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Review

Two-way coupled turbulence simulations of gas-particle flows using point-particle tracking

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ABSTRACT

This paper addresses computational models for dilute gas-particle multiphase flow in which the three dimensional, time-dependent fluid motion is calculated in an Eulerian frame, and a large number of particles are tracked in a Lagrangian frame. Point forces are used to represent the back effect of the particles on the turbulence. The paper describes the early development of the technique, summarizes several experiments which show how dilute particle loadings can significantly alter the turbulence, and demonstrates how the point-particle method fails when the particles are comparable in scale to the small scale turbulence. High-resolution simulations and experiments which demonstrate the importance of the flow details around individual particles are described. Finally, opinions are stated on how future model development should proceed.

1. Introduction

Research on particle-laden multiphase flow at Stanford began in the early 1980s with an experiment on air flow through vertical diffusers located above a fluidized bed (Kale and Eaton, 1985). We found that the presence of a relatively dilute loading of particles in the diffuser profoundly affected the mean velocity field. The flow through a wide-angle diffuser was fully stalled in single-phase flow, but it was fully attached with the addition of a light loading of 75 μm diameter glass beads. This experiment is representative of a broad class of two-phase flows, namely gas flows with a dilute loading of fine solid particles. In such flows, the motion of the particles is controlled by the gas-phase flow with only minor affects of particle collisions with walls or other particles. At the same time, the particles can have a very strong effect on the gas-phase flow, even at particle volume fractions below 0.1%.

In trying to understand the diffuser results, we developed a code following the particle-source-in cell (PSIC) method published by Crowe et al. (1977). In this approach, the gas-phase motion is computed on a regular Eulerian grid, while Lagrangian calculations are done for the motion of representative particles taking account of the drag force of the gas on the individual particles. A simple, quasi-steady drag law, either Stokes flow or an empirical correlation is used to calculate the magnitude and direction of the drag force at each point along the particle trajectory. The "back-effect" of the particles on the gas flow is incorporated by calculating source terms for each computational volume. For example, a momentum source term is calculated by finding the net change in momentum of all particles passing through a given grid cell. A mass source term can be calculated similarly for evaporating droplets, etc.

Our model used the Reynolds-averaged Navier–Stokes (RANS) equations with a conventional single-phase turbulence model. Experiments[1] had shown that a dilute particle loading could drastically alter the turbulence statistics. However, there was no consensus on how to incorporate this effect into turbulence models. We believed this deficiency caused the failure of our model to accurately predict the diffuser flow. This launched our group at Stanford into a two-decade research effort combining experiments and simulations attempting to understand and model turbulence modification by dispersed solid particles. The simulation efforts have focused on incorporating point particles into direct numerical simulation (DNS) and large eddy simulation (LES) codes and on fully resolved simulations to understand how we can capture turbulence modulation effects in a point-particle simulation.

This paper provides a summary of research in our group on simulation of particle-laden turbulent gas flows. Some reference is made to the work of others, but this paper is not intended to be

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[1] For an extensive review see article 12.6 by J.K. Eaton on Turbulence Modulation by Particles in Crowe, C.T., ed. *Multiphase Flow Handbook*, Taylor & Francis, Boca Raton, FL, 2006.

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a comprehensive review of the field. The paper will first describe our early work on incorporating Lagrangian particle tracking and point-force two-way coupling into existing single-phase DNS and LES codes for homogeneous turbulent flows. I will next give a brief summary of experimental evidence for turbulence modification by particles, since prediction of this phenomenon has been the main focus of our subsequent simulation work. There will be an extensive discussion on the implementation of two-way coupling in simulations of realistic flows where the particle size may be comparable to single-phase grid scales. Finally, I will discuss simulations and experiments that resolve the flow around individual particles and discuss how these findings may be incorporated into future simulation models.

2. Homogeneous flow simulations

Our work on simulating particle-laden gas flows began with a study of inertial particles moving in homogeneous, isotropic turbulence. This work was motivated by the need for fluid velocity statistics measured along the path of an inertial particle for incorporation into models for turbulent particle dispersion and turbulence modification by particles. The simulations resulted in several papers (Squires and Eaton, 1989, 1990, 1991a,b,c, 1994). Earlier, Riley and Patterson (1974) had tracked inertial particles in low Reynolds number turbulence simulations to compute Lagrangian statistics. By the late 1980s, DNS codes for simple flows were well established, and adequate supercomputing resources were available to allow tracking a large number of particles. Several efforts started in parallel with our own work. Yeung and Pope (1989) obtained Lagrangian statistics by tracking massless particles in DNS simulations and McLaughlin (1989) studied the deposition of fine aerosol particles in simulated channel flow. Elghobashi and Truesdell (1992) examined particle dispersion in decaying isotropic turbulence.

We used the pseudospectral DNS code developed by Rogallo (1981) for simulating homogeneous–isotropic turbulence and homogeneous shear flows. Neither of these flows is statistically stationary which complicated analysis of the results. Therefore, a forcing scheme was adopted which provided a continuous source of energy allowing the isotropic turbulence simulations to reach a statistically stationary state. Particles were treated as points, and characterized only by an aerodynamic time constant. The particles had no volume displacement, so it was impossible for a particle to occupy more than one computational cell. Particles were tracked by integrating the simple particle equation of motion

$$\frac{dv_i}{dt} = \frac{1}{\tau_p}(u_i[X(t),t] - v_i(t) + g\tau_p\delta_{i2}).$$

Here, v is the particle velocity, $u(X(t),t)$ is the fluid velocity at the position of the particle, τ_p is the particle aerodynamic time constant, and g is the acceleration of gravity assumed to be oriented in the x_2 direction. This implies a linear drag law that is appropriate for small particles at low Reynolds numbers.

With the assumptions above, there are only two issues to consider; the interpolation of the fluid velocity field to the particle position at each time step, and the numerical time advancement of the particle equations of motion. We chose to use second-order accurate Runge–Kutta time advancement for consistency with the Eulerian fluid simulation. Several different interpolation schemes ranging from tri-linear interpolation to fourth order accurate cubic splines and fifth order Lagrange polynomials were tested. There was little effect of the interpolation scheme on the resulting Lagrangian statistics, and third order Lagrange polynomials were used for all the main runs. Yeung and Pope (1989) made a more extensive study of interpolation schemes and arrived at a similar conclusion. Using the simple interpolation schemes, the particle tracking used only a small fraction of the total computing resource. Therefore, it was possible to track large numbers of particles. Numerical experiments were performed in which many sets of particles (each containing 4096 independent particles) were run simultaneously.

The unique aspect of Squires work was the implementation of two-way coupling using an adaptation of Crowe's PSIC method to a 3D, time-dependent simulation. For an incompressible, Newtonian fluid laden with point particles the equations of motion are:

$$\frac{\partial u_i}{\partial x_i} = 0$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_i u_j}{\partial x_j} = \frac{-1}{\rho}\frac{\partial p}{\partial x_i} + \nu\frac{\partial^2 u_i}{\partial x_j \partial x_j} - \frac{1}{\rho}f_{pi}$$

where f_{pi} is the local force applied by the fluid onto the particles, ρ is the fluid density, and the effects of gravity have been neglected. It is important for later discussions to realize that there is a significant problem with interpretation of this equation. Under the point-particle assumption, f_{pi} should be zero everywhere except for a delta function at the location of each particle. Generally, this has been interpreted as a smooth continuous function that is a filtered version of the actual point-force distribution. However, the filtering has not been done explicitly.

Our implementation involved computing the force on every particle at every time step of the simulation. The force on each particle was interpolated back to the eight grid points surrounding the particle using a volume-weighting method. The effects of all particles were summed to give the discrete force field needed to advance the fluid equation of motion. Tracking of a very large number of particles was needed to obtain a reasonably smooth force field. Forced, homogeneous, isotropic turbulence was simulated using either 32^3 or 64^3 collocation points to calculate the fluid velocity field. These cases used 3.73×10^5 and 1 million particles respectively. Thus, on average 30 particles (8×1 million/64^3) contributed to the computed particle force at each point for the 64^3 cases. Simulations were done for 10%, 50% and 100% mass loading ratio, and two different particle-time constants. All cases showed significant attenuation of the turbulent kinetic energy. For 100% mass loading and a particle aerodynamic time constant of 0.15 times the turbulence integral scale, a 47% reduction in the turbulent kinetic energy was observed. The turbulence attenuation was similar to reductions observed in some experiments. However, the results could not be directly compared to experiments because there is no precise physical analog to forced homogeneous, isotropic turbulence. The turbulence energy spectra showed broad attenuation in the energy-containing range, and substantial augmentation in the high wave number range. Similar behavior has been observed in many subsequent experiments and simulations. However, in most experiments there is mean relative motion between the particle and fluid phases due to gravity, and it is often assumed that this is responsible for energy input at small scales. The mean velocity for both phases was zero in our simulations, so the augmentation at small scales can only be due to local non-uniformity of the coupling force term.

The large number of particles tracked in the two-way coupled simulations allowed us to accurately resolve the instantaneous particle concentration distribution. This allowed us to observe preferential concentration of particles by turbulence (Squires and Eaton, 1990, 1991c) in which particles with aerodynamic time constants near the Kolmogorov time scale were found to have very high concentrations in localized regions of the turbulence. Maxey (1987) had previously predicted this analytically, and our study allowed quantitative assessment of the degree of concentration as a function of time constant. The simulations also allowed analysis of