LES of the particle-laden turbulent channel flow using partially smoothed dynamics of particles

Chtab A. and Gorokhovski M.

CORIA UMR-6614 CNRS University of Rouen, Site Universitaire du Madrillet, BP 12, 76801 Saint Etienne du Rouvray, France. E-mail: gorokhovski@coria.fr, chtab@coria.fr

The Boltzman equation for the particle distribution function has been written considering the gas-solid turbulent flow as an ensemble of stochastic interacting both liquid and solid particles. Then the motion equation for the solid particle partially averaged (smoothed) over all collisions has been derived. Similar to the kinetic theory, the statistical temperature has been introduced for the solid particle and for the turbulence. The relaxation-type relation was assumed for these two "temperatures". The smoothed particles dynamics was then coupled with LES approach for turbulent gas flow in "two-way". The calculated results are compared with the experiment of Kulick *et. al.* and with LES/particle computation of Yamomoto *et. al.* that consider the inter-particle interaction in the framework of hard-sphere collisions.

1. Motivation and objective

The experimental study [1,2] of dispersed two-phase developed turbulent flow in the vertical channel motivated to validate in [3] the LES approach with Lagrangian tracking of particles. The computed mean and r.m.s. velocity of flow and particles showed that while the gas flow has been predicted relatively well, the computed particle velocity differed from measurements. In the framework of discrete particles [4, 5] and continuum [6] approaches, this discrepancy motivated the further developments with inter-particle collisions. For example, along discrete particles approach, the collisions have been computed analogously to Monte Carlo simulation in the rarified gas [7, 8]. To this end, the computation by LES/particles in [9] was specifically performed to model the experiment [1, 2]. Accounting for inter-particle collisions, [9] improved the particle velocity distribution however requiring at the same time, significantly more CPU resources than one needs for the gas flow computation [4]. If the simulation of the particle laden turbulent flow is specifically target for the computation of two-phase combustion (which is our purpose in the future work), then such a computational model is too expensive. Therefore, the need comes to account for the inter-particle collision 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 measurements [1, 2] and with computation in [9] is the objective of the present paper.

2. Partially averaged equation for the particle motion along trajectory

In the high-Reynolds number flows, two random forces act on the motion of solid particle. The first one is due to the turbulence in flow and the second one is due to inter-particle interactions. These two processes are interrelated: the turbulence affects both the relative trajectory of two interacting particles (in terms of particle collisions efficiency) and the acceleration of the moving particle. When the particle is larger than the Kolmogorov microscale, it is too difficult to account for all details of such interactions. The problem is how to describe effectively the random Lagrangian motion of solid particle. By analogy with kinetic theory, one may average the motion of the particle over all unknown stochastic interactions. Then the trajectory of particle becomes partially smoothed. The smoothed acceleration of solid particle changes the local momentum in the gas phase, thereby affecting on the acceleration of neighboring solid particles. This is similar to the consideration of third body in many-body interaction problem with long-range forces. Also, the turbulence itself is often described in terms of Lagrangian stochastic variables [10]. In this spirit, we may consider the dispersed two-phase turbulent flow as a time evolution of a system of interacting stochastic both fluid and solid particles. The kinetic description is then specified by the distribution function of particles with position $\vec{\mathbf{r}}(x_1, x_2, x_3)$ and velocity $\vec{\mathbf{v}}(\mathbf{v}_1, \mathbf{v}_2, \mathbf{v}_3)$, $f(\vec{\mathbf{r}}, \vec{\mathbf{v}}, t)$, in the six-dimensional space, for each sort of particles, solid particles, $f_p(\vec{\mathbf{r}}_p, \vec{\mathbf{v}}_p, t)$ and fluid particles, $f_g(\vec{\mathbf{r}}_g, \vec{\mathbf{v}}_g, t)$. For solid particles, the Boltzman equation can be written in the following form:

$$\frac{\partial f_p}{\partial t} + \vec{\mathbf{v}}_p \cdot \frac{\partial f_p}{\partial \vec{\mathbf{r}}_p} = I(f_p, f_p) + I(f_p, f_g) \tag{1}$$

where $I(f_p, f_p)$ and $I(f_p, f_g)$ are operators for solid-solid and solid-liquid particles collisions, correspondingly. The first collision operator in (1) is usually modeled assuming pair hard sphere collisions with prescribed efficiency [11-16]. The form of the second operator of multi-particles collisions 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 does not change due to solid-solid collisions:

$$\int d^3\mathbf{v}_p \, I(f_p, f_p) = 0 \tag{2}$$

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

$$\int d^3\mathbf{v}_p \, I(f_p, f_p)\mathbf{v}_p = 0 \tag{4}$$

However

$$\int d^3\mathbf{v}_p \, I(f_p, f_g)\mathbf{v}_p \neq 0 \tag{5}$$

Introducing the solid particles density, n_p (in usual terms of kinetic approach [17]) 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 particles collision occurs enough frequently in a way that the correlation of fluctuations of solid particle velocities can be identified with the particle temperature of ordinary statistical mechanics, T_p:

$$\left\langle \mathbf{v}'_{p\alpha}\mathbf{v}'_{p\beta}\right\rangle_{f_p} = \frac{1}{3}\left\langle \mathbf{v}'^{\,2}_{p}\right\rangle_{f_M}\delta_{\alpha\beta} = \frac{1}{3}\frac{T_p}{m_p} \tag{6}$$

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 (1) by the velocity of particle, integrating over all these velocities and using (6), one yields:

$$\frac{d\left\langle \mathbf{v}_{p,\beta}\right\rangle_{f_p}}{d\,t} = -\frac{1}{n_p}\frac{\partial}{\partial x_\beta}\left(\frac{n_p T_p}{3m_p}\right) + \frac{1}{n_p}\int \mathbf{v}_{p,\beta}\, I\left(f_p, f_g\right) d^3\mathbf{v}_{p,\beta} \tag{7}$$

where the first term implies the change of the "particle pressure" along the smoothed particle trajectory and the second term is the mean rate of the particle velocity change due to collisions of solid particle with fluid turbulent particles. 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:

$$T_{tur,g} = \frac{2}{3}\rho_g\, VOL_L \left\langle \mathbf{v}'^2_g\right\rangle / 2 \tag{8}$$

where ρ_g is the gas density, VOL_L is a volume over Lagrangian integral spatial scale and $\left\langle \mathbf{v}'^2_g\right\rangle / 2$ 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:

$$\frac{d\,T_p}{d\,t} = \beta\left(T_{tur,g} - T_p\right) \tag{9}$$

where β is an exchange frequency parameter. If β is a very large value, then $\frac{d\,T_p}{d\,t} = 0$, *i.e.* the statistical temperature of particle either keeps the memory on its previous value or is locally in a "thermodynamic" equilibrium with the surrounding turbulence:

$$T_p = \max\left(T_{tur,g}, T_p\right) \tag{10}$$

Concerning the second term in (7), it can be presented by the draft force:

$$\left(\left\langle \mathbf{v}_{g,\beta}\right\rangle_{f_g} - \left\langle \mathbf{v}_{p,\beta}\right\rangle_{f_p}\right) / \tau_p \tag{11}$$

where τ_p is the response time, which is usually taken from the Stokes relaxation of the particle motion to the laminar flow with undisturbed velocity. With the particle Reynolds dependency of [18] , it writes:

$$\tau_p = \frac{\rho_p d_p^2}{18 \rho_g \nu_g} \frac{1}{1 + 0.15 \mathrm{Re}_p^{0.687}} \tag{12}$$

In this formulation, the equation (7) without the first term reduces to the usual LES/particle tracking procedure [3].

3. Computation procedure

The LES simulations were performed under conditions chosen to much the experiments [1,2]. In this experiment, a set of measurements has been performed on a vertical fully-developed air-channel flow laden with spherical particles of different levels of mass loading. In this measurement, the particles larger than the Kolmogorov microscale, were the particles of cooper with density $\rho_p = 8800 \, kg/m^3$ and diameter $d_p = 70 \, \mu m$. This case with 20% of mass loading was used in the present computation for validation of the model. The numerical code from [19] (called at CTR, Stanford University, as Chack's code), was adapted for IBM PC and used for the gas flow computation. In this code, the governing filtered Navier Stokes equations were solved using the second-order-accurate central- finite-difference scheme on staggered grids and the semi-implicit iterative for integration of those equations. A Newton-Raphson iterations were applied for time marching. The Poisson equation for pressure was solved using Fourier series expansions in the streamwise and spanwise directions together with tridiagonal matrix inversion. The subgrid momentum transport term was modeled by the dynamic approach developed in [20-22]. In the present work, this code has been coupled in "two-ways" with Lagrangian particles solver, specifically to (7) - (11). To define the local statistical temperature of turbulence in (8), the volume over Lagrangian integral spatial scale was associated with the control volume of the finite-difference mesh. The expressions for the instantaneous local kinetic energy of turbulence

$$k = \sum_{\alpha} \left(\mathbf{v}_{g,\alpha} - \overline{\mathbf{v}}_{g,\alpha} \right)^2 / 2 \tag{13}$$

and for the mean one

$$\overline{k} = \sum_{\alpha} \left\langle \left(\mathbf{v}_{g,\alpha} - \overline{\mathbf{v}}_{g,\alpha} \right)^2 \right\rangle / 2 \tag{14}$$

has been attempted to calculate (8), where the mean values were obtained from the fluid velocity time statistics. The numerical algorithm of two-way momentum coupling was implemented similar to fractional step method in KIVA2 numerical code [23]**.** 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 according to [3] with 65x66x65 grid points for the flow resolution in the x, y, and z directions, respectively, that covered the computational domain $8\delta \ x \ 2\delta \ x \ 2\delta$. In the streamwise and spanwise directions, the uniform grid was used. In the direction normal to the wall, the non-uniform stretched grid has been used with first velocity position at $y^+ = 0.88$. The periodic boundary conditions were used for gas phase and for particles at free boundaries.

4. Results

Fig.1a shows the mean streamwise gas-velocity profile obtained in experiment [1, 2] for unladen and laden turbulent flow. As it has been noted in [1, 2], the particles practically do not change the mean velocity profile. In this Figure, the mean flow velocity is shown from LES unladen and LES/particles with hard sphere collisions obtained in [9], as well as from LES unladen and LES/smoothed particles tracking, (7)-(11), computed with (13) and (14), in the present work. These cases are presented also in all Figures hereafter. It is seen from Fig. 1a that the mean gas velocity field is practically not influenced by the presence of particles. Fig. 1b shows the streamwise turbulence intensity. The experiment predicted attenuation of turbulence by particles. The calculated results in [9] do not show this effect regardless of whether inter-particle collision was included or not. The present computation show the turbulence attenuation effect but the intensity of this attenuation is strongly underestimated. Similar conclusion can be made from the computation of the wall-normal turbulence intensity, which is shown in Fig. 1c (in [9], such distribution was not presented). Underestimation of the turbulence attenuation effect by particles motivates the future study of the influence of particles on the subgrid turbulence. A model of particle/subgrid turbulence interaction will be presented in [24]. Fig. 2a shows profiles of the particle mean streamwise velocity. From measurements, it is clearly seen that the particle mean streamwise velocity profile is much flatter than one of the gas phase. Results of computations with (7)-(11) show the strong tendency towards the experiment, contrary to the computation by the usual LES/particle tracking procedure. It is also seen that making use of the instantaneous kinetic energy (13) in (8), leads to the distribution of velocity close to experimental one. In Fig. 2b and 2c, the computed r.m.s. streamwise and wall-normal particle velocities are compared with measurements. It is seen that similar to [9], the calculated results for streamwise velocity r.m.s. agree well with experimental results except in the channel center. At the same time, it is seen that computed here r.m.s. of wall-normal velocity is overestimated against the measured values while the data from [9] shows an underestimation of measurements.

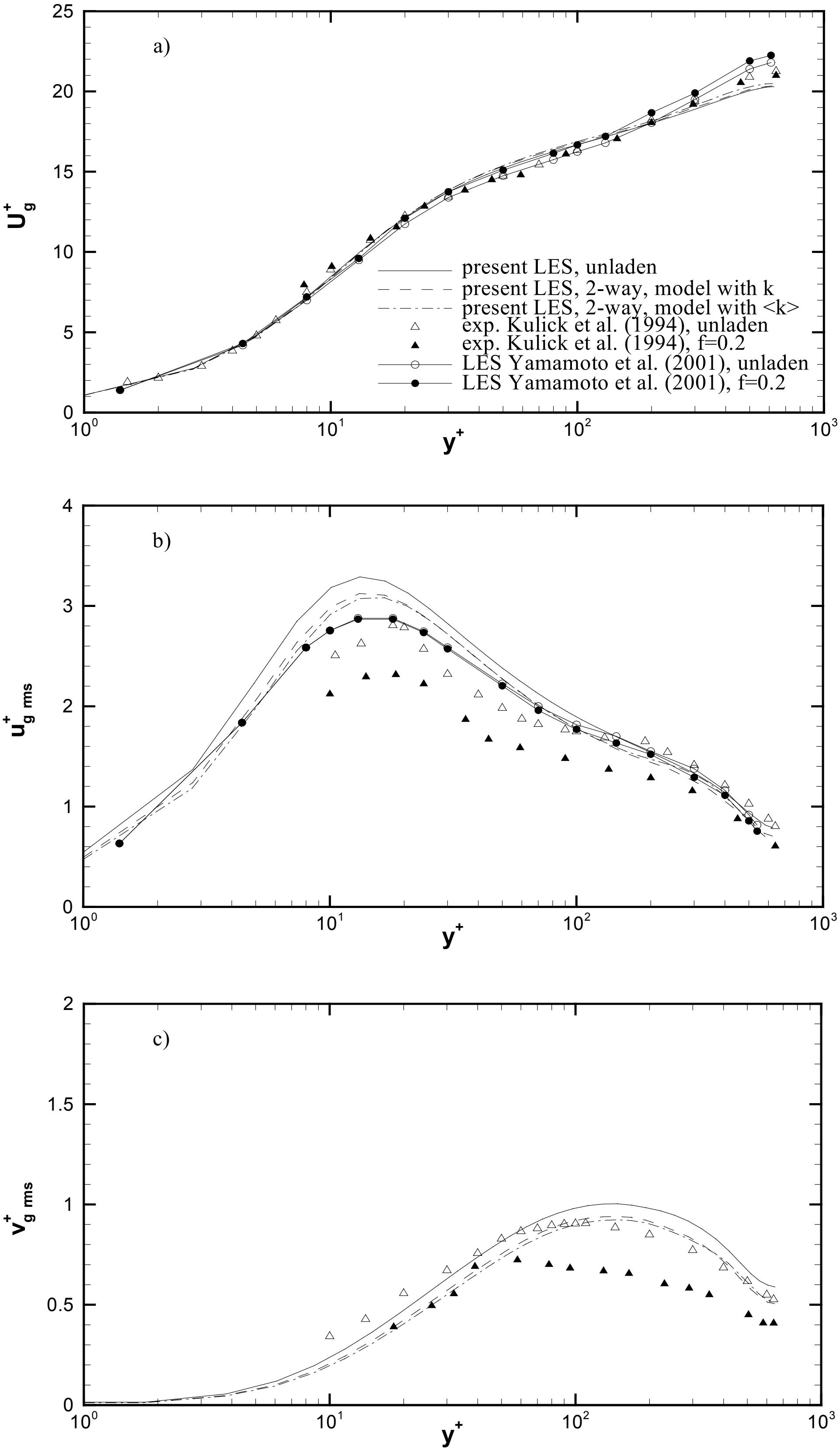

Fig.1 Comparison of computed gas velocity profiles (LES and (7)-(11)) with measurements of Kulick *et. al.*[1,2] and results from Yamomoto *et.al.* [9] with inter-particle collisions: a) streamwise mean velocity; b) r.m.s. of streamwise velocity; c) r.m.s. of wall-normal velocity.

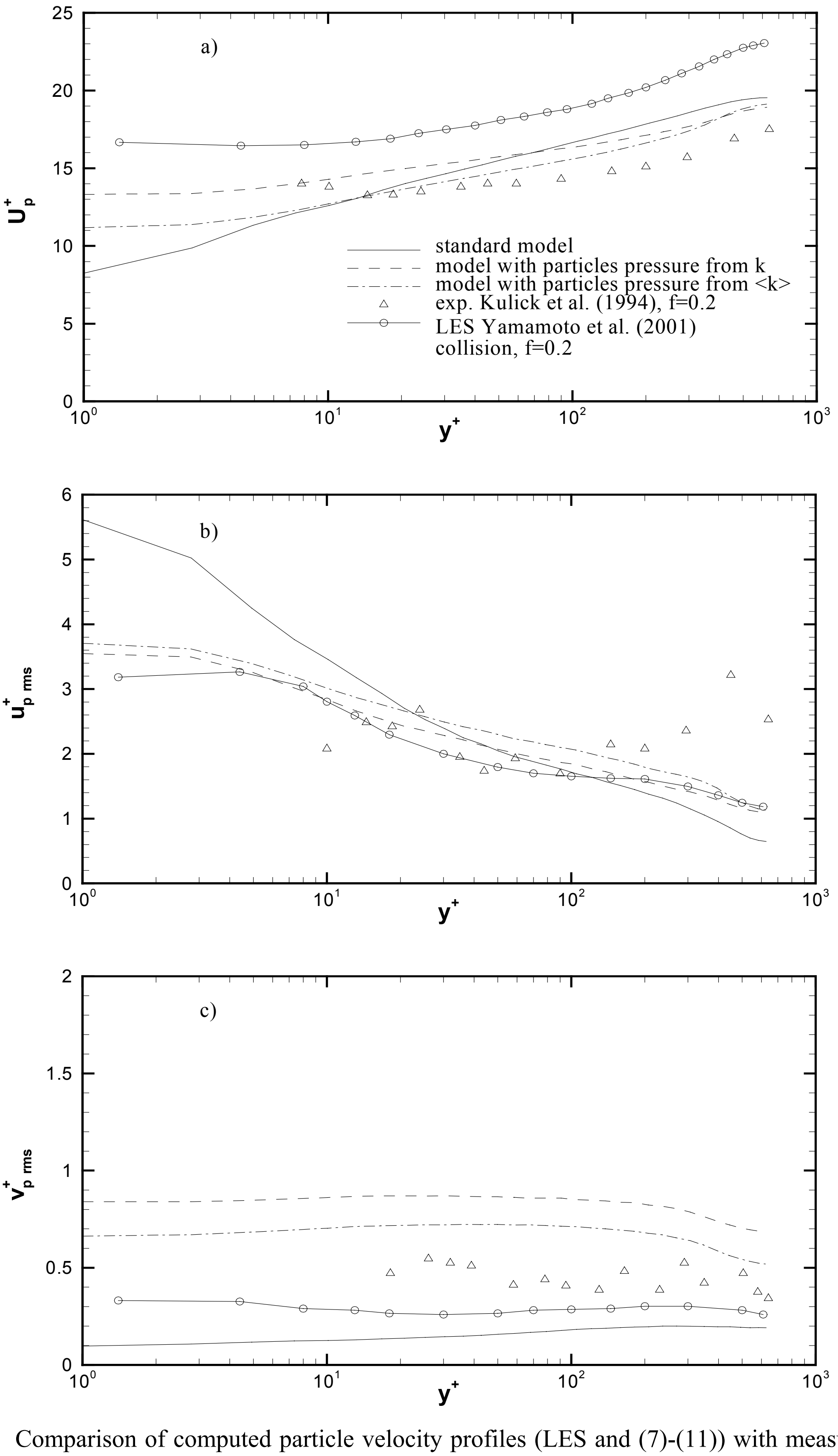

Fig.2 Comparison of computed particle velocity profiles (LES and (7)-(11)) with measurements of Kulick *et. al.*[1,2] and results from Yamomoto *et.al.* [9] with inter-particle collisions: a) streamwise mean velocity; b) r.m.s. of streamwise velocity; c) r.m.s. of wall-normal velocity.

5. References

[1] Kulick D, Fesler J R and Eaton J K 1994 *J. Fluid Mech.* **277**, 109-134

[2] Fesler J R, Kulick J D and Eaton J K 1994 *Phys. Fluids* **6**, 3742-3749

[3] Wang Q and Squires K 1996 *Phys. Fluids* **8**, 1207-1223

[4] Vance M W and Squires K D 2002 *ASME* July 14-18, 2002, Monreal, Quebec, Canada, FEDSM2002-31225

[5] Laveliéville J, Simonin O, Berlement A and Chang Z 1997 *Proc. 7th Int. Symp. on Gas-Particle Flows*, ASME FEDSM97-3623

[6] Simonin O, Février P and Laveliéville J 2002 *J. of Turbulence*, **3-040**

[7] Adler B J and Wainwright T E 1959 *J. Chem. Phys.* **31**, 2, 459-466

[8] Sigurgeirsson H, Stuart A and Wan W-L 2001 *J. Comput. Phys.* **172**, 766-807

[9] Yamamoto Y, Potthoff M, Tanaka T, Kajishima T and Tsuji Y 2001 *J. Fluid Mech.* **442**, 303-334

[10] Pope S 2000 *Turbulent flows* (Cambridge University Press)

[11] Williams J J E and Crane R I 1983 *Int. J. Multiphase Flow* **9**, **4**, 421-435

[12] Saffman P G and Turner J S 1956 *J. Fluid Mech.* **1**, 16-30

[13] Abramson J 1975 *Chem. Eng. Sci.* **30**, 1371-1379

[14] Sommerfeld M 2001 *Int. J. Multiphase Flow* **27**, 1829-1858

[15] Wang L-P, Wexler A S and Zhou Y 2000 *J. Fluid. Mech.* **415**, 117-153

[16] Mei R and Hu K C 1999 *J. Fluid. Mech.* **391**, 67-89

[17] Lifshitz E M and Pitaevskii L P 1981 *Physical Kinetics* (Butterworth-Heinemann

[18] Clift R, Grace J R and Weber M 1978 *Bubbles, Drops and Particles* (Academic Press)

[19] Pierce C D and Moin P 2001 *Stanford University Report* **TF-80**

[20] Germano M, Piomelly U, Moin P and Cabot W H 1990 *Proc. Summer Workshop, CTR, Stanford CA*

[21] Moin P, Squires K, Cabot W and Lee S 1991 *Phys. Fluids A* **3**, 2746-2757

[22] Lilly D K 1992 *Phys. Fluids A* **4**, 633-635

[23] Amsden A A, O'Rourke P J and Butler T D 1989 *The KIVA-II: A Computer Program for Chemically Reactive Flows with Sprays*, LA-11560-MS

[24] Gorokhovski M, Chtab A *Model of smoothed motion of interacting particles in LES of turbulent dispersed two-phase flow in channel* In Proc. of Int. Conf. on Multiphase flow 2003, 3-5 November, 2003, Sante Fe, New Mexico, USA