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Technical Note

Evaluation and modification of gas-particle covariance models by Large Eddy Simulation of a particle-laden turbulent flows over a backward-facing step

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ABSTRACT

Three-dimensional numerical investigation of a low speed particle-laden turbulent flow over a backward-facing step has been carried out. An assumption of incompressibility of the flow is used due to low Mach number of the flow. The gas phase is performed by Large Eddy Simulation (LES) and the particle phase is solved by a Lagrangian particle tracking model. The simulation results such as mean streamwise velocities and fluctuation velocities for the both phase are validated by experimental results performed by Fessler and Eaton (1999) [1]. Reynolds number of the gas phase over the backward-facing step with an expansion ratio of 5:3 is 18,400, based on the maximum inlet velocity and step height. The flow is considered as dilute. Hence a one-way coupling method is applied, in which we only consider the effect of fluid on the particle. Particle–particle collisions are also neglected. The success of simulation in predicting a particle-laden turbulent flow using LES and Lagrangian trajectory model provides a numerical basis for revisiting the gas-particle correlations models. Four second-order closure models for gas-particles covariance are evaluated in the present study. A modified better gas-particle covariance model is proposed in this paper.

1. Introduction

Two-phase flows occur frequently in many engineering and natural processes. A typical application to natural processes involves predicting pollutants dispersion in our living environment. Hunt [2] gave a review on environmental particulate problems. Engineering applications of two-phase flow include pulverized-coal combustion, spray combustion and solid transport. A detailed discussion of such two-phase flow problems can be found in Sirignano [3] and Ghosh and Hunt [4]. Almost all particle-laden flows in engineering are turbulent in nature and contain eddies in size from Kolmogorov scales to the integral scales. Eddies of the continuous phase have an important effect on particle dispersion. The interaction between particles and fluid eddies is therefore a fundamental problem in turbulent two-phase flows, and so accurate prediction of particle-laden turbulence is important in order to gain a better understanding of particle transport by turbulent flow as well as ultimately improve engineering devices in which two-phase flows occur.

In dealing with two-phase flow simulations, Pourahmadi and Humphrey [5] proposed a second-order closure for gas-particle covariance terms based on the equation of motion for a single particle with the drag force as the only force. The gas-particle covariance was modeled as a function of fluid turbulent kinetic energy, particle response time and fluid integral time scale. Another gas-particle covariance model similar to Pourahmadi's model was proposed by Chen and Wood [6]. The gas-particle covariance decays exponentially with the ratio of particle response time and fluid integral time scale. Both Pourahmadi's and Chen's models considered the fluid turbulent kinetic energy as a main variable to model gas-particle covariance. Chang and Wu [7] first claimed that the two-phase correlation should be related not only to the fluid kinetic energy, but also the particle kinetic energy.

A numerical simulation has been carried out in the present study to investigate quantitatively and qualitatively a two-phase turbulent flow over a backward-facing step with Reynolds number of 18,400. The simulation is validated by comparing the first and second-order statistical averages with experimental data of Fessler and Eaton [1]. A numerical simulation of the same configuration was also carried out by Wang [8], they studied the characteristics of a particle response to turbulent flow. In the present studied, four gas-particle covariance models used in two-phase flow simulation based on two-fluid assumption are evaluated in the present study. Gas-particle covariance represents the correlation between the particle velocity fluctuation and gas velocity fluctuation measured at the particle location. The prediction of gas-particle covariance is very important [9] for the closure of two-phase flow model based on two-fluid assumption. Although some gas-particle covariance models are in good agreement with the LES results, a proper

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empirical constant is needed for an individual flow configuration and particle diameters, but there is no formula to determine the constant. A modified model that gives more emphasis on the effect of particle kinetic energy has been proposed in the present study. The predicted results by the modified model without empirical constant give good agreement with LES result.

2. Simulation methods and code validation

Large Eddy Simulation (LES) is used to simulate the gas phase of the flow. The flow field variables are separated into a large-scale component and a subgrid scale (SGS) component by filtering. The effect of the subgrid scales on the resolved scales is modelled by the SGS stress according to the Smagorinsky [10] model. The Smagorinsky model parameter are chosen as 0.04 in the simulation. The equations have been nondimensionalized, using the step height as the length scale, the maximum inlet velocity as the velocity scale and the ratio of step height and maximum inlet velocity as the time scale.

The governing equations are discretized spatially on a staggered Cartesian grid. The flow was resolved using $514 \times 66 \times 65$ grid points in the x, y, and z directions for the simulation. Derivatives are approximated using central difference for the diffusion terms while the advection terms are discretized by a skew-symmetric form [11]. Time integration of the governing equations is carried out with a third-order Runge-Kutta method. The time step is taken as 0.005 in the simulation. Chorin's fractional-step projection method [12] is adopted in solving the incompressible gas-phase equations. The Poisson equation for pressure correction is formed and solved directly using Fourier series expansion in the streamwise and spanwise directions with tri-diagonal matrix inversion [13]. The inlet velocity profile is from a separate LES of a channel flow. No slip boundary condition for velocity is applied at the top and bottom solid walls where the pressure gradient is set as zero for the normal direction of the wall. Periodicity boundary condition is assumed in the spanwise direction in the 3D simulation. In order to prevent waves reflecting from the outlet, a convective open boundary condition [14] is applied at the outlet.

Lagrangian approach is employed to predict the properties of each particle directly from the equations of motion. The other assumptions for the particle motion are

1. All particles are rigid spheres with equal diameter and density of 2500 kg/m^3.
2. The density of the particles is assumed large compared with that of the fluid.
3. Particle–particle interactions are negligible.
4. Dilute two-phase particle-laden flow is assumed and effect of the particles on the flow structures is neglected.
5. Collisions with boundaries are assumed to be elastic.

The backward-facing step has an expansion ratio of 5:3. Reynolds number of the air flow over the backward-facing step is 18,400, based on the maximum inlet velocity U_0 of 10.5 ms^{-1} and step height H 26.7 mm. The predicted mean and fluctuating velocity profiles of the gas phase are in good agreement with experimental results of Fessler and Eaton [1].

3. Evaluation and modification of gas-particle covariance in second-order moment models

In two-fluid models, the gas phase and particulate phase are regarded as two separate continuous flows which are governed by separate transport equations. The approach will lead to closure problems for gas-particle covariance due to gas-particle interaction in two-phase flow. The prediction of gas-particle covariance is very important [9] in the closure of two-phase turbulent models with two-fluid assumption. The gas-particle covariance represents the correlation between the particle velocity fluctuation and the gas velocity fluctuation measured at the particle location. Physically, gas-particle covariance represents the interaction between the gas phase and particle Reynolds stresses or turbulent kinetic energies by the drag and other forces.

In experimental measurements, there is always a time delay between determining fluid velocity and particle velocity. So there are very few existing experimental data [15] to evaluate the said algebraic model for closure studies of gas-particle correlations. Large Eddy Simulation and Lagrangian particle tracking model can provide an efficiency numerical method for evaluation of the closure models used for practical applications.

The numerical results are used here to evaluate second-order moment closure for gas-particle correlations of Pourahmadi [5], Chen [6] and Chang and Wu [7]. In general, the predicted results by Chen's model are much better than Pourahmadi's. However, an empirical constant is needed in Chen's model for different situations. So we proposed a modified model which does not need an empirical constant and the predicted results are as good as those based on Chen's model.

The different second-order moment models for gas-particle covariance are represented as follows:

Pourahmadi and Humphrey's model [5]

$$\overline{u'_{gi}u'_{pi}} = 2k_g \frac{\tau_L}{\tau_p + \tau_L} \quad (1)$$

Chen and Wood's model [6]

$$\overline{u'_{gi}u'_{pi}} = 2k_g e^{(-B\tau_p/\tau_L)} \quad (2)$$

Modified Pourahmadi's model [7]

$$\overline{u'_{gi}u'_{pi}} = (k_g + k_p)\frac{\tau_L}{\tau_p + \tau_L} \quad (3)$$

Modified Chen and Wood's model [7]

$$\overline{u'_{gi}u'_{pi}} = (k_g + k_p)e^{(-B\tau_p/\tau_L)} \quad (4)$$

where k_g is turbulent kinetic energy of the gas phase, k_p is turbulent kinetic energy of the particle phase, τ_p is particle relaxation time, τ_L is fluid Lagrangian integral time scale, B is an empirical constant decided by two-phase properties.

In this chapter, the above four different second-order moment closure models for gas-particle covariance are evaluated by comparing with LES simulation results. Figs. 1 and 2 show the results calculated by different models based on LES for different particle diameters of 20 μm and 100 μm. The short notations to represent different models used in the figures for simplicity are as follows:

LES: Calculated by LES and Lagrangian simulation;
PH: Calculated with Pourahmadi and Humphrey's [5] model;
Chen: Calculated with Chen and Wood's [6] model;
ChangPH: Calculated with the modified [7] Pourahmadi and Humphrey model;
ChangChen: Calculated with the modified [7] Chen and Wood model;

LES results show the value of gas-particle covariance decreases with increasing particle diameter. Because the particle relaxation time becomes larger for larger particles than the local gas time scale, a relatively weak correlation between the two phases is expected.

Discrepancy occurs for gas-particle covariance calculated with PH and ChangPH models as shown in Figs. 1 and 2. The degree

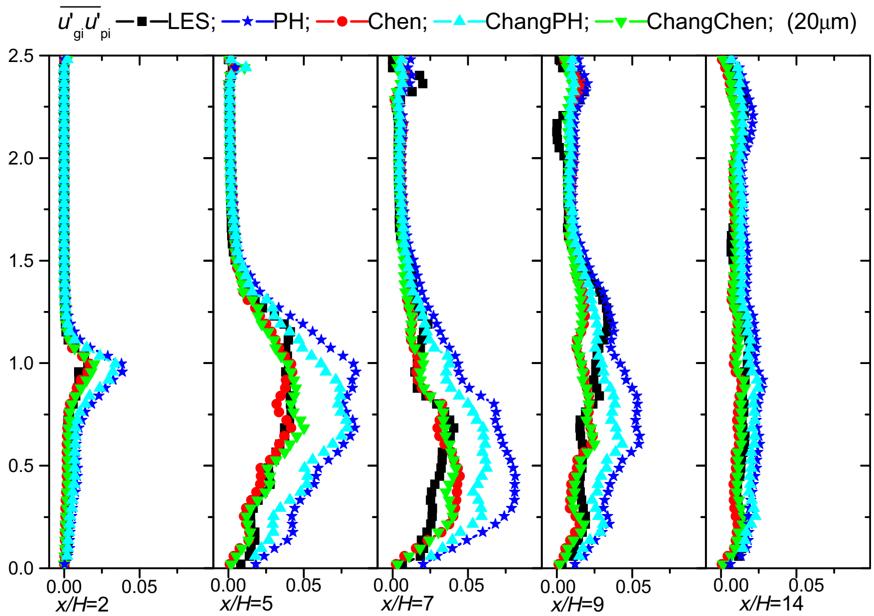

Fig. 1. $\overline{u'_{gi}u'_{pi}}$ calculated by LES and different models for 20 μm particles

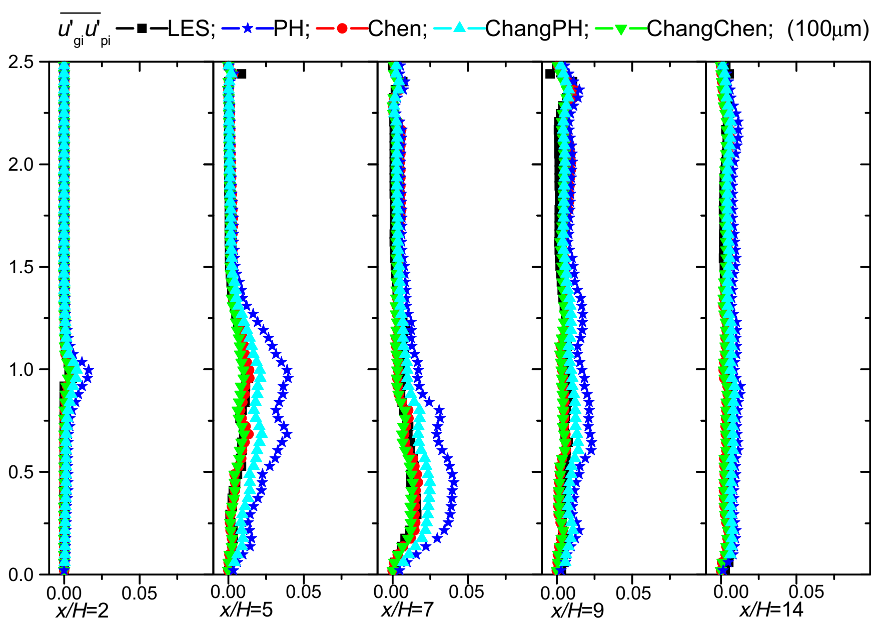

Fig. 2. $\overline{u'_{gi}u'_{pi}}$ calculated by LES and different models for 100 μm particles

of discrepancy increases with increasing particle diameter. Therefore, a conclusion is that both PH and ChangPH models are not capable to predict gas-particle covariance with larger particles. However, the result predicted with ChangPH's model gives better agreement with LES than PH's model. This is because particle kinetic energy has been added into the gas-particle covariance in ChangPH's model. It gives us a clue that particle kinetic energy may have substantial effect on gas-particle covariance. The effect of particle kinetic energy on gas-particle covariance is demonstrated in the next section by modifying PH's model.

Both Chen's and ChangChen's models give good agreement with LES results as shown in Figs. 1 and 2. The agreement is mainly due to the empirical constant B that modifies the effect of fluid or particle kinetic energy. The value of the empirical constant B depends mainly on the particle diameter and B is determined by comparing the results between the prediction by LES and the models. The relationship between the empirical constant B and particle diameter is shown in Fig. 3. A smaller value of B in ChangChen's model than that in Chen's model represents smaller modification is needed for ChangChen' model. This is another evidence of the importance of the effect of particle kinetic energy on the gas-particle covariance.

Although both Chen's and ChangChen's models give good agreement with LES results, an empirical constant B is needed in the models. The value of the empirical constant B depends on flow configuration and particle size. It is difficult to decide the correct value of B, and hence the generalization of the models is difficult. It would be ideal to find a model which can give good agreement with LES results without resorting to an empirical constant. As mentioned in the previous section, particle kinetic energy has substantial effect on gas-particle covariance as shown by the results based on ChangPH's model and ChangChen's model. The model proposed by Pourahmadi and Humphrey [5] is then modified with different proportions of gas and particle kinetic energies.

Case 1: Gas-particle covariance is governed by 100% particle kinetic energy only. The model is denoted by Modified PH 1:

$$\overline{u'_{gi}u'_{pi}} = 2k_p \frac{\tau_L}{\tau_p + \tau_L} \tag{5}$$

Case 2: Gas-particle covariance is governed by 25% of gas kinetic energy and 75% of particle kinetic energy. The model is denoted by Modified PH 2:

$$\overline{u'_{gi}u'_{pi}} = \left(\frac{k_g + 3k_p}{2}\right) \frac{\tau_L}{\tau_p + \tau_L} \tag{6}$$

Case 3: Gas-particle covariance is governed by 50% of gas kinetic energy and 50% of particle kinetic energy, which is the ChangPH's model shown in the previous paragraph.

Case 4: Gas-particle covariance is governed by 100% of gas kinetic energy, which is the PH's model shown in the previous paragraph.

The results of gas-particle covariance calculated by Modified PH 1 and Modified PH 2 are shown in Figs. 4 and 5 for different particle diameters of 20 μm and 100 μm, respectively. There is significant improvement compared with PH's model and ChangPH's model as shown in Figs. 1 and 2. Modified PH 1 gives a better agreement with LES results than Modified PH 2. Therefore, a con-

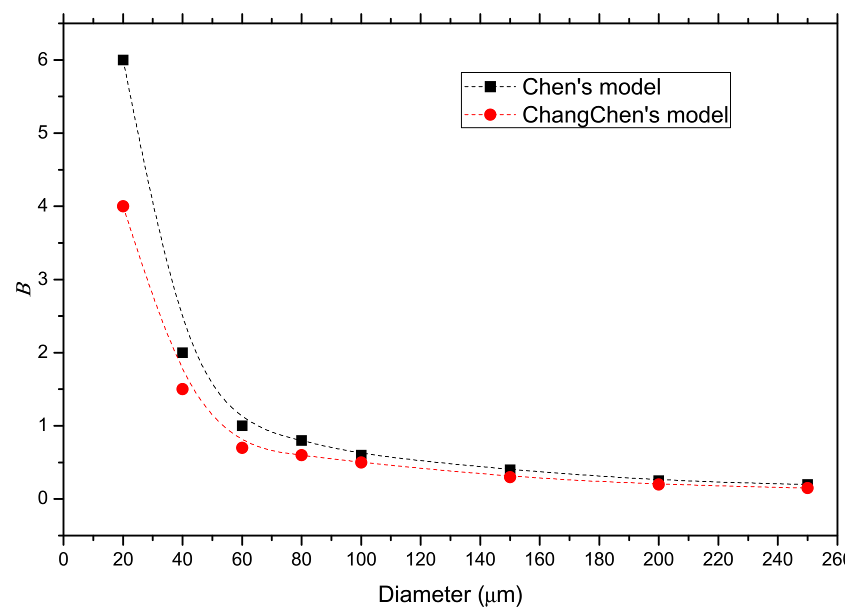

Fig. 3. Empirical constant *B* against diameter with Chen's and ChangChen's model

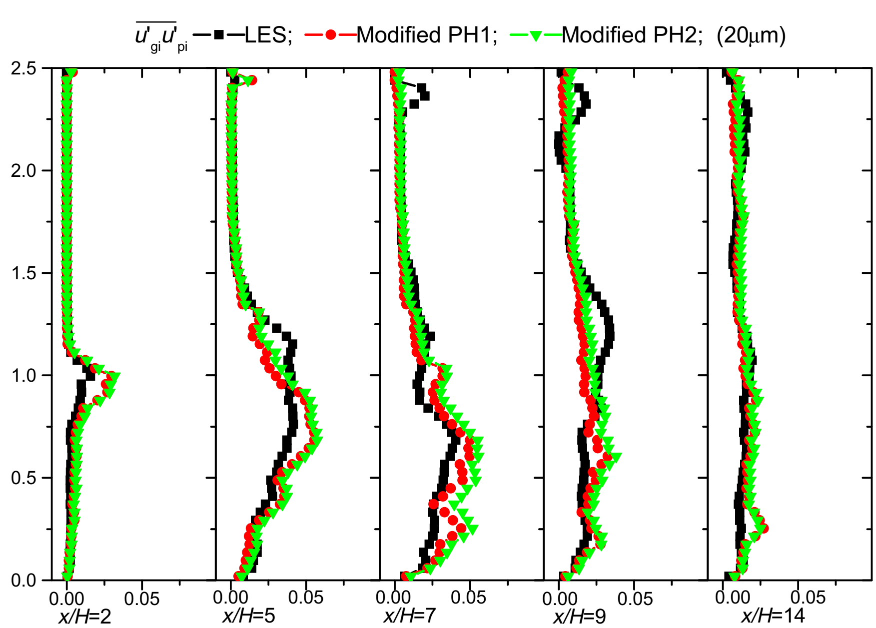

Fig. 4. $\overline{u'_{gi}u'_{pi}}$ calculated by LES and modified models for 20 μm particles

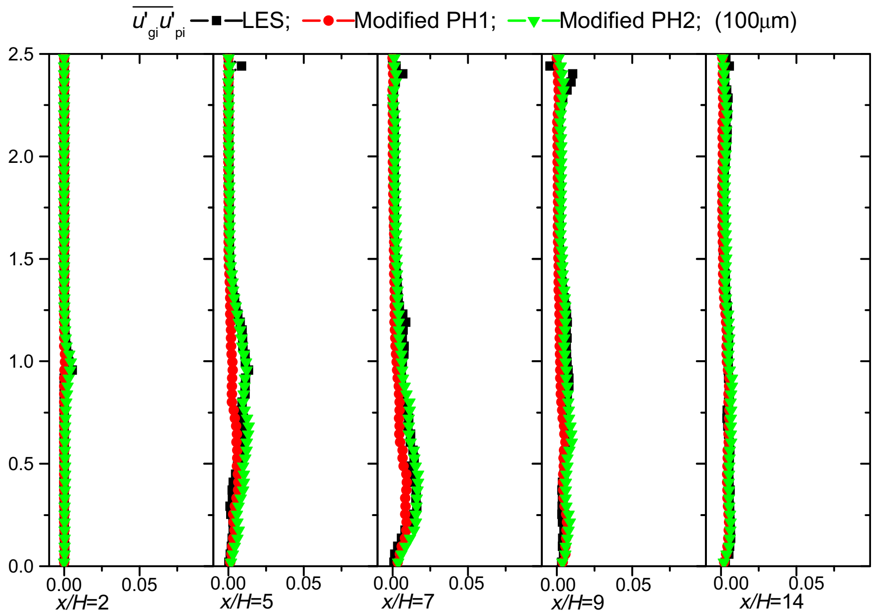

Fig. 5. $\overline{u'_{gi}u'_{pi}}$ calculated by LES and modified models for 100 μm particles

clusion is that the gas-particle covariance should be mainly related to particle kinetic energy and Modified PH 1 can be used effectively without resorting to any empirical constant.

Gas-particle covariance represents the correlation between the particle fluctuating velocity and the gas fluctuating velocity experienced by the particles. Gas fluctuating velocity can be regarded as the velocity unmodified by particles in dilute two-phase flow. Particle fluctuating velocity largely depends on particle diameter. The fluctuating velocity for small particles is similar to that of the gas phase due to their sufficient interacting time to respond to gas fluctuation. However, the fluctuating velocity for large particles is less than that of the gas phase because large particles do not have sufficient time to respond to the gas fluctuation. As a result, the value of gas-particle covariance is dominated by the fluctuation of the particle phase. Therefore, it is reasonable that the value of gas-particle covariance is governed mainly by the particle kinetic energy.

4. Conclusions

Numerical simulation of two-phase flow over a backward-facing step with Reynolds numbers of 18,400 has been successfully investigated by Large Eddy Simulation for the gas phase and a Lagrangian tracking model for the particle phase. Simulation results show that the one-way coupling assumption is effective in predicting dilute two-phase turbulent flow. The simulation results are in good agreement with the experimental results for the first and second-order statistical averages including mean and fluctuating results for both phases.

Several models for gas-particle covariance used in two-phase flow with the two-fluid assumption are evaluated by comparing with LES simulation results. The model proposed by Pourahmadi and Humphrey gives poor agreement with LES results. The model proposed by Chen and Wood gives better agreement with LES results, but an empirical constant is needed in Chen's model for different flow configurations and particle size. It is difficult to decide the correct value of the empirical constant. A modified model has been proposed in this study by claiming that gas-particle covariance is governed mainly by particle kinetic energy. The modified model gives good agreement with LES results and an empirical constant is no longer necessary.

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