INTER-PARTICLE COLLISIONS IN TURBULENT FLOWS: A STOCHASTIC LAGRANGIAN MODEL

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ABSTRACT

A stochastic inter-particle collision model to be applied in the frame of the Euler/Lagrange approach is introduced, which accounts for the correlated motion of particles in turbulent flows. The model relies on the generation of a fictitious collision partner, whereby no information is required on the actual position and direction of motion of the surrounding particles. The occurrence of a collision is decided based on the collision probability according to kinetic theory, but considering the correlation of the velocities of colliding particles. For validating the collision model results from large eddy simulations are used for monodisperse particles and a binary mixture of particles being dispersed in a homogeneous isotropic turbulence.

INTRODUCTION

Turbulent gas-solid flows with high particle loading are frequently found in technical and industrial processes. Examples are pneumatic conveying, fluidized beds, vertical risers, particle separation in cyclones, mixing devices, and others. In such particle-laden flows the particle behavior may be considerably affected by inter-particle collisions in addition to aerodynamic transport and turbulence effects if the mass loading is high or regions of high concentration develop as a result of inertial effects (Sommerfeld, 1995). Quite a number of theoretical studies on the collision rate of particles or droplets in turbulent flows have been published in the past. A detailed review was given for example by Williams and Crane (1983) and Pearson et al. (1984). Here only the limiting cases are considered which are also compared with the model calculations presented in this paper. In turbulent flows the two limiting cases may be identified by using a particle Stokes number which is defined as the ratio of particle response time, τ_p, to the relevant time scale of turbulence, T_t :

$$St = \frac{\tau_p}{T_t} \tag{1}$$

For particles which are small compared with the smallest scales of turbulence, i.e. the Kolmogorov length scale, and completely follow the turbulence (i.e. St $\rightarrow$ 0), Saffman and Turner (1956) have provided an expression for the collision rate of droplets in atmospheric turbulence. The collision rate (i.e. collisions per unit volume and time) for two droplet size classes with the radii R_{p1} and R_{p2} and with the number concentrations n_1 and n_2 (i.e. particles per unit volume) is given by:

$$N_c = \left(\frac{8\,\pi}{15}\right)^{\frac{1}{2}} n_1\, n_2\, \left(R_{p1} + R_{p2}\right)^3 \left(\frac{\varepsilon}{\nu}\right)^{\frac{1}{2}} \tag{2}$$

where ε is the dissipation rate of turbulent energy and ν is the kinematic viscosity. Hence, for this limiting case the collision rate depends solely on droplet size, concentration and the local velocity gradient.

The other extreme case is the kinetic theory limit for St $\rightarrow \infty$, where the particle motion is completely uncorrelated with the fluid and hence the velocity of colliding particles is also uncorrelated. This case was analysed by Abrahamson (1975) for heavy particles in high intensity turbulence. The resulting collision rate between two particle classes is given by:

$$N_c = 2^{\frac{3}{2}} \pi^{\frac{1}{2}} n_1 n_2 \left(R_{p1} + R_{p2}\right)^2 \sqrt{\sigma_{p1}^2 + \sigma_{p2}^2} \tag{3}$$

where σ_p is the fluctuating velocity of the particles assuming that all components are identical (i.e. isotropic fluctuating motion $\sigma_p^2 = \overline{u_p'^2} = \overline{v_p'^2} = \overline{w_p'^2}$). In practical two-phase flows the two limits are rarely met, rather the particles may partially respond to turbulence. Hence, the velocities of colliding particles will be correlated to a certain degree, since they are transported in the same turbulent eddy upon collision. The degree of correlation depends on the turbulent Stokes number defined above (Eq. 1). An analysis of this effect was performed by Williams and Crane (1983) and an analytic expression for the collision rate of particles in turbulent flows covering the entire range of particle Stokes numbers and accounting for a possible correlation of the velocities of colliding particles. The expression for the collision rate is given in terms of particle concentration, particle relaxation times (i.e. Stokes numbers), turbulence intensities, and turbulent scales.

$$N_c = (162\,\pi)^{\frac{1}{2}}\; n_1\; n_2\; \nu\; L_t \frac{\rho\; U_{rel}}{\rho_p\; \sigma_p} \left(St_1^{0.5} + St_2^{0.5}\right)^2 \quad (4)$$
$$\frac{2}{\pi} \tan^{-1}\left\{ \frac{1}{3} \frac{\rho_p}{\rho} \frac{\sigma_p\; L_t}{\nu} \left(\frac{U_{rel}}{\sigma_p} \right)^2 \frac{St_1\; St_2}{\left(St_1^{0.5} + St_2^{0.5}\right)^2} \right\}$$

Here L_t is the integral length scale of turbulence, U_{rel} the mean relative velocities between colliding particles and σ_p the fluctuating velocity of the fluid assuming isotropic turbulence. The Stokes number of the two particle classes is defined in terms of the integral time scale of turbulence.

Modeling of inter-particle collisions in the frame of the Euler/Lagrange method for the numerical calculation of two-phase flows has been based mainly on two approaches, a direct simulation and a modeling concept based on kinetic theory of gases. The most straight forward approach to account for inter-particle collisions is the direct simulation approach (Tanaka and Tsuji 1991). This requires that all particles are tracked simultaneously through the flow field. Thereby, the occurrence of collisions between any pair of particles can be judged based on their positions and relative motion. Once a collision occurs the change in linear and angular particle velocities can be determined by solving the equations for the conservation of linear and angular momentum in connection with Couloumbs law of friction.

For practical calculations based on the Euler/Lagrange approach stochastic inter-particle collision models are more suitable (Sommerfeld and Zivkovic, 1992; Oesterle and Petitjean, 1993). This approach is based on the generation of a fictitious second particle according to the local probability density functions of particle diameter and velocities. With this information the collision probability in analogy with kinetic theory of gases can be determined. From the value of the collision probability it is decided whether a collision takes place. By solving the conservation equations for linear and angular momentum the post-collision velocities of the considered particle are calculated. The post-collision properties of the fictitious particle are not of further interest in the calculations. So far in most of the modeling approaches, the correlation of the velocities of colliding particles was not respected.

In the present paper a model is presented which accounts for the correlation effect Sommerfeld (1998). The model calculations are validated on the basis of data obtained by large eddy simulations (LES) for an isotropic homogeneous turbulence (Lavieville et al. 1995; Gourdel et al. 1998).

FLUID FLOW AND PARTICLE TRACKING

In both test cases considered here, the flow field, i.e. turbulence intensities and turbulence length and time scales are prescribed according to the LES. The mean continuous phase velocity is zero in both cases. The particle trajectories are calculated sequentially and the particle phase properties are ensemble averaged for each control volume of the computational domain. The forces which are considered in the equation of motion for the particles are the drag and gravity forces only. Hence the following ordinary differential equations are solved along the particle trajectory:

$$\frac{d\vec{x}_p}{dt} = \vec{u}_p \quad (5)$$
$$\frac{d\vec{u}_p}{dt} = \frac{3}{4} \frac{\rho}{\rho_P\; D_P}\; c_D \left(\vec{u} - \vec{u}_p\right)\left|\vec{u} - \vec{u}_p\right| + \vec{g}$$

For the drag coefficient the standard correlation is used (Sommerfeld, 1995). In order to generate the instantaneous fluid velocity along the particle trajectory the so-called Langevin equation model is applied (Sommerfeld et al. 1993). In this approach the fluid fluctuation at the new particle position is correlated with that at the pervious position through a Lagrangian and an Eulerian correlation function. The latter is only considered in the case with gravity in order to model the crossing trajectories effect. Periodic boundary conditions are applied for the particles according to the approach adopted in the LES. The time step for solving the equations of motion was fixed with a value of 0.5 ms.

INTER-PARTICLE COLLISION MODEL

The developed stochastic inter-particle collision model relies on the generation of fictitious collision partners and the calculation of the collision probability according to kinetic theory. The advantage of this model is that it does not require information on the location of the surrounding particles and hence it is also applicable if a sequential tracking of the particles is adopted, as usually done when applying the Euler/Lagrange approach to stationary flows. During each time step of the trajectory calculation of the considered particle a fictitious second particle is generated. The size and velocity of this fictitious particle are randomly sampled from local distribution functions. In generating the fictitious particle velocity components the correlation with the velocity of the considered particle due to turbulence has to be respected. The degree to which the particle velocities are correlated depends on their response to the turbulent fluctuations. The velocities of small particles will be strongly correlated while those of very large particles are completely uncorrelated. The response of particles to turbulent fluctuations is characterized in terms of the Stokes number, i.e. the ratio of the particle response time to the Lagrangian integral time scale (see Eq. 1). The particle response time is determined from the calculations accounting for non-linear drag and the Lagrangian integral time scale is obtained from the turbulent dispersion model (Sommerfeld et al. 1993). In the developed collision model, the correlation of the velocity components of the fictitious particle $u_{fict,i}$ with those of the real particle $u_{real,i}$ is accounted for in the following way by using the turbulent Stokes number:

$$u_{fict,i} = R(St_t)\, u_{real,i} + \sigma_{p,i} \sqrt{1 - R(St_t)^2}\; \xi \quad (6)$$

Here $\sigma_{p,i}$ is the local rms value of the particle velocity component i and ξ is a Gaussian random number with zero mean and a rms value of one. Hence, the sampled velocity components are composed of a correlated and a random part.

With increasing Stokes number the correlated term (first term in Eq. (6)) decreases and the random term increases accordingly. Comparing model calculations with large eddy simulations (which will be introduced below) the following dependence of the correlation function $R(St_t)$ on the Stokes number was found.

$$R(St_t) = \exp\left(-0.55\ St_t^{0.4}\right) \qquad (7)$$

The next step in the collision model is the determination for the probability for the occurrence of a collision between the considered and the fictitious particle within the time step. The probability is obtained as the product of the time step size Δt and the collision frequency given by kinetic theory:

$$P_{coll} = f_c\ \Delta t = \frac{\pi}{4}\ \left(D_{p1} + D_{p2}\right)^2 \left|\vec{u}_{p1} - \vec{u}_{p2}\right| N_{p2}\ \Delta t \quad (8)$$

where, D_{p1} and D_{p2} are the particle diameters, $\left|\vec{u}_{p1} - \vec{u}_{p2}\right|$ is the instantaneous relative velocity between the considered and the fictitious particle and N_{p2} is the number of particles per unit volume in the respective control volume. In order to decide whether a collision takes place, a random number RN from a uniform distribution in the interval [0,1] is generated. A collision is simulated when the random number becomes smaller than the collision probability, i.e if:

$$RN < P_{coll}$$

It is more complicated to determine the position of the fictitious particle relative to the considered particle. Since both particles move, any point on the surface of the particles is a possible point of contact. Moreover, the probability density is not the same for every point on the surface and strongly depends on the relative motion of the particles. Therefore, it is very difficult to model the collision in the co-ordinate system of the flow field in which both particles move. When the problem is however transferred into a co-ordinate system in which the fictitious particle is fixed, the collision calculation becomes much simpler. In this situation, the point of impact on the surface of the fictitious particle can only be located on the hemisphere facing the considered particle. Now a collision cylinder is defined as the domain where the center of the fictitious particle must be located if a collision takes place (Fig. 1). It is physically obvious that the probability density of finding the center of the fictitious particle at some point in the perpendicular cross-section of the cylinder is uniform (note that this does not imply a uniform probability density for the points of the particle surface to be points of contact). By generating two uniform random numbers XX and ZZ in the range [0, 1], the location of the collision point in the longitudinal section of the collision cylinder is defined by the lateral displacement, L, and the angle ϕ (Fig. 1).

$$\begin{aligned} L &= \sqrt{XX^2 + ZZ^2} \qquad with:\ L < 1 \\ \phi &= \arcsin(L) \end{aligned} \qquad (9)$$

An additional random number, Ψ, with uniform distribution ($0 < \Psi < 2\ \pi$) is necessary to determine the angular position of the collision point.

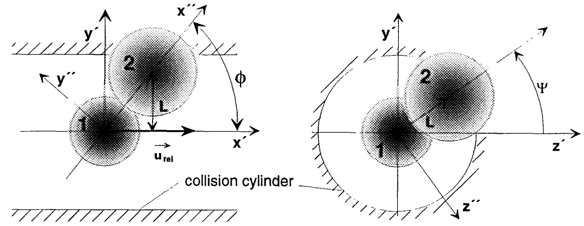

Figure 1. Particle-particle collision configuration and coordinate system

The relations for the calculation of the post-collision velocities of the considered particle in the co-ordinate system where the fictitious particle is stationary now reduce to the momentum equations for an oblique central collision. Hence, one obtains for the determination of the velocity components the following equations.

$$\begin{aligned} u'_{P1} &= u_{P1}\left(1 - \frac{1+e}{1 + m_{P1}/m_{P2}}\right) \\ v'_{P1} &= v_{P2} \end{aligned} \qquad (10)$$

Here, e is the coefficient of restitution, and m_{P1} and m_{P2} are the masses of the considered and the fictitious particle, respectively. Finally, the velocities of the considered particle are re-transformed in the original co-ordinate system.

An essential requirement for the collision model is however, that for each control volume the particle size and the velocity distribution functions have to be sampled and stored. The local distribution functions of the particle phase properties are updated after each Lagrangian calculation through an iterative procedure until these properties approach steady state values. Since in the first iteration no particle phase properties are available yet, the particle collision calculation begins with the second Lagrangian calculation. When the effect of the particles on the fluid flow is accounted for, this procedure is combined with the two-way coupling iteration procedure (Kohnen et al. 1993).

HOMOGENEOUS ISOTROPIC TURBULENCE

In order to validate the developed stochastic Lagrangian inter-particle collision model, data obtained by large eddy simulations (LES) were used (Lavieville et al. 1995). The first test case was a homogeneous isotropic turbulence field (i.e. a cube with periodic boundary conditions). The turbulence characteristics and the particle properties are summarized in Table 1. The collision detection algorithm adopted in the LES required to consider rather large particles (i.e. D_p = 656 µm). In order to have particle response times which are in the order of the integral time scale of turbulence, the density of the particles was selected accordingly (Table 1). The resulting turbulent Stokes numbers (Eq. 1) are between about 0.8 and 6.0. But the model calculations were also performed for a wider range of Stokes numbers. For this case no gravity was considered, whereby the particle motion is solely controlled by turbulence and collisions. The collision is assumed to be fully elastic (i.e. e = 1.0, μ = 0.0).

Gas phase rms velocity	0.3 m/s
Kinematic viscosity	$1.45 \cdot 10^{-5}$ m²/s
Lagrangian integral time scale	23 ms
Eulerian integral time scale	26 ms
Long. Eulerian length scale	7.25 mm
Lateral Eulerian length scale	3.71 mm
Particle diameter	0.656 mm
Particle density	25, 50, 100, and 200 kg/m³
Turbulent Stokes number	0.79, 1.5, 2.9, and 5.7
Volume fraction	0.005 – 0.05

Table 1. Turbulence characteristics and particle phase properties for the large eddy simulations

As expected, the energy of the particles` fluctuating motion decreases with increasing Stokes number, since the particles become less responsive to the turbulent fluctuations. Both the model calculations and the simulations follow the same trend, indicating that the particle-turbulence interaction is modeled properly (Fig. 2). The collisions between the particles have no strong influence on the particles fluctuating motion, i.e. the results for the different volume fractions are only slightly different.

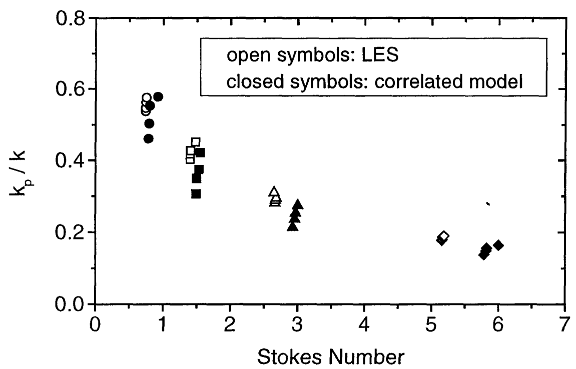

Figure 2. Kinetic energy of the particle fluctuating motion as a function of Stokes number (symbols of one kind indicate the results for the different volume fractions (see Table 1))

An important feature of the stochastic collision model is the consideration of the correlated motion of colliding particles. This effect is pronounced when the particle response time is in the order of the integral time scale of turbulence or even lower. The relative velocity distribution function (PDF) for particles with a Stokes number of 0.794, shown in Fig. 3, reveals the importance of accounting for this correlation. If the velocity of the fictitious particle is not correlated with that of the considered particle a rather wide velocity distribution with a mean value of 0.45 m/s is obtained. The correlated model in contrary gives a more narrow relative velocity distribution with a mean value reduced to 0.32 m/s. The comparison of the model calculations with the large eddy simulations shows a rather good agreement if the degree of correlation is modeled properly by appropriate specification of the model constants in the correlation function (Eq. 7).

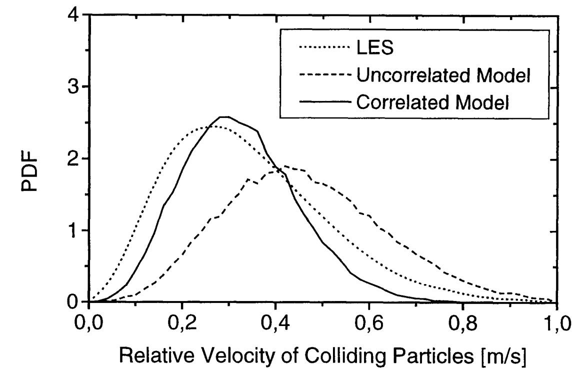

Figure 3. PDF of the relative velocity between colliding particles, comparison of the stochastic model with large eddy simulations (ρ_p = 25 kg/m³, St_t = 0.794, α = 0.0352)

The effect of Stokes number on the mean relative velocity of colliding particles is illustrated in Fig. 4 for model calculations with and without correlation. As a result of the higher agitation of small particles by turbulence the uncorrelated model considerably over-predict the mean relative velocity. The correlated model predicts an increase of the mean relative velocity with decreasing Stokes number up to a Stokes number of about 0.4. With further reducing particle size the velocity of colliding particles become more and more correlated and hence a decrease in the mean relative velocity is observed. For very small particles the mean relative velocity approaches the value obtained by Saffman and Turner (1956) for particles completely following the turbulent fluctuations. By not accounting for the velocity correlation for light particles, the mean relative velocity and hence the collision frequency is completely over-predicted. For heavy particles the same mean relative velocity is obtained for both model calculations as one would expect.

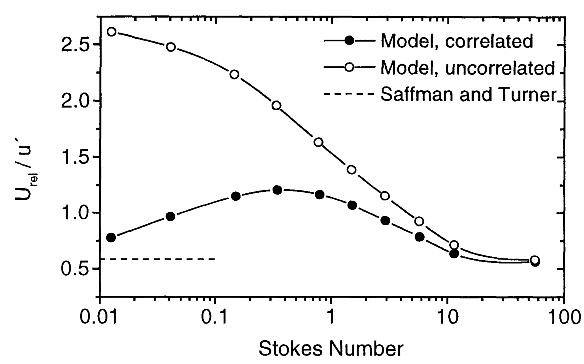

Figure 4. Mean relative velocity of colliding particles, comparison of uncorrelated and correlated model (α = 0.0176)

As a result of the reduction of the mean relative velocity due to the correlation effect, also the average collision frequency will be reduced. This effect may be illustrated by comparing the simulated average collision frequency with that resulting from the kinetic theory limit, which corresponds to the average collision frequency obtained without correlation. In Fig. 5 the ration of the calculated collision frequency to that predicted by kinetic theory is plotted versus Stokes number. For very large Stokes numbers the frequency ratio approaches unity. With decreasing Stokes number the frequency ratio is continuously reduced due to the increasing degree of correlated motion of colliding particles. The predicted increase of the frequency ratio with Stokes number is in very good agreement with the LES data.

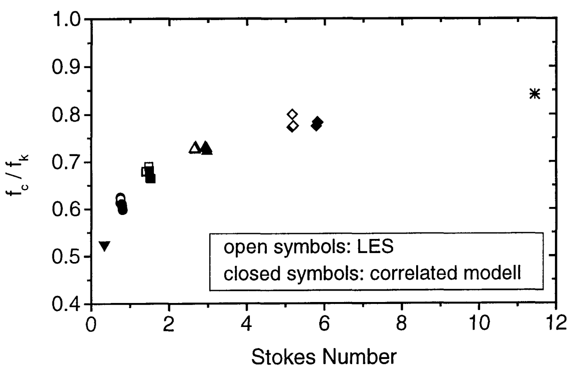

Figure 5. Dependence of the ratio of simulated collision frequency to the collision frequency obtained from the kinetic theory limit on the particle Stokes number

BINARY MIXTURE OF PARTICLES

The second test case for validating the stochastic inter-particle collision model was again an isotropic homogeneous turbulence. However, now a binary mixture of particles (fraction A and B) is considered. In the LES of Gourdel et al. (1998) the same turbulence properties were used as in the previous case (see Table 1). The particle size was 650 µm and two classes of particles (i.e. with different response time) were generated by using different densities (i.e. $\rho_A = 117.5$ kg/m^3 and $\rho_B = 235$ kg/m^3). The volume fraction of class A particles was fixed with $1.3 \cdot 10^{-2}$ and that of class B particles was varied between $6.5 \cdot 10^{-4}$ and $4 \cdot 10^{-2}$. Again completely elastic collisions were considered (i.e. $e = 1$, $\mu = 0$). The first series of calculations was performed for a granular medium without particle-fluid interaction under zero-gravity conditions. This implies that the particle motion is solely governed by inter-particle collisions and the initial fluctuation of the particles upon injection into the computational domain.

The particle fluctuating motion due collisions is characterized by the particle phase fluctuating energy (Fig. 6). As expected the energy of fluctuation is higher for the lighter particles (class A) than for the heavier particles (class B). With increasing total number density (i.e. in this case the number density of fraction A is constant and the number density of fraction B is increasing) the energy of particle fluctuation is increasing for both fractions due to the increase in total collision frequency. The model calculations are in good agreement with the LES-data. Only for large concentrations of fraction B, a slight over-prediction of the fluctuation of fraction A is observed.

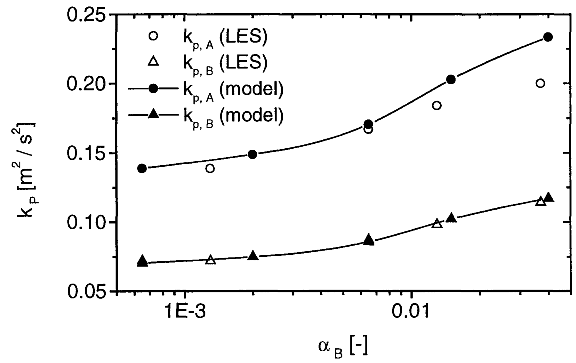

Figure 6. Kinetic energy of particle fluctuating motion for fraction A and B, comparison of model calculations with LES data

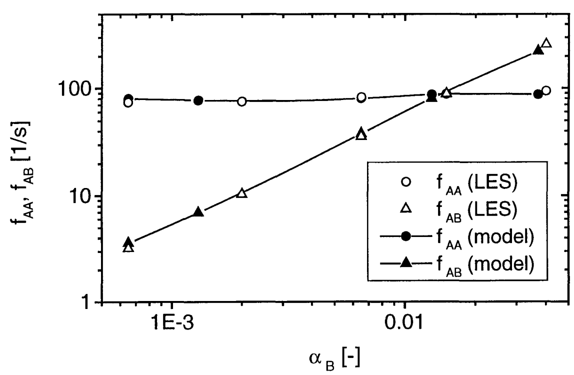

Figure 7. Collision frequencies for fraction A and between fraction A and B, comparison of model calculations with LES data

The calculated collision frequencies between particles of fraction A (f_{AA}) and between both fractions (f_{AB}) as a function of the volume fraction of class B particles are compared in Fig. 7 with the results of the LES. The collision frequency f_{AA} slightly increases with the volume fraction α_B, since the fluctuating intensity of fraction A particles is increasing (see Fig. 6). With increasing the fraction of B-particles also the collision frequency f_{AB} increases linearly. Both trends are very well captured by the model calculations and the agreement with the LES is very good.

In the second case with particle-flow interaction and a gravity of $g_x = 49.05$ m/s^2, a mean relative velocity between the two particle classes is induced due to their different terminal velocity. As a result of the collisions between the two particle fractions a momentum transfer is caused, whereby the mean velocity (i.e. in the direction of gravity) is smaller than the terminal velocity for the light particles (fraction A) and larger for the heavy particles (Fig. 8). At low volume fractions of class B, the heavy particles are strongly dragged by the light ones and hence the heavy particle mean velocity is about 19 % smaller than their terminal velocity. With increasing volume fraction of class B, the heavy particles drag the light particles and their mean velocity increases, while the mean velocity of the heavy particles also increases and approaches the expected terminal velocity. These effects are well reproduced in the model calculations and the agreement with the LES-results is reasonably good.

Considering the collision frequencies for this case (Fig. 9), it is obvious that f_{AA} is much smaller than for the case without flow (Fig. 7), which is caused by the particle-turbulence interaction. With increasing concentration of fraction B the collision frequency of fraction A (f_{AA}) increases at a higher rate compared to the result in Fig. 7 due to a stronger fluctuating motion resulting from the momentum transfer with the fraction B. The collision frequencies between fraction A and B are about the same than for the case without flow. This indicates that the reduction of collision frequency due to particle-turbulence interaction is balanced by the increase due to the mean relative drift between both fractions. The agreement of the model calculations with the LES-results is also for this case quite good.

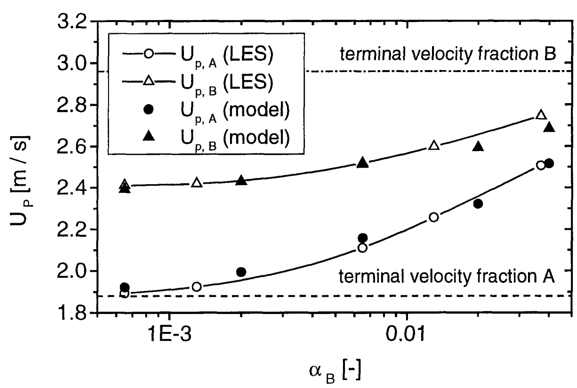

Figure 8. Mean particle velocities for fraction A and B, comparison of model calculations with LES data

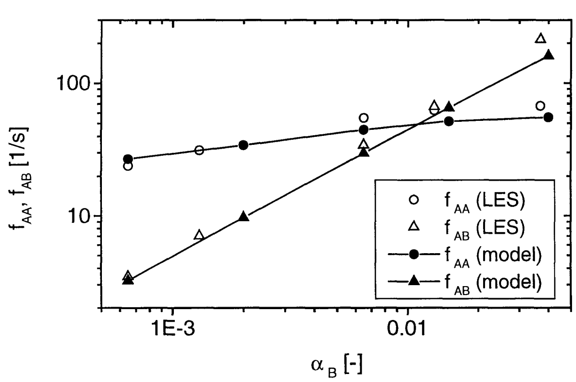

Figure 9. Collision frequencies for fraction A and between fraction A and B, comparison of model calculations with LES data

CONCLUSIONS

It has been demonstrated that the developed stochastic inter-particle collision model predicts the correct particle phase statistics if the correlation of the velocities of colliding particles is accounted for. For both test cases considered, the agreement with LES-data is very good. For a further validation of the model a homogeneous shear flow will be considered.

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