"Hypothetical" heavy particles dynamics in LES of turbulent dispersed two-phase channel flow

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1. Motivation and objectives

The extensive experimental study of dispersed two-phase turbulent flow in a vertical channel has been performed in Eaton's research group in the Mechanical Engineering Department at Stanford University (see Kulick *et al.* (1994) and Fessler *et al.* (1994)). In Wang & Squires (1996), this study motivated the validation of LES approach with Lagrangian tracking of round particles governed by drag forces. While the computed velocity of the flow have been predicted relatively well, the computed particle velocity differed strongly from the measured one. Using Monte Carlo simulation of inter-particle collisions, the computation of Yamamoto *et al.* (2001) was specifically performed to model Eaton's experiment. The results of Yamamoto *et al.* (2001) improved the particle velocity distribution. At the same time, Vance & Squires (2002) mentioned that the stochastic simualtion of inter-particle collisions is too expensive, requiring significantly more CPU resources than one needs for the gas flow computation. Therefore, the need comes to account for the inter-particle collisions in a simpler and still effective way. To present such a model in the framework of LES/Lagrangian particle approach, and to compare the calculated results with Eaton's measurement and modeling of Yamamoto is the main objective of the present paper.

2. Equation for the particle motion along smoothed trajectory

In the high-Reynolds number flows, three random forces act on the motion of solid particles: (i) particle-small scale turbulence interaction (affecting mostly light particle dynamics); (ii) inter-particle collisions (important for relatively heavy particle motion; this randomness motivated the present work); (iii) particle-wall interaction (due to the wall roughness). Accounting for all details of this randomness in LES is formidable. The problem is how to describe effectively the random Lagrangian motion of solid particles. One of the possibilities is as follows: By analogy with kinetic theory, we may introduce a 'hypothetical' particle, which is moving along the smoothed trajectory averaged over random collision trajectories. The smoothed acceleration of such solid particle changes the local momentum in the gas phase, thereby affecting the acceleration of neighboring solid particles. To derive the equation of such a smoothed motion, let us consider the dispersed two-phase turbulent flow as a time evolution of a system of interacting stochastic fluid (Pope 2000) and solid particles. The kinetic description is then specified by the distribution function of particles with position $\overrightarrow{\mathbf{r}}(x_1, x_2, x_3)$ and velocity $\overrightarrow{\mathbf{v}}(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$, $f(\overrightarrow{\mathbf{r}}, \overrightarrow{\mathbf{v}}, t)$, in the six-dimensional space, for solid particles, $f_p(\overrightarrow{\mathbf{r}}_p, \overrightarrow{\mathbf{v}}_p, t)$ and fluid particles, $f_g(\overrightarrow{\mathbf{r}}_g, \overrightarrow{\mathbf{v}}_g, t)$. For solid particles, the Boltzman equation can be written in the

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following form:

$$\frac{\partial f_p}{\partial t} + \overrightarrow{\mathbf{v}}_p \cdot \frac{\partial f_p}{\partial \overrightarrow{\mathbf{r}}_p} = I(f_p, f_p) + I(f_p, f_g) \tag{2.1}$$

where $I(f_p, f_p)$ and $I(f_p, f_g)$ are operators for solid-solid and solid-liquid particle collisions, respectively. The first collision operator in (2.1) is usually modeled assuming pair hard sphere collisions with prescribed efficiency (see Vance & Squires (2002), Lavelieville *et al.* (1997), Simonin *et al.* (2002), Sommerfeld (2001), Wang *et al.* (2000), Mei & Hu (1999), Sigurgeirsson *et al.* (2001)). The form of the second operator is principally unknown. The total number of solid particles does not change due to any collisions, as well as the total momentum of solid particles is unchanged due to solid-solid collisions,*i.e.*:

$$\int d^3\mathbf{v}_p I(f_p, f_p) = 0 \tag{2.2}$$

$$\int d^3\mathbf{v}_p I(f_p, f_g) = 0 \tag{2.3}$$

$$\int d^3\mathbf{v}_p I(f_p, f_p)\mathbf{v}_p = 0 \tag{2.4}$$

However

$$\int d^3\mathbf{v}_p I(f_p, f_g)\mathbf{v}_p \neq 0 \tag{2.5}$$

Introducing the solid particles density, n_p (in usual terms of kinetic approach) and the particle velocity averaged by f_p, $\langle\mathbf{v}_p\rangle_{f_p} = \frac{1}{n_p}\int d^3\mathbf{v}_p f_p\mathbf{v}_p$, let us assume that the solid-solid particle collision occurs frequently such that the correlation of fluctuations of solid particle velocities can be identified with the particle temperature of ordinary statistical mechanics, T_p:

$$\langle\mathbf{v}'_{p,\alpha}\mathbf{v}'_{p,\beta}\rangle_{f_p} = \frac{1}{3}\langle\mathbf{v}'^2_p\rangle_{f_M}\delta_{\alpha\beta} = \frac{T_p}{m_p} \tag{2.6}$$

Here f_M is Maxwellian distribution, m_p is the mass of the considered solid particle and $\delta_{\alpha\beta}$ is the Kronecker delta. Multiplying (2.1) by the velocity of particle, integrating over all these velocities and using (2.6), one yields:

$$\frac{d\langle\mathbf{v}_{p,\beta}\rangle_{f_p}}{dt} = -\frac{1}{n_p}\frac{\partial}{\partial x_\beta}\left(\frac{n_p T_p}{m_p}\right) + \frac{1}{n_p}\int\mathbf{v}_{p,\beta}I(f_p, f_g)d^3\mathbf{v}_{p,\beta} \tag{2.7}$$

where the first term implies the change of the 'particle pressure' along the smoothed trajectory of the particle and the second term is the mean rate of the particle velocity change due to particle-turbulence interaction. These two terms have to be modeled. The first term is modeled as follows. We introduce the 'temperature' of stochastic fluid particles, $T_{tur,g}$. According to its kinetic definition, one writes:

$$T_{tur,g} = \frac{2}{3}\rho_g VOL_L\langle\mathbf{v}'^2_g\rangle/2 \tag{2.8}$$

where ρ_g is the gas density, VOL_L may be viewed as a volume over integral spatial scale and $\langle\mathbf{v}'^2_g\rangle/2$ is the kinetic energy of turbulence in gas flow. Assuming a relaxation of the statistical temperature of solid particle to the statistical temperature of liquid one, one writes:

$$\frac{dT_p}{dt} = \beta(T_{tur,g} - T_p) \tag{2.9}$$

where β is an exchange frequency parameter. If β is very large, the statistical temperature

of particle may be assumed to be locally in a 'thermodynamic' equilibrium with the surrounding turbulence:

$$T_p = T_{tur,g} \tag{2.10}$$

Concerning the second term in (2.7), for heavy particles, it can be presented by the draft force:

$$\left(\langle \mathbf{v}_{g,\beta} \rangle_{f_g} - \langle \mathbf{v}_{p,\beta} \rangle_{f_p} \right) / \tau_p \tag{2.11}$$

where τ_p is the Stokes time. With the particle Reynolds dependency from Clift *et al.* (1978), it writes:

$$\tau_p = \frac{\rho_p d_p^2}{18 \rho_g \nu_g} \frac{1}{1 + 0.15 Re_p^{0.687}} \tag{2.12}$$

In this formulation, the equation (2.7) without the first term represents usual LES/ particle tracking procedure.

3. Computation procedure

LES of particle-laden flow is performed for conditions corresponding to the Eaton's experiment. In this experiment, a set of measurements has been performed on a vertical fully-developed air-channel flow laden with spherical particles of different mass loading. From this measurement, we chose the case with particles of copper (density $\rho_p = 8800 \, kg/m^3$, diameter $d_p = 70 \, \mu m$ and 20% of mass loading). The numerical code developed at CTR, Stanford University by Pierce & Moin (2001), was adapted in this paper for IBM PC. In this code, the sub-grid momentum transport term was modeled by dynamic approach of Germano *et al.* (1990). In the present work, this code has been coupled in 'two-ways' with Lagrangian particle solver, according to (2.7)-(2.11). The second order Runge-Kutta scheme has been used for computation of the particle motion.

To define the local statistical temperature of turbulence in (2.8), the volume was associated with the control volume of the finite-difference mesh. Two different expressions for the 'temperature' of turbulence have been used to calculate (2.8):

$$T_{turb,g} = \frac{2}{3} \rho_g \Delta_x \Delta_y \Delta_z \sum_{\alpha} (\mathbf{v}_{g,\alpha} - \overline{\mathbf{v}}_{g,\alpha})^2 / 2 \tag{3.1}$$

and for the mean one

$$\langle T_{turb,g} \rangle = \frac{2}{3} \rho_g \Delta_x \Delta_y \Delta_z \sum_{\alpha} \left\langle (\mathbf{v}_{g,\alpha} - \overline{\mathbf{v}}_{g,\alpha})^2 \right\rangle / 2 \tag{3.2}$$

The numerical algorithm of two-way momentum coupling was implemented. The particle equations have been solved using the second order Runge-Kutta method. For the gas velocity at a particle position, the linear interpolation scheme has been used. The implementation of higher order schemes of interpolation did not give an explicit advantage, requiring at the same time a substantial computational effort. The computations were performed at Reynolds number based on friction velocity and channel half-width of 644 (corresponding to Reynolds numbers of 13800 based on centerline velocity and channel half-width). Parameters of the computation have been chosen similar to Wang & Squires (1996) with $64 \times 65 \times 64$ grid points for the flow resolution in the x, y and z directions, respectively, that covered the computational domain $5\pi\delta/2 \times 2\delta \times \pi\delta/2$. In the streamwise and spanwise directions, uniform grid was used. In the direction normal to the wall, the non-uniform stretched grid has been used with first velocity position at

$y^+ = 0.88$. Periodic boundary conditions were used for gas phase and for particles at free boundaries.

4. Results

For unladen and laden turbulent flow with different mass loading, Fig.1a shows the mean stream-wise gas-velocity obtained in Eaton's experiment and in the present computation. It has been noted in the experiment that particles do not change practically the mean velocity profile of gas. As it is seen from Fig.1a, the computed mean gas velocity field is also not influenced by the presence of particles. Fig.1b and 1c show the turbulence intensity in stream-wise and wall-normal directions. The Eaton's experiment predicted an attenuation of the turbulence by particles. This is also seen from computation in Fig.1b and 1c. To demonstrate the strong effect of the turbulence attenuation, the centreline experimental and computed values of kinetic energy and viscous dissipation are presented in Fig.2. versus different mass loading. In Fig.3, the profiles of mean particle velocity and of its variance are shown. Fig.3a gives the particle mean streamwise velocity. It is clearly seen that similar to measurements and computations of Yamamoto *et al.* (2001), the present computation gives the flattened profile. In Fig.3b, the computed r.m.s. streamwise particle velocity is compared with the measurements. The computation is in agreement with experiment except near the channel centre. At the same time, it is seen from Fig.3c, that computed r.m.s. of wall-normal velocity is overestimated against the measured values (the data from Yamamoto *et al.* (2001) show an underestimation of measurements).

5. Conclusion and future work

The recent LES computation of particle-laden turbulent flow showed that the particle velocity distribution can be predicted relatively well, if the inter-particle collisions are included in the simulation. However the Monte Carlo simulation of inter-particle collisions, which is used in those computations, is too expensive for practical applications. In this paper, a simplified approach of two-phase flow simulation is proposed. By analogy with kinetic theory, we introduced a 'hypothetical' particle, which is moving along the smoothed trajectory averaged over random collision trajectories. An equation of such a smoothed motion has been derived, using hypothesis of a 'thermodynamic' equilibrium between the statistical temperature of the particle and the surrounding turbulence. The Lagrangian tracking of 'hypothetical' particles was performed along LES computation of a vertical fully-developed air-channel flow (experiment in Eaton's research group). It has been shown that our computation is in agreement with Eaton's experiment and computation, where the inter-particle interaction has been simulated by hard-sphere collisions with prescribed efficiency. At the same time, to account for inter-particle interactions, the presented model does not require additional CPU time. Our future work concerns the further development of this approach for interaction between particles & rough wall.
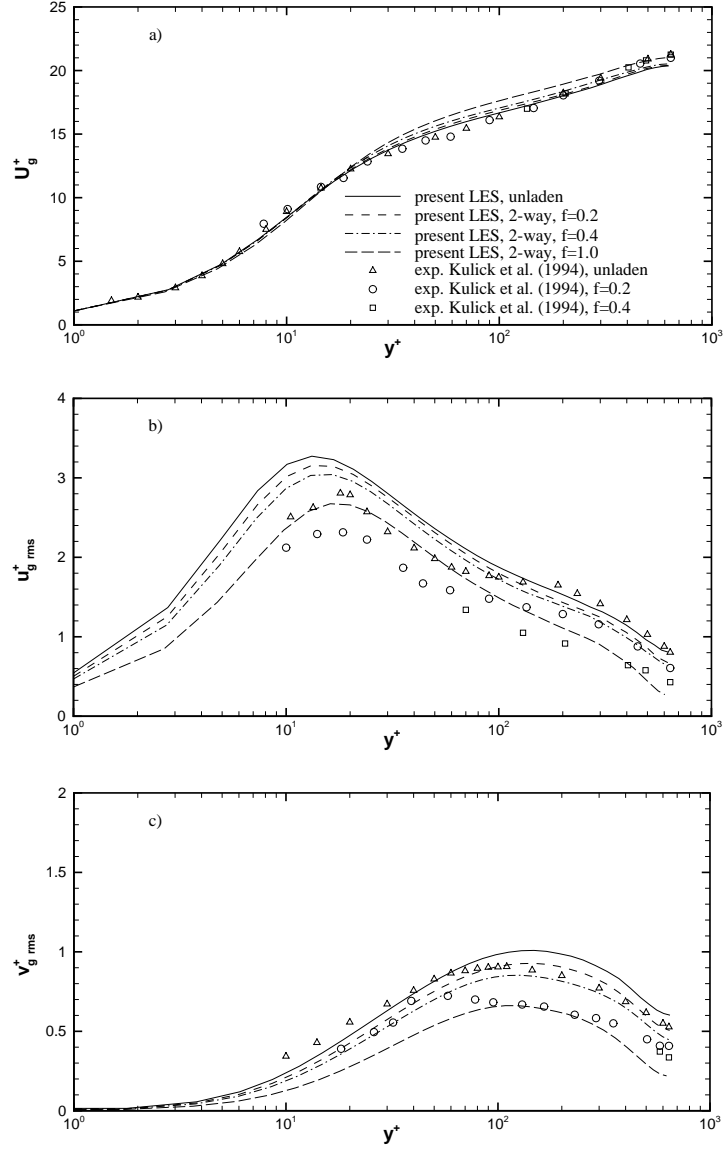
FIGURE 1. Comparison of computed gas velocity profiles with measurements of Kulick *et al.* (1994) at different mass loading: a) streamwise mean velocity; b) r.m.s. of streamwise velocity; c) r.m.s. of wall-normal velocity.

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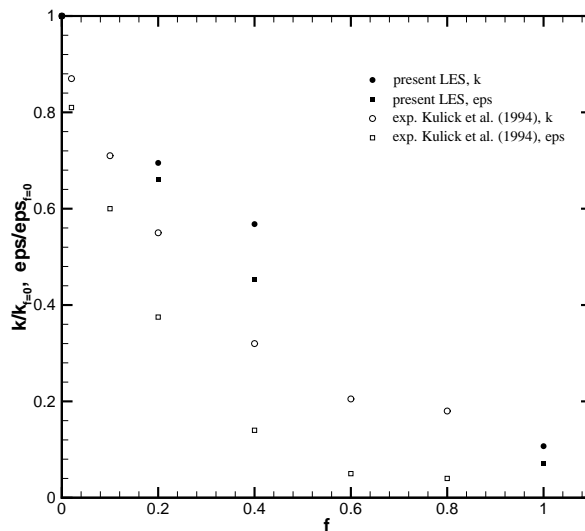
FIGURE 2. Attenuation of gas-phase turbulent kinetic energy and dissipation with particle mass loading: filled symboles - computation; empty symbols - measurement.

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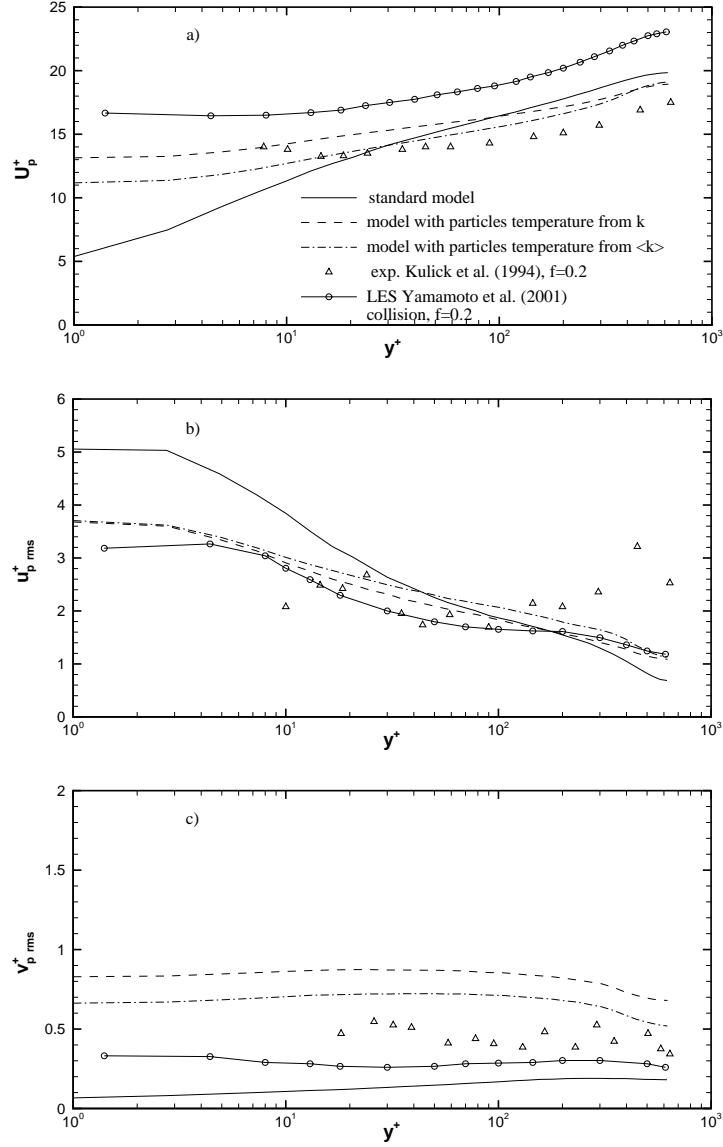CLIFT, R., GRACE, J. R., WEBER, M. 1978 *Bubbles, Drops and Particles.* Academic Press.

FIGURE 3. Comparison of computed particle velocity profiles with measurements of Kulick *et al.* (1994) and results from Yamamoto *et al.* (2001) with inter-particle collisions: a) streamwise mean velocity; b) r.m.s. of streamwise velocity; c) r.m.s. of wall-normal velocity.

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