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Turbulent particle dispersion in arbitrary wall-bounded geometries: A coupled CFD-Langevin-equation based approach

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ABSTRACT

A Lagrangian continuous random walk (CRW) model is developed to predict turbulent particle dispersion in arbitrary wall-bounded flows with prevailing anisotropic, inhomogeneous turbulence. The particle tracking model uses 3D mean flow data obtained from the Fluent CFD code, as well as Eulerian statistics of instantaneous quantities computed from DNS databases. The turbulent fluid velocities at the current time step are related to those of the previous time step through a Markov chain based on the normalized Langevin equation which takes into account turbulence inhomogeneities. The model includes a drift velocity correction that considerably reduces unphysical features common in random walk models. It is shown that the model satisfies the well-mixed criterion such that tracer particles retain approximately uniform concentrations when introduced uniformly in the domain, while their deposition velocity is vanishingly small, as it should be. To handle arbitrary geometries, it is assumed that the velocity rms values in the boundary layer can locally be approximated by the DNS data of fully developed channel flows. Benchmarks of the model are performed against particle deposition data in turbulent pipe flows, 90° bends, as well as more complex 3D flows inside a mouth-throat geometry. Good agreement with the data is obtained across the range of particle inertia.

1. Introduction

Turbulent flows which transport particulates are quite often encountered in a vast array of environmental, industrial, and medical applications. Examples of particle-laden flows can be found in atmospheric dispersion of pollutants, sediment transport in rivers, drug delivery in human airways, fouling in compressor and turbine blades, chemical pulping, nuclear fission products transport, etc. Hence, an accurate description of particle transport is of great practical importance. While particle transport in isotropic and homogeneous turbulent fields has been extensively studied (Yeung and Pope, 1989; Squires and Eaton, 1991), wall-bounded flows have not comparatively attracted the same attention. In the latter, boundary layers form close to the walls, and turbulence is strongly anisotropic and inhomogeneous, which renders the problem quite a bit more complicated. Of particular importance in boundary layer flows is the understanding of mechanisms responsible for particle preferential concentration (Marchioli and Soldati, 2002), which in turn explain many macroscopic features such as the particle deposition rates on the walls. The heart of the particle dispersion problem resides in modeling the random velocity fluctuations which particles encounter along their trajectories.

As summarized by Dehbi (2008), one can distinguish two main families of methods to treat particle dispersion in fluid flows: Eulerian and Lagrangian. In the Eulerean or "two-fluid" approach, the particles are regarded as a continuous phase for which the averaged conservation equations (continuity, momentum and energy) are solved in similar fashion to the carrier gas flow field (Zhang and Prosperetti, 1994). The Eulerean approach is particularly suitable for denser suspensions when particle–particle interactions are important and the particle feedback on the flow is too large to ignore. The main challenge facing Eulerian-type, two-fluid approaches resides in accurately defining the inter-phase exchange rates and closure laws which arise from the averaging procedures (Drew, 1983). In addition, the strong coupling between the phases renders the Eulerean approach quite delicate to handle, especially at boundaries where the solid phase may be removed or reflected.

The Lagrangian approach (Maxey, 1987) treats particles as a discrete phase which is dispersed in the continuous phase. The particle volume loading is usually assumed negligible, so that particles have no feedback effect on the carrier gas and particle–particle interactions are neglected. In the Lagrangian framework, the controlling phenomena for particle dispersion in the field are assessed using a rigorous treatment of the forces acting on the particle. In general, the detailed flow field is computed first, then a representatively large number of particles are injected in the domain, and their trajectories determined by following individual particles until

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they are removed from the gas stream or leave the computational space. Particle motion is extracted from the time integration of Newton's second law, in which all the relevant forces can be incorporated (drag, gravity, lift, thermophoretic force, etc.). The Lagrangian approach is computationally intensive, because it entails tracking a large number of particles until stationary statistics are achieved. On the other hand, the results of Lagrangian particle tracking (LPT) are physically easier to interpret. Therefore, in the following investigation, the LPT methodology is used, along with the assumption that the dispersed phase is dilute enough not to affect the continuous flow field (one-way coupling).

Many methods have been developed to take into account velocity fluctuations in the turbulent flow. In principle, the simplest and more "physical" method is Direct Numerical Simulation (DNS) (McLaughlin, 1989) in which turbulence is "reproduced" by solving the transient Navier–Stokes continuity and momentum equations on a sufficiently fine grid and with a sufficiently small time step. In such a way, all relevant spatial and temporal scaled are resolved. Large-Eddy Simulations (LES) (Wang and Squires, 1997) are conceptually similar to DNS, except that the computational effort is reduced somewhat by requiring the grid to be only so fine as to resolve the largest eddies, whereas the smaller, quasi isotropic eddies are modeled. While being widely used, DNS-LES/LPT methods remain computationally expensive, and their extension to general geometries poses very tough and sometimes intractable computational challenges.

An alternative method, which borrows from the family of stochastic models, attempts to simulate turbulence using complementary equations whereby the instantaneous turbulent velocities are calculated from local quantities such as the mean turbulent kinetic energy, the Eulerian time scale and the distance to the wall. Examples of these treatments are random walk models which have been popular due to their relative ease of implementation and reasonable computational expense.

In Discrete Random Walk (DRW) models (Gosman and Ioannides, 1983), the turbulent dispersion of particles is modeled as a succession of interactions between a particle and eddies which have finite lengths and lifetimes. It is assumed that at time t_0, a particle with velocity U_p is captured by an eddy which moves with a velocity composed of the mean fluid velocity, augmented by a random "instantaneous" component which is piecewise constant in time. When the lifetime of the eddy is over or the particle crosses the eddy, another interaction is generated with a different eddy, and so forth. In wall-bounded flows, the original isotropic DRW model of Gosman and Ioannides (1983) has been improved to account for anisotropic turbulence in the near-wall regions. This improved DRW model has been used with some success to predict turbulent particle deposition in isothermal 2D channels (Kallio and Reeks, 1989), in general 3D isothermal flows (Dehbi, 2008) or in cooled pipes (Kröger and Drossinos, 2000).

Continuous Random Walk (CRW) models provide a more physically sound picture of fluid turbulence, as they represent the instantaneous velocities in a continuous way. CRW models, which are usually based on the Langevin equation, have been shown to provide more realistic predictions of turbulent particle dispersion than DRW, in particular in flows where inhomogeneous effects are important such as mixing layers (MacInnes and Bracco, 1992) or free shear flows (Bocksell and Loth, 2001). Hence a CRW model will be adopted in this investigation.

One of the main goals of this investigation is to describe turbulent particle dispersion in general wall-bounded geometries. Mean flow parameters in complex turbulent flows can only be predicted on a routine basis using standard Computational Fluid Dynamics (CFD) tools based on the Reynolds Averaged Navier Stokes (RANS) equations. Ideally then, turbulent particle dispersion in general 3D geometries could be done by coupling CFD with reliable particle dispersion models in a single application. However, as shown recently by Tian and Ahmadi (2007), the use e.g. of DRW in combination with the state-of-the-art anisotropic Reynolds Stress Model (RSM) still led to large overpredictions of particle deposition rates in 2D parallel ducts. This is due to the fact that the RSM calculated root mean square (rms) of the normal velocity near the wall overpredicts the profiles determined by DNS studies, and no grid refinement can remedy this problem. Using the same RSM-DRW framework, Parker et al. (in press) were able to obtain dimensionless deposition velocities that overestimated the experimental data by less than one order of magnitude, which is the best that can be achieved with today's CFD codes in their default mode. Better results were however obtained when Tian and Ahmadi (2007) combined the use of RSM for the mean flow field, the Langevin equation for the turbulent fluctuations, and a DNS-supplied correlation for the normal velocity rms close to the wall.

Based on the above, it becomes clear that quantitatively accurate predictions of turbulent particle dispersion in general 3D geometries can only be achieved through a substantial improvement in the treatment of particle-turbulence interactions in the boundary layer. This treatment needs to be developed and incorporated in the CFD tools in order to properly account for near-wall effects which control to a large extent the physics of particle deposition. In this investigation, the fluid fluctuations will be computed from a Langevin equation based model, which will be combined with the mean flow data obtained from the Fluent 6.3 code (Fluent, 2006). Fluent 6.3 is a state of the art code based on finite volume methods that provides a wide choice of turbulence models (k–ε, k–ω, RSM, etc). The necessary Eulerian statistics to close the Lagrangian particle tracking model will be supplied by the available DNS databases of channel flows.

2. Particle equations of motion

Let a spherical particle be entrained in a turbulent flow. Assuming only drag and gravity are significant, the vector force balance on that particle is written as follows:

$$\frac{dU_p}{dt} = F_D(U - U_p) + g\left(1 - \frac{\rho_f}{\rho_p}\right) \tag{1}$$

where the drag force per unit mass may be expressed as

$$F_D = \frac{18\mu}{\rho_p d_p^2} C_D \frac{Re_p}{24} \tag{2}$$

In the above, U is the fluid velocity, U_p is the particle velocity, ρ_p the particle density, ρ_f the fluid density, g the gravity acceleration vector, d_p the particle geometric diameter, μ the fluid molecular viscosity, and Re_p the particle Reynolds number defined as

$$Re_p = \frac{d_p \mid U - U_p \mid}{\nu} \tag{3}$$

ν being the fluid kinematic viscosity. The drag coefficient is computed in the Fluent code from the following equation:

$$C_D = \beta_1 + \frac{\beta_2}{Re_p} + \frac{\beta_3}{Re_p^2} \tag{4}$$

where the β's are constants which apply to spherical particles for wide ranges of Re_p. The trajectory $x(x_1, x_2, x_3, t)$ of the particle is obtained by integration of the following velocity vector equation with respect to time:

$$U_p = \frac{dx}{dt} \tag{5}$$

The expressions (1)–(5) are all one needs to compute the trajectory of individual particles in laminar flows. The particle concentration