Dispersed particles in turbulent flow and the effects of subgrid-scales in LES: stochastic models, perspectives for kinematic simulations

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Introduction. Turbulent two-phase flows with solid particles or liquid droplets are of industrial importance in power, chemical, and process engineering. At the same time, the modelling of such flows remains an open issue. Recently, the Large-Eddy Simulation (LES) has become an alternative to Reynolds-based approaches, at least for geometrically-simpler cases. In LES, there has been a long discussion about the impact of subgrid scales (SGS) of the flow on the dynamics of the dispersed phase [7], and there is an agreement now that these effects may be considerable for smaller-inertia particles, in particular for preferential concentration statistics, turbulent kinetic energy, collision rates or deposition velocity in wall-bounded flows.

In the present contribution, we briefly recall the state-of-the art in SGS particle dispersion coupled to LES of the carrier phase. Then, we present our proposals and results to date concerning the models based on the stochastic diffusion processes for the SGS fluid velocity along the particle trajectories. At last, we consider a relatively simple approach to mimic the SGS fluid turbulence: it is the so-called kinematic simulation (KS) based on the Fourier velocity modes.

Stochastic models. Heavy, point-particles in turbulent flow are treated using the Lagrangian approach (only the drag force term is retained):

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{V}_p \,, \quad \frac{d\mathbf{V}_p}{dt} = \frac{\mathbf{U}(\mathbf{x}_p, t) - \mathbf{V}_p}{\tau_p} \tag{1}$$

where τ_p is the particle momentum relaxation time. The fluid velocity along particle trajectories can be decomposed into the filtered part (resolved in LES and interpolated to particles), and the SGS contribution: $\mathbf{U}(\mathbf{x}_p, t) = \overline{\mathbf{U}}(\mathbf{x}_p, t) + \mathbf{u}^*$ where the SGS contribution $\mathbf{u}^*$ may need a separate model. The SGS dispersion can safely be neglected when it comes to large-inertia particles or to long-time dispersion from the point source. In cases where SGS contribution may change the behaviour of the dispersed phase (e.g., the wall-deposition rate), we have used a stochastic analogue of advection-diffusion equation, namely the Langevin equation, to model for the SGS fluid velocity at particle position, $\mathbf{u}^*$ [5]. We have then extended the model to the anisotropic formulation, accounting also for possible correlations among SGS velocity components [6]. Following the exact formulation of the deterministic drift terms that account for non-homogeneity of fluid velocity statistics, shown to appear in LES [1], we have recently proposed a general model for the SGS fluid velocity at particle position, $\mathbf{u}^*$, in the form [3]:

$$d\mathbf{u}^* = \left(-(\mathbf{u} \cdot \nabla)\overline{\mathbf{U}} + \nabla \cdot \boldsymbol{\tau}\right)^* dt - \frac{\mathbf{u}^*}{\tau_{sg}} dt + \boldsymbol{\sigma} \cdot d\mathbf{W}, \tag{2}$$

where $\boldsymbol{\tau}$ is the SGS stress tensor, $d\mathbf{W}$ is a vector of independent increments of the Wiener process, $\boldsymbol{\sigma}$ is a diffusion matrix, τ_{sg} is a characteristic timescale of SGS velocity fluctuations along particle trajectories and also the autocorrelation time of the resulting stochastic process.

The model parameters that need to be estimated are τ_{sg} and $\boldsymbol{\sigma}$, the latter being related to the SGS fluid kinetic energy. The choice of these parameters comes from the statistical description of the smallest flow scales; various proposals for τ_{sg} and $\boldsymbol{\sigma}$ will be shown at the Colloquium and validated with DNS reference data. The simulation results that we have obtained so far are reasonably good and show improvements in the statistics of particle velocity and mean concentration profiles. However, the preferential segregation patterns for lower-inertia particles are not reproduced correctly because of the diffusive character of the model, Eq. (2).

Kinematic simulations. Stochastic models belong to so-called functional approaches in LES, in analogy to single-phase flows where the effect of residual scales on the resolved flow is modelled with the extra viscosity corresponding to a diffusion-type Lagrangian model for the residual fluid velocity. An alternative is offered by so-called structural approaches that aim at reconstructing or mimicking (part of) the residual scales themselves. The advantage of these approaches is that they account for two-point correlations and are thus able to simulate the impact of the SGS flow effects on relative particle dispersion or their collisions/coalescence. Proposals to date include approximate deconvolution of fluid velocity field [4], fractal reconstruction ideas (Salvetti, Marchioli & Soldati 2006) and the use of kinematic simulation [2].

The incompressible velocity field in KS is constructed as a sum of N_k separate random modes with prescribed wavevectors $\mathbf{k}_n$ and frequencies (or inverse time scales) ω_n:

$$\mathbf{u}(\mathbf{x},t) = \sum_{n=1}^{N_k} [\mathbf{a}_n \times \mathbf{k}_n \cos(\mathbf{k}_n \cdot \mathbf{x} + \omega_n t) + \mathbf{b}_n \times \mathbf{k}_n \sin(\mathbf{k}_n \cdot \mathbf{x} + \omega_n t)] \; . \qquad (3)$$

The random coefficients $\mathbf{a}_n$ and $\mathbf{b}_n$ are chosen so that the magnitude of the cross-products, $|\mathbf{a}_n \times \mathbf{k}_n|^2 = |\mathbf{b}_n \times \mathbf{k}_n|^2 = E(k_n)\Delta k_n$, should yield the pre-defined energy spectrum of the flow beyond the cut-off, i.e. a part of the inertial range $E(k) \sim k^{-5/3}$.

As contrasted to the application of KS for simplest homogeneous turbulence in periodic domains, its use for more realistic flow cases involves considerable implementation difficulties. The possibilities to apply KS for the SGS particle dispersion in channel flow will be discussed.

Acknowledgment. The work has been funded by the National Science Centre (NCN, Poland) through the research project 2011/03/B/ST8/05677.

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