Title: A New Dynamic SGS Model for Large Eddy Simulation of Particle-Laden Turbulent Flows

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A NEW DYNAMIC SGS MODEL FOR LARGE EDDY SIMULATION OF PARTICLE-LADEN TURBULENT FLOWS

KANGBIN LEI
Computer and Information Division, Advanced Computing Center
The Institute of Physical and Chemical Research (RIKEN)
2-1, Hirosawa, Wako-shi, Saitama 351-0198, Japan
lei@riken.go.jp

NOBUYUKI TANIGUCHI
Super Computing Division, Information Technology Center
University of Tokyo
2-11-16, Yayoi, Bunkyo-Ku, Tokyo, 113-8658, Japan
taniguchi@cc.u-tokyo.ac.jp

TOSHIO KOBAYASHI
The 2nd Department, Institute of Industrial Science
University of Tokyo
4-6-1, Komaba, Meguro-ku, Tokyo 153-8505, Japan
kobaya@iis.u-tokyo.ac.jp

Abstract

The paper presents a new dynamic SGS model of two-way coupling for large eddy simulation of particle-laden turbulent flow. The advantage of this new model is that coupling of fluid-particles SGS components was taken into account and at the same time the coefficient of proposed SGS model can be optimized by Germano's (1991) dynamic procedure\(^1\). To investigate the capability of this model, numerical simulations of particle-laden turbulent flow at Re=644 in a vertical channel were performed using this new dynamic SGS model. By comparing the calculation results with that using single-phase SGS models which didn't consider coupling of SGS components the role of particles SGS components played in the turbulence modulation of fluid flow was clarified for particle-laden channel turbulent flows. In addition, the subgrid-scale stresses obtained using the proposed model vanish at wall boundary, and have the correct asymptotic behavior in the near-wall region of the turbulent boundary.

1. Introduction

In large eddy simulation of single-phase turbulent flows, one major deficiency of the Smagorinsky\(^2\) subgrid-scale stress models is their inability to represent correctly with a single universal constant to different turbulent fields in rotating
or sheared flows, near solid walls, or in transitional regimes. Usually additional modifications to the Smagorinsky model were made in the near-wall region to force the subgrid-scale stresses to vanish at the wall boundary with a standard Van Driest(3) damping function. The dynamic SGS model proposed by Germano(1) et al. (1991) overcomes these deficiencies by locally calculating the eddy viscosity coefficient to reflect closely the state of the flow. In large eddy simulation of multi-phase turbulent flows, it is being expected that the fluid turbulence modulation SGS model can be evaluated by Germano’s dynamic procedure as in the single-phase turbulent flows.

In particle-laden turbulent flow, a kind of multi-phase turbulent flows that occur in a wide range of engineering and scientific research, interaction of particles and gas-phase turbulent carrier flow is a problematic research topic of both fundamental importance and practical interest. In addition, it is the most interesting problem in developing numerical simulation models. A two way coupling SGS model was present by Yuu(4) (1997), in which coupling of fluid-particles SGS component was considered. However, the model coefficient was simply decided in the same way as previous works for the single-phase turbulent flows.

We present here a new dynamic SGS model for two way coupling LES of particle-laden turbulent flow based on Yuu’s SGS model. The couplings of fluid-particles SGS component on fluid turbulence modulation in LES was taken into account and at the same time the coefficient of proposed SGS model can be dynamically decided by assuming that the small scales are in equilibrium, so that energy production, dissipation and interaction of fluid-particles are in balance.

The main objective of this paper is to introduce this model and at the same time to report the results of investigation about the capability and limitation of present SGS mode in predicting the fluid turbulence modulation for particle-laden turbulent flows through numerical simulations, which were performed in downward particle-laden turbulent flows at Re=644 in a vertical channel using Van Driest wall function model and the proposed new dynamic SGS model.

2. Improvement of Two Way Coupling SGS model

For dilute particle-laden turbulent flow, in which particle volume fraction is very small but the particle mass loading is large, momentum equations governing transport of the large eddies was oriented by filtering the incompressible Navier-Stokes equations with the particle source term, where the Leonard and Cross terms were neglected.

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = \frac{1}{\rho_f} \frac{\partial \bar{p}}{\partial x_i} + \frac{\mu}{\rho_f} \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j} - F[N(\bar{u}_i - \bar{u}_m) + n \bar{u}_i - n \bar{u}_m] \tag{1}
\]

The effect of the SGS on the resolved eddies in EQ (1) is represented by SGS stress \( \tau_{ij} = \bar{u}_i \bar{u}_j - \bar{u}_i \bar{u}_j \). In this work, \( \tau_{ij} \) is parameterized using an eddy viscosity
hypothesis expressed by Eq. (2), and the particles turbulent dispersion flux terms \( n u_i \) and \( n u_{pi} \) adopt gradient dispersion model as presented in Eq. (3) and Eq. (4).

\[
\tau_{ij} - \frac{1}{3} \delta_{ij} \tau_{kk} = -2 \nu_T \overline{S}_{ij} \tag{2}
\]

\[
\frac{n u_i}{\mu} = -\nu_T \frac{\partial N}{\partial x_i} \tag{3}
\]

\[
\frac{n u_{pi}}{\mu} = -\nu_{tp} \frac{\partial N}{\partial x_i} \tag{4}
\]

Here, the viscosity taking into account fluid particles interactions needs to be parameterized.

The governing equation of kinetic energy for subgrid-scale flow considering the interaction of fluid and particles can be derived as follow.

\[
\frac{Dk}{Dt} + \frac{\partial k}{\partial x_j} \frac{\partial k}{\partial x_j} = -u_i u_j \Delta_{ij} - \frac{1}{2} \mu_j u_i + \frac{1}{\rho_f} u_j p - \nu \frac{\partial k}{\partial x_j} \frac{\partial n u_i}{\partial x_j} - \nu \frac{\partial n u_{pi}}{\partial x_j} \frac{\partial n u_i}{\partial x_j} - F[N(u_i u_j - u_{pi}(u_i - u_{pi})) + n u_i(u_i - u_{pi})] \tag{5}
\]

From Eq. (5), however, the third order fluctuating terms were neglected, Yuu (1997) proposed a two way coupling SGS model applying a local equilibrium assumption expressed as Eq. (6) that energy production, dissipation and interaction of fluid-particles are in balance.

\[
2 \nu_T \overline{S}_{ij} \overline{S}_{ij} - C_v k^{3/2} \Delta^4 - 2 NF \frac{1 - b}{a T_{Li} + 1} k + F \nu_T \frac{\partial N}{\partial x_i} (\overline{u}_i - \overline{u}_{pi}) = 0 \tag{6}
\]

From Eq. (6), the viscosity taking into account of fluid-particles interaction was derived and expressed as Eq. (7)

\[
\nu_T = \nu_{Tc} C_e^{1/3} \sqrt{\frac{A_1 + \sqrt{A_2^2 + 4A_3(A_4 + A_5)}}{2A_4}} \tag{7}
\]

Where

\[
A_1 = C_e \Delta^{-1} \quad A_2 = 2 NF \frac{1 - b}{a T_{Li} + 1}
\]

\[
A_3 = 2C_v C_e^{1/3} \Delta \overline{S}_{ij} \overline{S}_{ij} \quad A_4 = FC_v C_e^{1/3} \frac{\Delta}{\sigma_s} \frac{\partial N}{\partial x_i} (\overline{u}_i - \overline{u}_{pi})
\]

\[
T_{Li} = \frac{L_e}{(2k/3)^{1/2}} = \frac{\alpha_1}{C_e} \Delta \left( \frac{2}{3} k \right)^{1/2} \tag{8}
\]

However, it is difficult to decide the coefficient \( C_v \) dynamically in Yuu’s model because the filter width \( \Delta \) are mixed in Eq. (7). In this study, we take the place of Eq. (6) \( T_{Li} \) with Eq. (8) and get Eq. (9) as follows
The SGS turbulence energy $k$ can be modeled as follows according to dimensional analysis

$$k = \frac{C_v}{C_e} 2^{3/2} \Delta^2 (2 \bar{S}_y \bar{S}_y) = \frac{C_v}{C_e} 2^{3/2} \Delta^2 |\bar{S}|^2$$

(10)

Substitution of EQ (10) into the third term denominator of EQ (9) and put it in order, the new eddy viscosity is then given by

$$\nu_T = C_{vt}^{3/2} \Delta^2 \left[ \frac{|\bar{S}|^2 + \frac{F}{\sigma_s} \frac{\partial N}{\partial x_i} (\bar{u}_i - \bar{u}_{pi})}{1 + \frac{2NF(1-b)}{\sqrt{3/2\alpha_F + \sqrt{C_sC_e}|\bar{S}|}}} \right]^{1/2}$$

(11)

Because the filter width $\Delta$ appears at only one place in the EQ (11) similar to the standard Smagrinisky model of single-phase turbulent flows, the coefficient $C_{vt}$ of proposed model can be easily decided by Germano’s (1991) dynamic procedure.

3. A proposal of new dynamic SGS model of Two Way Coupling

Now substitute EQ (11) into EQ (2) to get the new dynamic eddy viscosity subgrid-scale stress expressed as EQ (12), which takes into account of the interaction of particles-fluid SGS components in LES.

$$\tau_{ij} = u_i u_j - \bar{u}_i \bar{u}_j$$

$$= -2\nu_T \bar{S}_{ij} = -2 C_{vt}^{3/2} \Delta^2 \left[ \frac{|\bar{S}|^2 + \frac{F}{\sigma_s} \frac{\partial N}{\partial x_i} (\bar{u}_i - \bar{u}_{pi})}{1 + \frac{2NF(1-b)}{\sqrt{3/2\alpha_F + \sqrt{C_sC_e}|\bar{S}|}}} \right]^{1/2} \bar{S}_{ij}$$

(12)

$$= -2(C_m \Delta)^3 g(\bar{u}_i, \bar{u}_{pi}, N) \bar{S}_{ij}$$

According to the Germano’s dynamic procedure (1), the test filter level SGS stress can be defined as

$$T_{ij} = u_i \bar{u}_j - \bar{u}_i \bar{u}_j = -2 C_{vt}^{3/2} \Delta^2 \left[ \frac{|\tilde{S}|^2 + \frac{F}{\sigma_s} \frac{\partial N}{\partial x_i} (\tilde{u}_i - \tilde{u}_{pi})}{1 + \frac{2NF(1-b)}{\sqrt{3/2\alpha_F + \sqrt{C_sC_e}|\tilde{S}|}}} \right]^{1/2} \tilde{S}_{ij}$$

(13)

$$= -2(C_m \Delta)^3 g(\tilde{u}_i, \tilde{u}_{pi}, N) \tilde{S}_{ij}$$
A NEW DYNAMIC SGS MODEL FOR LES

Where, $\Delta$ is the characteristic filter width associated with the grid level filtering operator, and $\Delta_s$ is the filter width associated with the test level filtering operator. Considering the similarity between the SGS stresses at the grid and test levels, which are modeled using the same functional expression, it was assumed that the coefficient $C_{vt}$ or $C_{m5}$ in EQ (12) and EQ (13) are same, then grid filter stress $\tau_{ij}$, test filter stress $T_{ij}$ and resolved turbulent stress can be related in algebraic relation EQ (14)

$$T_{ij} - \tau_{ij} = 2C_{vt}^3 2C_{vt}^\frac{3}{4} \left[ g(\bar{u}, u_{pi,N}) S_{ij} - \alpha^2 g(\bar{u}, u_{pi,N}) \tilde{S}_{ij} \right]$$

From EQ (14), $C_{vt}(x,y,z,t)$ can be obtained in principle. The quantity in square brackets, however, can become zero, which would make $C_{vt}$ indeterminate or ill-conditioned. For the channel flow, therefore, it was assumed that $C_{vt}$ is only a function of $y$ and $t$. The average of both sides of EQ (14) are taken over a plane parallel to the wall to yield

$$C_{m5} = C_{vt}^{3/4} = \left[ \frac{\langle \bar{u}_{ij} u_{ij} - \bar{u}_{ij} \tilde{u}_{ij} \rangle}{2\Delta^3 < g(\bar{u}, u_{pi,N}) S_{ij} - \alpha^2 g(\bar{u}, u_{pi,N}) \tilde{S}_{ij} >} \right]^{1/2}$$

The new dynamic eddy viscosity subgrid-scale stress model, which takes into account of the interaction of particles-fluid SGS components in LES, is then given by

$$\tau_{ij} = \left[ \frac{\langle \bar{u}_{ij} u_{ij} - \bar{u}_{ij} \tilde{u}_{ij} \rangle}{\alpha^2 g(\bar{u}, u_{pi,N}) S_{ij} - g(\bar{u}, u_{pi,N}) \tilde{S}_{ij}} \right] g(\bar{u}, u_{pi,N}) \tilde{S}_{ij}$$

4. Simulation overview
4.1 Calculation of fluid phase
The particle-laden turbulent flows between plane channels driven by uniform pressure gradient and particles gravity were calculated by large eddy simulations at Reynolds numbers based on friction velocity and channel half-width of 644. Van Driest damping function model and dynamic SGS models with (the present model) or without (Germano's model) couplings of SGS components were applied respectively. The governing equation EQ (1) and continuity equation were solved numerically by SMAC method on a staggered grid. Second-order central difference scheme was used for the advection and diffusion terms, and second-order Adams-Bashforth method was adopted for time advancement. The Poisson equation for pressure was solved using ICCG method. The flow was resolved using $32 \times 64 \times 32$ grid points in the $x$, $y$ and $z$ directions, respectively. The channel domain for the calculation was $\pi \delta \times 2 \delta \times \pi \delta / 2$. For fully developed channel flow, periodic boundary conditions for the dependent variables were applied in the streamwise and spanwise directions, whereas the no-slip condition was applied on the channel walls.
4.2 Calculation of particle phase
The motion of particles was integrated using second-order Adams-Bashform in
time, and third-order Lagrange polynomials were used to interpolate the fluid
velocity to the particle position since it is only by chance that a particle is located
at a grid point where the Eulerian velocity is available. For particles that moved
out of the channel in the streamwise or spanwise directions, the periodic
boundary conditions were used to introduce them into the computational domain.
The channel walls were perfectly smooth and a particle was assumed to contact
the wall when its center was one radius from the wall. Elastic collisions were
assumed for particles contacting the wall.
The initial condition of single phase Eulerian velocity field was given by a
statistically developed solution. Then the particles were assigned to random
locations throughout the canal, where the initial particle velocity was assumed
to be the same as the fluid velocity at the particle location. Similar to the fluid
flow, statistics of the particle velocity were averaged over two homogeneous
directions, both channel halves and time. To distinguish the effect of two way
coupling, the 70 μm Copper particles were blended at mass loading ratio 1.0.

5. Calculation results

The numerical simulations were carried out using Van Driest wall function and
the present dynamic SGS model, while the SGS coupling was taken into account
or not respectively. The streamwise mean velocities of fluid are shown in Figure
1, the root-mean-square velocity fluctuations of fluid in streamwise are shown in
Figure 2. As may be observed in figures above, in spite of the SGS coupling is
taken into account or not, the mean velocities are predicted larger, and the
root-mean-square velocity fluctuations are also slightly larger using proposed
dynamic SGS models than using Van Driest wall function. Since this
characteristic is similar to single-phase turbulent flow using standard dynamic
SGS model, we can say that the present SGS model has proper asymptotic
behavior near the wall without the use of ad hoc damping function in case of
multiphase turbulent flow. As shown in Figure 2, the turbulence intensities of
particle-laden flow are clearly decreased than ones of particle-unladen flow for the coupling of GS components of particle-laden flow, but the turbulence intensities of particle-laden flow are hardly decreased when the SGS coupling was taken into account.

The eddy viscosity model coefficients that were calculated by proposed dynamic SGS model are shown in Figure 3. In the channel buffer region, the dynamic SGS model coefficient of particle-laden flow is smaller than that of particle-unladen flow. On the contrary, in the channel center area, the former is higher than the latter. Since the effects of two-way coupling of GS and SGS components correspond the profile of turbulence intensity of fluid in wall normal, the coefficient of proposed dynamic SGS model obtains the correct asymptotic behavior in the near-wall region. In logarithm law region (y+ ~ 100), where concentration of the local particles is lowest, the proposed model obtains the fittest value Cm’ ~ 0.1 in single-phase channel turbulent flows. It reflects the local structure of small eddies, showing that the capability of proposed model is validated.

The mean distributions of eddy viscosity are shown in Figure 4. In the near-wall region (y+ < 30), as the effects from SGS component to GS component are relatively small, the distribution of model coefficients correspond the profile of eddy viscosity as they are. While in the logarithm law region, though the model coefficients are roughly same, the effect of two-way coupling of GS components is significant, which may result from the difference of strain velocity S. As a result of taking into account of two-way coupling of SGS component, the model coefficients become bigger, which is agreed with the tendency that dissipation of turbulence is enhanced in high frequency.

The cascade profile of GS turbulence energy with or without SGS component coupling is shown in Figure 5, the energy cascade becomes slightly stronger owing to SGS coupling as expected. This indicates that the contribution of SGS component to GS component is shown as dissipation of GS component. According to this simulation result, the efficiency of presented dynamic two-way coupling SGS Model is verified. Intriguingly, contrary to the conjecture of Yamamoto (1998), the spatial spectra of fluctuation energy becomes a
little stronger with SGS coupling than that without it as shown in Figure 6.

Figure 5. Cascade Profile of GS turbulence energy

Figure 6. Streamwise spatial spectra of fluctuation energy at y+=5

6. Concluding remarks

(1) A new dynamic SGS model has been proposed for two way coupling LES of particle-laden turbulent flow based on Yuu's SGS model, in which the couplings of fluid-particles SGS component on fluid turbulence modulation was taken into account and at the same time the coefficient of proposed SGS model can be dynamically obtained as the calculations progress rather than input a priori.

(2) As a result of taking into account of two-way coupling of SGS component, the dynamic model coefficients become bigger, and in the channel buffer region, the proposed dynamic model coefficient of particle-laden flow is smaller than that of particle-unladen flow, on the contrary, the former is higher than latter in the channel center area.

(3) Numerical simulation results using the new dynamic model proposed reflected the local structure of small eddies of particle-laden, showing that the capability of proposed model was validated.

Reference