(0)} + \mathbb{C}_{ij}^{\alpha\beta(1)}$ , which are based on an anisotropic PDF. The strong directional anisotropy of the kinetic stresses calls attention. This is due two mechanisms of the production of particle velocity fluctuations. In the first place, the collision production mechanisms manifest itself mainly in the drift direction (i.e., in the vertical direction). Second, as is clear from (33) and (34), the "crossing trajectory effect" causes the particles to be more responsible to the vertical fluid velocity fluctuations than to the horizontal ones. Both of these effects result in considerably higher values of the vertical stress components as compared to those in the horizontal direction. Comparing Fig. 7(a) and (b) demonstrate how taking into account the anisotropy of the PDF influences the particle kinetic stresses. As is seen, the inclusion of  $\mathbb{C}_{ii}^{\alpha\beta(1)}$  leads to a noticeable reduction in the particle fluctuating velocity anisotropy of both species. Although the results of both collision models are found to be very close, the predictions obtained on the basis of the FP model are in slightly better agreement with the simulations of Gourdel et al. (1998) than those based on the TP model.

To gain insight into why the TP and FP models predict close results, notice that, in the locally equilibrium approximation (30), the coefficients appearing in (B9) and (C3) coincide (namely,  $A_{ij} = \tilde{A}_{ij}$ ,  $B_{ij} = \tilde{B}_{ij}$ , and  $C_{ij} = \tilde{C}_{ij}$ ) and hence the collision terms given by both models for bidisperse particles coincide as well. Because the locally equilibrium approximation is quite correct for predicting the turbulent characteristics of the flow considered in this section, it is not surprising that the results obtained using the TP and FP collision models are in close agreement.

#### 8. Summary

Two statistical models for predicting the effect of collisions on particle velocities and stresses in a binary mixture of inertial particles dispersed in turbulent flow were advanced. The first model is based on a Grad-like expansion for the two-particle velocity distribution. The second model starts from a Grad-like expansion for the joint fluid–particle velocity distribution. Both of these collision models incorporate the effects of the mean velocity drift, the particle velocity correlation, and the anisotropy of particle fluctuating velocities. In spite of apparent complexity, both models provide algebraic relationships for the collision terms that quantify the contributions of collisions to the balance equations of particulate momentum and stresses. These collision terms can be easy implanted in any CFD code designed for simulating particle-laden turbulent flows on the basis of the Eulerian two-fluid approach with using a differential model of particulate stresses.

The validity of the models is established by means of comparisons with numerical simulations performed in uniformly sheared and isotropic homogeneous turbulent flows. The collision models being developed compare reasonably well with numerical simulations and properly reproduce the crucial trends of computations. Although the results predicted by both collision models for homogeneous flows considered in the paper are found to be very close, the second model is more complete because it provides the direct contribution of the anisotropy of fluid velocity fluctuations and fluid–particle velocity covariances.

It is significant that the models presented are applicable for simulating not-too-dense bidisperse turbulent flows laden with heavy not-too-low-inertia particles. Thus, the collision terms entering into the momentum and stress balance equations would hold when  $\rho_{\alpha}/\rho \gg 1$ ,  $\Phi < 0.1$ , and  $\tau_{\alpha}/\tau \gg 1$ .

A potential extension of the collision models includes the modelling of more complicated inhomogeneous turbulent flows. In this case, one might expect a more considerable distinction between the predictions of both models.

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#### Appendix A

The diffusion tensors appearing in Eq. (3) have the following form:

$$\begin{aligned} \lambda_{ij}^{\alpha} &= \left\langle u_{i}^{\prime}u_{k}^{\prime}\right\rangle \left\{ \frac{f_{u}^{\alpha}k_{j}}{\tau_{\alpha}} + l_{u}^{\alpha}k_{n}\frac{\partial U_{j}}{\partial x_{n}} + \tau_{\alpha}m_{u}^{\alpha}k_{l}\frac{\partial U_{n}}{\partial x_{l}}\frac{\partial U_{j}}{\partial x_{n}} \right) \\ &- \frac{1}{2}\frac{D_{p}\left\langle u_{i}^{\prime}u_{k}^{\prime}\right\rangle}{Dt}\left( f_{u1}^{\alpha}k_{j} + \tau_{\alpha}l_{u1}^{\alpha}k_{j}\frac{\partial U_{j}}{\partial x_{n}} \right), \end{aligned}$$
(A1)

$$\mu_{ij}^{\alpha} = \left\langle u_{i}^{\prime}u_{k}^{\prime}\right\rangle \left(g_{u\ kj}^{\alpha} + \tau_{\alpha}h_{u\ kn}^{\alpha}\frac{\partial U_{j}}{\partial x_{n}}\right) - \frac{\tau_{\alpha}}{2}\frac{D_{p}\left\langle u_{i}^{\prime}u_{k}^{\prime}\right\rangle}{Dt}g_{u1\ kj}^{\alpha},\tag{A2}$$

$$\frac{D_{\alpha}\left\langle u_{i}^{\prime}u_{j}^{\prime}\right\rangle}{Dt}=\frac{\partial\left\langle u_{i}^{\prime}u_{j}^{\prime}\right\rangle}{\partial t}+U_{\alpha k}\frac{\partial\left\langle u_{i}^{\prime}u_{j}^{\prime}\right\rangle}{\partial x_{k}},\quad U_{\alpha i}=U_{i}-\tau_{\alpha}\mu_{ij}^{\alpha}\frac{\partial\ln\Phi}{\partial x_{j}}$$

with  $\langle u'_i u'_j \rangle$  being the turbulent stresses of the fluid, and  $U_{\alpha i}$  being the mean fluid velocity viewed by the particles of species  $\alpha$ . In (A1) and (A2), the tensor coefficients  $f^{\alpha}_{u ij}$ ,  $g^{\alpha}_{u ij}$ ,  $l^{\alpha}_{u ij}$ ,  $h^{\alpha}_{u ij}$ ,  $m^{\alpha}_{u ij}$ ,  $f^{\alpha}_{u ij}$ ,  $f^{\alpha}_{u ij}$ ,  $g^{\alpha}_{u ij}$ , and  $l^{\alpha}_{u 1 ij}$  measure the response of particles of species  $\alpha$  to velocity fluctuations of the fluid, i.e., coupling between the particulate and fluid phases. By making use of matrix notation, these response coefficients are written as follows:

$$\begin{split} & \mathbf{f}_{u}^{\alpha} = \mathbf{M}_{u0}^{\alpha}, \quad \mathbf{g}_{u}^{\alpha} = \mathbf{N}_{u0}^{\alpha} - \mathbf{f}_{u}^{\alpha}, \quad \mathbf{l}_{u}^{\alpha} = \mathbf{g}_{u}^{\alpha} - \mathbf{f}_{u1}^{\alpha}, \\ & \mathbf{h}_{u}^{\alpha} = \mathbf{N}_{u1}^{\alpha} + \mathbf{M}_{u1}^{\alpha} - 2\mathbf{g}_{u}^{\alpha}, \\ & \mathbf{m}_{u}^{\alpha} = \mathbf{N}_{u1}^{\alpha} + 2\mathbf{M}_{u1}^{\alpha} + \mathbf{M}_{u2}^{\alpha} - 3\mathbf{g}_{u}^{\alpha}, \quad \mathbf{f}_{u1}^{\alpha} = \mathbf{M}_{u1}^{\alpha}, \\ & \mathbf{g}_{u1}^{\alpha} = \mathbf{N}_{u1}^{\alpha} - \mathbf{f}_{u1}^{\alpha}, \quad \mathbf{l}_{u1}^{\alpha} = \mathbf{g}_{u1}^{\alpha} - 2\mathbf{M}_{u2}^{\alpha}, \end{split}$$
(A3)

$$\begin{split} \mathbf{M}_{un}^{\alpha} &= \frac{1}{n!\tau_{p\alpha}^{n+1}} \int_{0}^{\infty} \mathbf{\Psi}_{Lp}^{\alpha}(\tau) \tau^{n} \exp\left(-\frac{\tau}{\tau_{p\alpha}}\mathbf{I}\right) d\tau = \frac{(-1)^{n}}{n!\tau_{p\alpha}^{n+1}} \frac{d^{n}\mathbf{F}_{\alpha}(s)}{ds^{n}}, \\ \mathbf{N}_{un}^{\alpha} &= \frac{1}{n!\tau_{p\alpha}^{n+1}} \int_{0}^{\infty} \mathbf{\Psi}_{Lp}^{\alpha}(\tau) \tau^{n} d\tau = \frac{(-1)^{n}}{n!\tau_{p\alpha}^{n+1}} \lim_{s \to 0} \frac{d^{n}\mathbf{F}_{\alpha}(s)}{ds^{n}}, \quad s = \tau_{p}^{-1}, \end{split}$$

where  $\mathbf{F}_{\alpha}(s)$  denotes the Laplace transformation over the Lagrangian fluid velocity autocorrelation matrix  $\Psi_{Lp}^{\alpha}(\tau)$  viewed by the particles of species  $\alpha$ , and  $\mathbf{I}$  is the unit matrix. If the particle response time is much greater than the temporal turbulence microscale, the autocorrelations may be taken in the form of the exponential approximation

$$\Psi_{Lp}^{\alpha}(\tau) = \exp\left(-\tau \mathbf{T}_{Lp}^{-1}\right) \tag{A4}$$

with  $T_{Lp}^{-1}$  being the inverse of the eddy-particle interaction time matrix. Substituting (A4) into (A3) leads to the following expressions for the response coefficients:

$$\begin{aligned} \mathbf{f}_{u}^{\alpha} &= \left(\mathbf{I} + \tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)^{-1}, \quad \mathbf{g}_{u}^{\alpha} &= \left(\mathbf{T}_{Lp}/\tau_{p\alpha}\right)\left(\mathbf{I} + \tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)^{-1}, \\ \mathbf{I}_{u}^{\alpha} &= \left(\mathbf{T}_{Lp}/\tau_{p\alpha}\right)\left(\mathbf{I} + \tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)^{-2}, \quad \mathbf{h}_{u}^{\alpha} &= \left(\mathbf{T}_{Lp}/\tau_{p\alpha}\right)^{2}\left(\mathbf{I} + \tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)^{-2}, \\ \mathbf{m}_{u}^{\alpha} &= \left(\mathbf{T}_{Lp}/\tau_{p\alpha}\right)^{2}\left(\mathbf{I} + \tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)^{-3}, \quad \mathbf{f}_{u1}^{\alpha} &= \left(\mathbf{I} + \tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)^{-2}, \\ \mathbf{g}_{u1}^{\alpha} &= \left(\tau_{p\alpha}^{-1}\mathbf{T}_{Lp}\right)^{2} - \left(\mathbf{I} + \tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)^{-2}, \\ \mathbf{I}_{u1}^{\alpha} &= \left(\mathbf{I} + 3\tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)\left(\tau_{p\alpha}^{-1}\mathbf{T}_{Lp}\right)^{2}\left(\mathbf{I} + \tau_{p\alpha}\mathbf{T}_{Lp}^{-1}\right)^{-3}. \end{aligned}$$
(A5)

Note that, when the terms containing the response coefficients  $l_{u\ ij}^{x}$ ,  $h_{u\ ij}^{x}$ ,  $m_{u\ ij}^{z}$ ,  $f_{u\ ij}^{x}$ ,  $g_{u\ ij}^{x}$ ,  $ad l_{u\ ij}^{z}$ , are neglected, (A1) and (A2) reduce to the diffusion tensors appearing in the kinetic equation obtained by Derevich and Zaichik (1988) and Reeks (1991) for a homogeneous unsheared flow field. Mention should be also made of another way of the functional formalism employed by Hyland et al. (1999) to derive a PDF kinetic equation for the transport of particles in turbulent flow. The difference between the approaches is in the way of solving the set of integral equations for functional derivatives. In the present approach, the iteration procedure was employed to solve this equation set (Zaichik, 1999; Zaichik et al., 2004), which allows the diffusion tensors to be got in the form of (A1) and (A2). In Hyland et al. (1999), this problem was solved using the technique of Green's functions. Both approaches become equivalent for times large enough compared to the eddy–particle interaction timescale.

#### **Appendix B**

In (12), the coefficients  $\mathcal{R}_{\alpha i}$  and  $\mathcal{R}_{\alpha ij}$  are found from the following conditions:

$$\begin{aligned} \frac{1}{\Phi_1\Phi_2} \int \int v'_{\alpha i} P(\mathbf{v}_1, \mathbf{v}_2) d\mathbf{v}_1 d\mathbf{v}_2 &= \langle v'_{\alpha i} \rangle = 0, \\ \frac{1}{\Phi_1\Phi_2} \int \int v'_{\alpha i} v'_{\alpha j} P(\mathbf{v}_1, \mathbf{v}_2) d\mathbf{v}_1 d\mathbf{v}_2 &= \left\langle v'_{\alpha i} v'_{\alpha j} \right\rangle, \\ \frac{1}{\Phi_1\Phi_2} \int \int v'_{\alpha i} v'_{\beta j} P(\mathbf{v}_1, \mathbf{v}_2) d\mathbf{v}_1 d\mathbf{v}_2 &= \left\langle v'_{\alpha i} v'_{\beta j} \right\rangle, \quad \beta \neq \alpha. \end{aligned}$$

Hence, in accordance with (9), (10) and (12), it follows that

$$\begin{aligned} \mathcal{R}_{\alpha i} &= 0, \quad \mathcal{R}_{\alpha i j} = \left\langle \nu'_{\alpha i} \nu'_{\alpha j} \right\rangle - \nu'^{2}_{\alpha} \delta_{i j}, \\ \mathcal{Q}_{i j} &= \frac{\left\langle \nu'_{1 i} \nu'_{2 j} \right\rangle + \left\langle \nu'_{1 j} \nu'_{2 i} \right\rangle}{2} - \zeta_{1 2} \nu'_{1} \nu'_{2} \delta_{i j}. \end{aligned} \tag{B1}$$

Further let us assume that the velocity correlations of the particles of different species are linearly related to those of the particles of the same species

$$\frac{\left\langle \nu_{1i}^{\prime}\nu_{2j}^{\prime}\right\rangle + \left\langle \nu_{1j}^{\prime}\nu_{2i}^{\prime}\right\rangle}{2} = C_{1}\left\langle \nu_{1i}^{\prime}\nu_{1j}^{\prime}\right\rangle + C_{2}\left\langle \nu_{2i}^{\prime}\nu_{2j}^{\prime}\right\rangle. \tag{B2}$$

Notice that (B2) is just the simplest relation, which permits the covariance between the velocities of different particles to be expressed in terms of their self-correlations. Since (10) gives  $\langle v'_{1k}v'_{2k}\rangle = 3\zeta_{12}v'_1v'_2$ , the trace of (B2) yields

$$C_1 v_1^{\prime 2} + C_2 v_2^{\prime 2} = \zeta_{12} v_1^{\prime} v_2^{\prime}. \tag{B3}$$

It is seen that the coefficients  $C_1$  and  $C_2$  are linked by only relation (B3). Therefore, there is one degree of freedom in choosing these coefficients. As an additional prerequisite to the determination of  $C_1$  and  $C_2$ , we require that the terms of the particles of the same species be independent of the properties of the particles of the other species. To do this requires as follows:

$$C_1 = \frac{\zeta_{12} v_2'}{2 v_1'}, \quad C_2 = \frac{\zeta_{12} v_1'}{2 v_2'}.$$
 (B4)

With due regard for (B1), (B2) and (B4), the first-order expansion term (12) is rewritten as

$$P^{(1)}(\mathbf{v}_{1},\mathbf{v}_{2}) = \left[\frac{\nu'_{1i}\nu'_{1j}\varphi_{1ij}}{\nu'_{1}^{2}} + \frac{\nu'_{2i}\nu'_{2j}\varphi_{2ij}}{\nu'_{2}^{2}} + \frac{(\nu'_{1i}\nu'_{2j} + \nu'_{1j}\nu'_{2i})\varphi_{12ij}}{\nu'_{1}\nu'_{2}}\right]\frac{P^{(0)}(\mathbf{v}_{1},\mathbf{v}_{2})}{2},$$
  

$$\varphi_{1ij} = \frac{\mathcal{R}_{1ij}}{(1-\zeta_{12}^{2})\nu'_{1}^{2}}, \quad \varphi_{2ij} = \frac{\mathcal{R}_{2ij}}{(1-\zeta_{12}^{2})\nu'_{2}^{2}},$$
  

$$\varphi_{12ij} = -\frac{\zeta_{12}}{2(1-\zeta_{12}^{2})} \left(\frac{\mathcal{R}_{1ij}}{\nu'_{1}^{2}} + \frac{\mathcal{R}_{2ij}}{\nu'_{2}^{2}}\right).$$
(B5)

In what follows we proceed to the new coordinates

$$\mathbf{q} = \kappa_1 \mathbf{v}_2 + \kappa_2 \mathbf{v}_1, \quad \mathbf{w} = \mathbf{v}_2 - \mathbf{v}_1, \quad \kappa_1 = \frac{\nu_1^2 - \zeta_{12} \, \nu_1' \, \nu_2'}{\nu_1'^2 + \nu_2'^2 - 2\zeta_{12} \, \nu_1' \, \nu_2'},$$
  

$$\kappa_2 = \frac{\nu_2'^2 - \zeta_{12} \, \nu_1' \, \nu_2'}{\nu_1'^2 + \nu_2'^2 - 2\zeta_{12} \, \nu_1' \, \nu_2'},$$
(B6)

which quantify two types of particle motion, namely, the transport of the binary mixture as a whole and the relative motion of twoparticle species. The form of **q** is chosen so that the argument of the exponential function in (10) can be presented as the sum of the kinetic energies of two motion types, and thereby this resembles the velocity of a mass centre of two particles in solid body mechanics. Then the two-particle PDF (9) along with (10) and (B6) is given by

$$P(\mathbf{w}, \mathbf{q}) = P^{(0)}(\mathbf{w}, \mathbf{q}) + P^{(1)}(\mathbf{w}, \mathbf{q}),$$
(B7)

$$P^{(0)}(\mathbf{w},\mathbf{q}) = \frac{\Phi_1 \Phi_2}{(2\pi \nu_1' \nu_2')^3 (1-\zeta_{12}^2)^{3/2}} \exp\left[-\frac{w^2 q_k' q_k'}{2(1-\zeta_{12}^2) \nu_1'^2 \nu_2'^2} - \frac{w_k' w_k'}{2w^2}\right],$$
(B8)

$$P^{(1)}(\mathbf{w},\mathbf{q}) = \left[A_{ij}q'_iq'_j + B_{ij}w'_iw'_j + C_{ij}\left(q'_iw'_j + q'_jw'_i\right)\right]P^{(0)}(\mathbf{w},\mathbf{q}), \quad (B9)$$

$$\begin{split} \mathsf{A}_{ij} &= \frac{\varphi_{1ij}}{2\,\nu_1^2} + \frac{\varphi_{2ij}}{2\,\nu_2^2} + \frac{\varphi_{12ij}}{\nu_1'\,\nu_2'} = \frac{1}{2(1-\zeta_{12}^2)} \bigg[ \frac{\mathcal{R}_{1ij}}{\nu_1'} \left( 1 - \zeta_{12}\frac{\nu_1'}{\nu_2'} \right) \\ &+ \frac{\mathcal{R}_{2ij}}{\nu_2'^4} \left( 1 - \zeta_{12}\frac{\nu_2'}{\nu_1'} \right) \bigg], \end{split}$$

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$$\begin{split} B_{ij} &= \frac{\kappa_1^2 \varphi_{1jj}}{2\nu_1'^2} + \frac{\kappa_2^2 \varphi_{2ij}}{2\nu_2'^2} - \frac{\kappa_1 \kappa_2 \varphi_{12ij}}{\nu_1' \nu_2'} \\ &= \frac{1}{2(1-\zeta_{12}^2)} \bigg[ \frac{\kappa_1^2 \mathcal{R}_{1ij}}{\nu_1'^4} \bigg( 1 + \zeta_{12} \frac{\kappa_2 \nu_1'}{\kappa_1 \nu_2'} \bigg) + \frac{\kappa_2^2 \mathcal{R}_{2ij}}{\nu_2'^4} \bigg( 1 + \zeta_{12} \frac{\kappa_1 \nu_2'}{\kappa_2 \nu_1'} \bigg) \bigg], \end{split}$$

$$\begin{split} C_{ij} &= \frac{\kappa_2 \varphi_{2ij}}{2 \nu_2^{\prime 2}} - \frac{\kappa_1 \varphi_{1ij}}{2 \nu_1^{\prime 2}} + \frac{(\kappa_2 - \kappa_1) \varphi_{12ij}}{2 \nu_1^{\prime} \nu_2^{\prime}} \\ &= \frac{1}{2(1 - \zeta_{12}^2)} \left\{ \frac{\mathcal{R}_{2ij}}{\nu_2^{\prime 4}} \left[ \kappa_2 + \frac{\zeta_{12}(\kappa_1 - \kappa_2) \nu_2^{\prime}}{2 \nu_1^{\prime}} \right] \\ &- \frac{\mathcal{R}_{1ij}}{\nu_1^{\prime 4}} \left[ \kappa_1 + \frac{\zeta_{12}(\kappa_2 - \kappa_1) \nu_1^{\prime}}{2 \nu_2^{\prime}} \right] \right\}. \end{split}$$

In (17), 
$$\mathbb{C}_{i}^{\alpha(0)}$$
 and  $\mathbb{C}_{i}^{\alpha(1)}$  are as follows:  

$$\mathbb{C}_{i}^{\alpha(0)} = \frac{\sigma^{2} N_{\beta} m_{\beta}(1+e)}{\Phi_{\alpha} \Phi_{\beta}(m_{\alpha}+m_{\beta})} \int_{\mathbf{w} \mathbf{k} < 0} \int_{\mathbf{w} \mathbf{k} < 0} (\mathbf{w} \cdot \mathbf{k})^{2} l_{i} P^{(0)}(\mathbf{w}, \mathbf{q}) d\mathbf{k} d\mathbf{w} d\mathbf{q}$$

$$= \frac{\pi \sigma^{2} N_{\beta} m_{\beta}(1+e) W}{2(m_{\alpha}+m_{\beta})} W_{i} F_{1}(z), \qquad (B10)$$

$$\mathbb{C}_{i}^{\alpha(1)} = \frac{\sigma^{2}N_{\beta}m_{\beta}(1+e)}{\Phi_{\alpha}\Phi_{\beta}(m_{\alpha}+m_{\beta})} \int \int \int W_{\mathbf{w}\mathbf{k}<0} (\mathbf{w}\cdot\mathbf{k})^{2}l_{i}P^{(1)}(\mathbf{w},\mathbf{q})d\mathbf{k}d\mathbf{w}d\mathbf{q}$$
$$= \frac{\pi\sigma^{2}N_{\beta}m_{\beta}(1+e)W^{4}}{(m_{\alpha}+m_{\beta})W^{2}} \bigg[ WB_{ik}W_{k}\Psi_{1}(z) - \frac{B_{jk}W_{i}W_{j}W_{k}}{2W}\Psi_{2}(z) \bigg], \quad (B11)$$

$$F_1(z) = \frac{\exp(-z)}{\sqrt{\pi z}} \left( 1 + \frac{1}{2z} \right) + \operatorname{erf} \sqrt{z} \left( 1 + \frac{1}{z} - \frac{1}{4z^2} \right),$$
  

$$\Psi_1(z) = 4F_0(z) - 3F_1(z),$$

$$\Psi_2(z) = \Psi_1(z) - \frac{2\Psi_0(z)}{z},$$

where  $N_{\beta}$  is the number concentration of the particles of species  $\beta$ . In (18),  $\mathbb{C}_{ij}^{\alpha\beta(0)}$  and  $\mathbb{C}_{ij}^{\alpha\beta(1)}$  are as follows:

$$\mathbb{C}_{ij}^{\alpha\beta(0)} = \frac{\sigma^2 N_\beta m_\beta (1+e)}{\Phi_\alpha \Phi_\beta (m_\alpha + m_\beta)} \int \int \int \int \left[ \frac{m_\beta (1+e)}{(m_\alpha + m_\beta)} (\mathbf{w} \cdot \mathbf{k})^3 k_i k_j - \kappa_\alpha (\mathbf{w} \cdot \mathbf{k})^2 (w_i k_j + w_j k_i) \right] \times P^{(0)} (\mathbf{w}, \mathbf{q}) d\mathbf{k} d\mathbf{w} d\mathbf{q} + \kappa_\alpha \left( \mathbb{C}_i^{\alpha(0)} W_j + \mathbb{C}_j^{\alpha(0)} W_i \right) \\
= \pi \sigma^2 N_\beta W \frac{m_\beta (1+e)}{m_\alpha + m_\beta} \left\{ \frac{m_\beta (1+e)}{4(m_\alpha + m_\beta)} \left[ \left( W_i W_j + \frac{W^2}{3} \delta_{ij} \right) F_2(z) - \left( W_i W_j - \frac{W^2}{3} \delta_{ij} \right) \frac{3F_1(z)}{2z} \right] - \kappa_\alpha \left[ W_i W_j \frac{2F_0(z)}{z} - \left( W_i W_j - \frac{W^2}{3} \delta_{ij} \right) \frac{3F_1(z)}{2z} \right] \right\},$$
(B12)

$$\begin{split} \mathbb{C}_{ij}^{z\beta(1)} &= \frac{\sigma^{2}N_{\beta}m_{\beta}(1+e)}{\Phi_{x}\Phi_{\beta}(m_{x}+m_{\beta})} \int \int_{\mathbf{w}\cdot\mathbf{k}<0} \left[ \frac{m_{\beta}(1+e)}{(m_{x}+m_{\beta})} (\mathbf{w}\cdot\mathbf{k})^{3} l_{i} l_{j} \right. \\ &\left. -\kappa_{\alpha}(\mathbf{w}\cdot\mathbf{k})^{2}(w_{i} l_{j}+w_{j} l_{i}) \right] \times P^{(1)}(\mathbf{w},\mathbf{q}) d\mathbf{k} d\mathbf{w} d\mathbf{q} + \kappa_{\alpha} \left( \mathbb{C}_{i}^{z(1)}W_{j} + \mathbb{C}_{j}^{z(1)}W_{i} \right) \right. \\ &= \frac{\pi\sigma^{2}N_{\beta}W(1+e)^{2}m_{\beta}^{2}}{4(m_{x}+m_{\beta})^{2}} \times \left\{ 2w'^{4}B_{ij}\Psi_{3}(z) + w'^{2} \left[ \delta_{ij}W_{k}W_{n}B_{kn} + 2(W_{i}B_{jk}+W_{j}B_{ik})W_{k} \right] \frac{\Psi_{4}(z)}{2z} - W_{i}W_{j}W_{k}W_{n}B_{kn} \times \frac{\Psi_{5}(z)}{4z^{2}} \right\} \\ &\left. -\pi\sigma^{2}N_{\beta}W\frac{(1+e)m_{\beta}}{m_{\alpha}+m_{\beta}} \left\{ \kappa_{\alpha} \left[ 2w'^{4}B_{ij}\Psi_{3}(z) - w'^{2}\delta_{ij}W_{k}W_{n}B_{kn} \frac{\Psi_{2}(z)}{4z^{2}} \right] \right. \\ &\left. +w'^{2}(W_{i}B_{jk}+W_{j}B_{ik})W_{k}\frac{\Psi_{6}(z)}{2z} - W_{i}W_{j}W_{k}W_{n}B_{kn}\frac{\Psi_{7}(z)}{2z^{2}} \right] \\ &\left. -\frac{v_{\alpha}^{2}v_{\beta}^{\prime}(1-\zeta_{12}^{2})}{w'^{4}} \left[ 2w'^{4}C_{ij}F_{1}(z) + w'^{2}(W_{i}C_{jk}+W_{j}C_{ik})W_{k}\frac{\Psi_{1}(z)}{2z} \right] \right\}, \end{split}$$
(B13)

$$\begin{split} F_2(z) &= F_1(z) + \frac{2F_0(z)}{z}, \quad \Psi_3(z) = F_1(z) + \frac{2\Psi_1(z)}{z}, \\ \Psi_4(z) &= \Psi_1(z) - \frac{\Psi_2(z)}{2z}, \\ \Psi_5(z) &= \Psi_1(z) - \frac{7\Psi_2(z)}{2z}, \quad \Psi_6(z) = \Psi_1(z) - \frac{\Psi_2(z)}{z}, \\ \Psi_7(z) &= \frac{\Psi_2(z) + \Psi_5(z)}{2}. \end{split}$$

# Appendix C

In (20), the coefficients  $A_{\alpha ij}$ ,  $B_{\alpha ij}$  and  $\Gamma_{\alpha ij}$  as well as the correlation coefficient  $\xi_{\alpha}$  are the following:

$$\begin{split} A_{\alpha ij} &= \frac{1}{\left(1-\xi_{\alpha}^{2}\right)^{2}} \left( \mathcal{R}_{ij} - \frac{2u'\xi_{\alpha}}{v'_{\alpha}} \mathcal{S}_{\alpha ij} + \frac{u'^{2}\xi_{\alpha}^{2}}{v'^{2}} \mathcal{R}_{\alpha ij} \right), \\ B_{ij} &= \frac{\xi_{\alpha}^{2}}{\left(1-\xi_{\alpha}^{2}\right)^{2}} \left( -\frac{v'_{\alpha}\xi_{\alpha}}{u'} \mathcal{R}_{ij} + (1+\xi_{\alpha}^{2}) \mathcal{S}_{\alpha ij} - \frac{u'\xi_{\alpha}}{v'_{\alpha}} \mathcal{R}_{\alpha ij} \right), \\ \Gamma_{\alpha ij} &= \frac{1}{\left(1-\xi_{\alpha}^{2}\right)^{2}} \left( \frac{v'_{\alpha}\xi_{\alpha}^{2}}{u'^{2}} \mathcal{R}_{ij} - \frac{2v'_{\alpha}\xi_{\alpha}}{u'} \mathcal{S}_{\alpha ij} + \mathcal{R}_{\alpha ij} \right), \\ \mathcal{R}_{ij} &= \left\langle u'_{i}u'_{j} \right\rangle - u'^{2}\delta_{ij}, \quad \mathcal{S}_{\alpha ij} = \frac{\left\langle u'_{\alpha i}v'_{\alpha j} \right\rangle + \left\langle u'_{\alpha j}v'_{\alpha i} \right\rangle}{2} - \xi_{\alpha}u'v'_{\alpha}\delta_{ij}, \\ u'^{2} &= \frac{\left\langle u'_{\alpha k}u'_{k} \right\rangle}{3}, \\ \xi_{\alpha} &= \frac{\left\langle u'_{\alpha k}v'_{\alpha k} \right\rangle}{\left\langle u'_{k}u'_{k} \right\rangle^{1/2}}, \end{split}$$

The first-expansion term appearing in (24) has the form

$$P^{(1)}(\mathbf{v}_1, \mathbf{v}_2) = \left[\frac{\nu'_{1i} \, \nu'_{1j} \phi_{1ij}}{\nu'_1^2} + \frac{\nu'_{2i} \, \nu'_{2j} \phi_{2ij}}{\nu'_2^2} + \frac{(\nu'_{1i} \, \nu'_{2j} + \nu'_{1j} \, \nu'_{2i}) \phi_{12ij}}{\nu'_1 \, \nu'_2}\right] \frac{P^{(0)}(\mathbf{v}_1, \mathbf{v}_2)}{2},$$
(C1)

$$\begin{split} \phi_{1ij} &= \frac{\left(A_{1ij} + A_{2ij} - \mathcal{R}_{ij}\right)\xi_1^2 \left(1 - \xi_2^2\right)^2}{u'^2 \left(1 - \xi_1^2\right)^2} + \frac{2B_{1ij} \left(1 - \xi_2^2\right)}{u' \, \nu_1' \, \xi_1 \left(1 - \xi_{12}^2\right)} + \frac{\Gamma_{1ij}}{\nu_1'^2}, \\ \phi_{2ij} &= \frac{\left(A_{1ij} + A_{2ij} - \mathcal{R}_{ij}\right)\xi_2^2 \left(1 - \xi_1^2\right)^2}{u'^2 \left(1 - \xi_{12}^2\right)^2} + \frac{2B_{2ij} \left(1 - \xi_{12}^2\right)}{u' \, \nu_2' \xi_2 \left(1 - \xi_{12}^2\right)} + \frac{\Gamma_{2ij}}{\nu_2'^2}, \end{split}$$

$$\phi_{12ij} = \frac{1}{u'(1-\zeta_{12}^2)} \left[ \frac{(A_{1ij}+A_{2ij}-\mathcal{R}_{ij})\xi_1\xi_2(1-\zeta_1^2)(1-\xi_2^2)}{u'(1-\zeta_{12}^2)} + \frac{B_{2ij}\xi_1(1-\xi_2^2)}{v'_2\xi_2^2} \right],$$

where the particle velocity correlation coefficient is determined as

$$\zeta_{12} = \xi_1 \xi_2. \tag{C2}$$

Note that, in isotropic homogeneous turbulence,  $\xi_{\alpha} = f_{u\alpha}^{1/2}$  and hence the particle velocity correlation coefficients defined by (11) and (C2) are coincident.

Changing to the coordinates defined in (B6), we can rewrite the two-particle PDF (24) along with (10) and (C1) in the form of (B7) with the zero-expansion term given by (B8) and the first-expansion term given by

$$P^{(1)}(\mathbf{w},\mathbf{q}) = \left[\widetilde{A}_{ij}q'_iq'_j + \widetilde{B}_{ij}w'_iw'_j + \widetilde{C}_{ij}\left(q'_iw'_j + q'_jw'_i\right)\right]P^{(0)}(\mathbf{w},\mathbf{q}), \quad (C3)$$

$$\begin{split} \widetilde{A}_{ij} &= \frac{\phi_{1ij}}{2\nu_1^2} + \frac{\phi_{2ij}}{2\nu_2^2} + \frac{\phi_{12ij}}{\nu_1'\nu_2'}, \quad \widetilde{B}_{ij} = \frac{\kappa_1^2\phi_{1ij}}{2\nu_1'^2} + \frac{\kappa_2^2\phi_{2ij}}{2\nu_2'^2} - \frac{\kappa_1\kappa_2\phi_{12ij}}{\nu_1'\nu_2'}, \\ \widetilde{C}_{ij} &= -\frac{\kappa_1\phi_{1ij}}{2\nu_1'^2} + \frac{\kappa_2\phi_{2ij}}{2\nu_2'^2} + \frac{(\kappa_2 - \kappa_1)\phi_{12ij}}{2\nu_1'\nu_2'}. \end{split}$$

It is clear that the first-order expansion term (C3) coincides with the one (B9) when replacing  $A_{ij}$ ,  $B_{ij}$ , and  $C_{ij}$  by  $\tilde{A}_{ij}$ ,  $\tilde{B}_{ij}$ , and  $\tilde{C}_{ij}$ . Because of this, all the relations for the collision rate as well as for the momentum and stress collision terms, which are obtained using the TP model, still stand for the FP model when replacing  $B_{ij}$  and  $C_{ij}$  by  $\tilde{B}_{ij}$  and  $\tilde{C}_{ij}$ .

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