FULL WAY COUPLING OF LARGE EDDY SIMULATION FOR PARTICLE-LADEN TURBULENT FLOWS USING NEW DYNAMIC SGS MODELS

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ABSTRACT

A new method named Full Way Coupling of Large Eddy Simulation (LES) for particle-laden turbulent flows using two modified dynamic Sub-Grid-Scale (SGS) models and considering particles collision based on a Eulerian-Lagrangian approach was presented. In order to simulate the interactions of SGS components, two new SGS models were introduced: Dynamic Random Walk SGS Model was used to calculate the particles diffusion by fluid SGS component, and the fluid turbulence modification of particle SGS component has been investigated using a proposed Dynamic Fluid-Particles SGS Coupling Model. The advantage of these new SGS coupling models is that the dimensional analysis coefficient of proposed SGS model could be decided by Germano's (1991) dynamic procedure. The effects of inter-particle collision on particles motion were taken into accounts using Direct Numerical Simulation (DNS). Using this Full Way Coupling method, the numerical simulations were performed for downward channel flow at Reynolds numbers of 644 that was identical to the experiments done by Kulick et al. in 1994. The effects of fluid-particles SGS component couplings and inter-particle collisions on solid particles dispersion and fluid turbulence modification in LES for particle-laden turbulent flows were then investigated.

INTRODUCTION

Particle-laden turbulent flows are classified by the material of fluid and particles, and also by flow conditions. Interaction between particles and gas-phase turbulent carrier flows is a problematic research topic of both fundamental importance and practical interest. In addition, it is the most intriguing problem for developing numerical simulation models.

The interactions are classified into One-Way Coupling (only the influence of fluid motion on particle motion was considered), Two-Way Coupling (the influence of particle motion on fluid motion are also taken account of) and Four-Way Coupling (addition to the above factors, the collisions between particles are also considered) in DNS according to Elghobashi's regimes (1994). It is known that addition of particles to a turbulent flow could change the intensities significantly, even at low volume fraction, but the practical modeling of such mechanisms remains an open question.

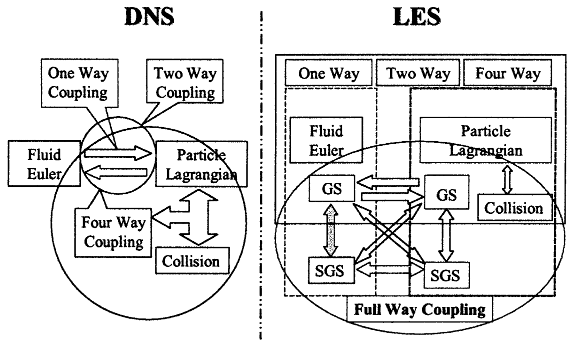
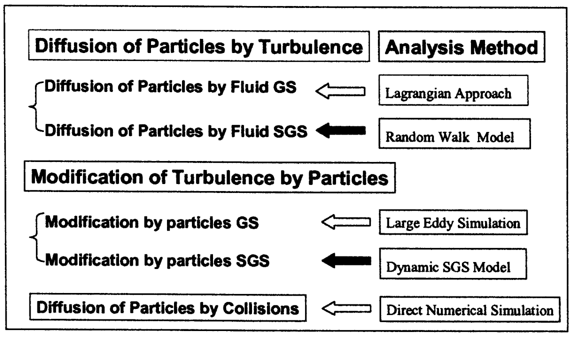


Figure 1: Comparison of coupling method between of DNS and LES

In LES of particle-laden turbulent flows, which is not as severely restricted in the range of Reynolds numbers as DNS, the interactions between particles and gas-phase turbulent carrier flows are much more complicated because they concern not only Grid-Scale (GS) components but also SGS components caused by LES filtering operation as well as particles collision as shown in figure 1. However, there are not yet well-developed modeling methodologies to take into account all of these factors. Recently we resolved this problem to some extent by establishing the new method named Full Way Coupling of LES, as shown in table 1, using new-developed Dynamic SGS Coupling Models.



Diffusion of Particles by Turbulence	Analysis Method
Diffusion of Particles by Fluid GS	Lagrangian Approach
Diffusion of Particles by Fluid SGS	Random Walk Model
Modification of Turbulence by Particles	
Modification by particles GS	Large Eddy Simulation
Modification by particles SGS	Dynamic SGS Model
Diffusion of Particles by Collisions	Direct Numerical Simulation

Table 1: Problems of LES for particle-laden turbulent flows and Method of Full Way Coupling

The main objective of the present study is to introduce these models and at the same time to investigate the capability and limitation of the Full Way Coupling method in predicting the particles dispersion and the fluid turbulence modification for particle-laden turbulent flows. Numerical predictions were compared with experimental measurements done by Kulick et al. (1994), who studied the statistical properties of particle-laden turbulent flow in a vertical channel at Re=644.

GOVERNING EQUATIONS

Equation of fluid flow

The particle-laden turbulent flow between plane channels driven by uniform pressure gradient and particles gravity was calculated using LES of the incompressible Navier-Stokes equations with the particle source term. The equations governing transport of the large eddies oriented by filtering the N-S equations are:

$$\frac{\partial \bar{u}_i}{\partial t}+\frac{\partial}{\partial x_j}(\bar{u}_i\bar{u}_j)=-\frac{1}{\rho_f}\frac{\partial \bar{p}}{\partial x_i}+\frac{\mu}{\rho_f}\frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j}-\frac{\partial \tau_{ij}}{\partial x_j} \quad (1)$$
$$-F[N(\bar{u}_i-\bar{u}_{pi})+\overline{n'u_i'}-\overline{n'u_{pi}'}]$$

The last term on the right hand side of EQ (1) is the particle source term, which indicates the one-way interaction from particles to fluid. The effect of the SGS on the resolved eddies in EQ (1) are represented by SGS stress, $\tau_{ij}=\overline{u_iu_j}-\bar{u}_i\bar{u}_j$. In this work τ_{ij} is parameterized using an eddy viscosity hypothesis as EQ (2), and the particles turbulent dispersion flux terms $\overline{n'u_i'}$ and $\overline{n'u_{pi}'}$ are adopted gradient dispersion model as EQ (3) and EQ (4).

$$\tau_{ij}-\frac{1}{3}\delta_{ij}\tau_{kk}=-2\nu_T\bar{S}_{ij} \quad (2)$$

$$\overline{n'u_i'}=-\nu_{TS}\frac{\partial N}{\partial x_i} \quad (3)$$

$$\overline{n'u_{pi}'}=-\nu_{TP}\frac{\partial N}{\partial x_i} \quad (4)$$

Here, the viscosity considering fluid-particles interaction needs to be parameterized.

Equation of particle motion

The dimensionless particle equation of motion used in the simulations describes the motion of particles with densities substantially larger than that of the surrounding fluid and small diameters compared to the Kolmogorov scale:

$$\frac{dv_i}{dt}=-\frac{f(v_i-u_i)}{\tau_p}+g_i\delta_{1i} \quad (5)$$

$$u=\bar{u}+u',u_i=\bar{u}_i+u_i' \quad (6)$$

Where, the $\bar{u},\bar{u}_i$ are the GS components of fluid, and the u',u_i' are the SGS components of fluid, respectively. The effect of SGS velocity fluctuations on particles transport should be taken account by Lagrangian SGS model because that only the large eddies (GS component) is directly available in LES computation.

Calculation of inter-particle collisions

Due to the preferential concentration of particles in turbulent flow, the inter-particle collisions may have a strong influence on the statistics of particle velocity even at low mass flow ratio. Therefore, inter-particles collisions were computed directly using the momentum conservation law below.

$$\vec{u}_{rji}^{*}=\vec{u}_{pj}^{*}-\vec{u}_{pi}^{*} \quad (7)$$

$$\vec{r}_{ji}=\vec{r}_j-\vec{r}_i \quad (8)$$

$$\vec{u}_{pi}^{c}=\vec{u}_{pi}^{*}+\frac{(\vec{r}_{ji}\cdot\vec{u}_{rji}^{*})\vec{r}_{ji}}{|\vec{r}_{ji}|^2} \quad (9)$$

$$\vec{u}_{pj}^{c}=\vec{u}_{pj}^{*}-\frac{(\vec{r}_{ji}\cdot\vec{u}_{rji}^{*})\vec{r}_{ji}}{|\vec{r}_{ji}|^2} \quad (10)$$

Where, the velocities superscripted with "*" indicate the velocities of particles before collisions and the velocities by the superscript "c" are velocities of particles after collisions.

PROPOSALS OF NEW DYNAMIC SGS MODELS

Eulerian Dynamic Fluid-Particles Coupling SGS Model for turbulence modification

A new viscosity SGS model EQ (11) considering fluid-particles coupling for turbulence modification were proposed based on the assumption (Yuu, 1997) of local energy equilibrium of SGS fluctuations (Lei et al. 2000).

$$\nu_T=C_{\nu T}^{3/2}\Delta^2\left[\frac{|\bar{S}|^2+\frac{F}{\sigma_s}\frac{\partial \bar{N}}{\partial x_i}(\bar{u}_i-\bar{u}_{Pi})}{1+\frac{2\bar{N}F(1-b)}{\sqrt{3/2}\alpha_1 a+\sqrt{C_\nu C_\varepsilon}|\bar{S}|}}\right]^{1/2} \quad (11)$$

The advantage of this SGS coupling model is that the dimensional analysis coefficient $C_{\nu T}$ of proposed SGS model could be decided by Germano's (1991) dynamic procedure as follows:

$$\tau_{ij}=\overline{u_i u_j}-\bar{u}_i\bar{u}_j=-2\nu_T\bar{S}_{ij}$$

$$=-2C_{vT}^{3/2}\Delta^2\left[\frac{\left|\bar{S}\right|^2+\dfrac{F}{\sigma_S}\dfrac{\partial\bar{N}}{\partial x_i}(\bar{u}_i-\bar{u}_{Pi})}{1+\dfrac{2F\bar{\bar{N}}(1-b)}{\sqrt{3/2}\alpha_1 a+\sqrt{C_v C_\varepsilon}\left|\bar{S}\right|}}\right]^{\frac{1}{2}}\bar{S}_{ij} \quad (12)$$

$$=-2(C_{ms}\Delta)^2 g(\bar{u}_i,\bar{u}_{Pi},\bar{N})\bar{S}_{ij}$$

$$T_{ij}=\widetilde{\overline{u_i u_j}}-\tilde{\bar{u}}_i\tilde{\bar{u}}_j$$

$$=-2C_{vT}^{3/2}\Delta_S^2\left[\frac{\left|\tilde{\bar{S}}\right|^2+\dfrac{F}{\sigma_S}\dfrac{\partial\tilde{\bar{N}}}{\partial x_i}(\tilde{\bar{u}}_i-\tilde{\bar{u}}_{Pi})}{1+\dfrac{2F\tilde{\bar{N}}(1-b)}{\sqrt{3/2}\alpha_1 a+\sqrt{C_v C_\varepsilon}\left|\tilde{\bar{S}}\right|}}\right]^{\frac{1}{2}}\tilde{\bar{S}}_{ij} \quad (13)$$

$$=-2(C_{ms}\Delta_S)^2 g(\tilde{\bar{u}}_i,\tilde{\bar{u}}_{Pi},\tilde{\bar{N}})\tilde{\bar{S}}_{ij}$$

$$T_{ij}-\tilde{\tau}_{ij}=\widetilde{\bar{u}_i\bar{u}_j}-\tilde{\bar{u}}_i\tilde{\bar{u}}_j$$
$$=2C_{vT}^{3/2}\Delta[\widetilde{g(\bar{u}_i,\bar{u}_{pi},\bar{N})\bar{S}_{ij}}-\alpha^2 g(\tilde{\bar{u}}_i,\tilde{\bar{u}}_{Pi},\tilde{\bar{N}})\tilde{\bar{S}}_{ij}] \quad (14)$$

$$C_{mS}=C_{vT}^{3/4}$$
$$=\left[\frac{<\widetilde{\bar{u}_i\bar{u}_j}-\tilde{\bar{u}}_i\tilde{\bar{u}}_j>}{2\Delta^2<\widetilde{g(\bar{u}_i,\bar{u}_{Pi},\bar{N})\bar{S}_{ij}}-\alpha^2 g(\tilde{\bar{u}}_i,\tilde{\bar{u}}_{Pi},\tilde{\bar{N}})\tilde{\bar{S}}_{ij}>}\right]^{\frac{1}{2}} \quad (15)$$

Lagrangian Dynamic Random Walk SGS Coupling Model for particles dispersion

According to Gaussian distribution and isotropic statistical properties of the SGS fluctuation, the fluid SGS fluctuation magnitude u', u_i' can be modeled as follows:

$$u'=L_{Gaussian}\otimes\sqrt{2/3k_s} \quad (16)$$

$$k_s=\frac{C_{vt}}{C_\varepsilon}\Delta^2\left|\bar{S}\right|^2 \quad (17)$$

Where, $L_{Gaussian}$ means scaling operation by random numbers sampled from a Gaussian distribution, which are generated by Box and Mullar method as follows.

$$y_i=\sigma\sqrt{-2\log(x_i)}\cos(2\pi x_{i+1})+\mu \quad (18)$$

$$y_{i+1}=\sigma\sqrt{-2\log(x_i)}\sin(2\pi x_{i+1})+\mu \quad (19)$$

The important dimensional analysis coefficient C_{vT} (where the $C_\varepsilon=1.0$ is constant) of this modified *Random Walk SGS Coupling Model* could also be derived by dynamic procedure as EQ (15). Subsequently, the particle motion was determined using the complete fluid velocity at the particle location in EQ (5).

SIMULATION OVERVIEW

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. The governing equations 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 and the flow was resolved using 32×64×32 grid points in the x, y and z directions, respectively. The channel domain for the calculation was πδ×2δ×πδ/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.

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 cannel, 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.

CALCULATION RESULTS AND ANALYSIS

FIRSTLY, to investigate the effect of fluid SGS component on particle motion, 5 types particle with response time τ_p^+ =0.13 (2 μ m Lycopodium), 1.6 (7 μ m Lycopodium), 27 (28 μ m Lycopodium), 300 (50 μ m Glass) and 2050 (70 μ m Copper) were calculated with or without Dynamic Random Walk SGS Coupling Model. Profiles of the mean streamwise velocity, streamwise fluctuation velocity and the distribution of particle number density obtained from the LES calculations are shown respectively in Fig.2, Fig.3, and Fig.4 for each particle type. Of all types of particle, the velocity of 70 μ m Copper is most significantly affected by fluid SGS component, while for the streamwise fluctuation velocity, 50 μ m Glass is most markedly subjected to the effect of SGS component in the near-wall region. But the particle number density of 28 μ m Lycopodium is most sharply relaxed by SGS component in all types of particle. Results observed above suggest that both the energy contain eddy and sub-grid eddies close to the Kolmogorov scale are responsible for the particles motion, moreover, fluid SGS component is strongly associated with particles motion because preferred particles were affected by preferred length scale of the eddy structure around.

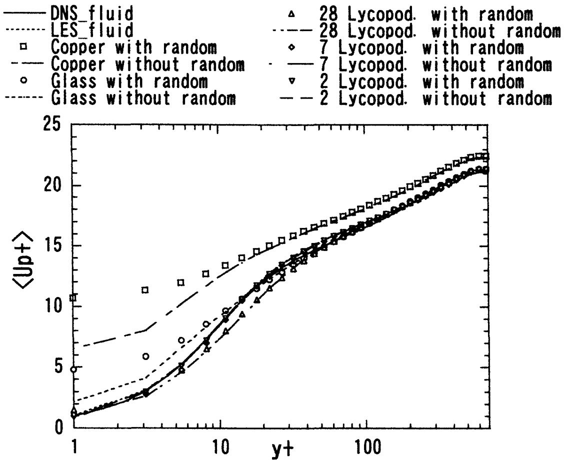


Figure 2: Profile of particles streamwise mean velocity with or without SGS component coupling

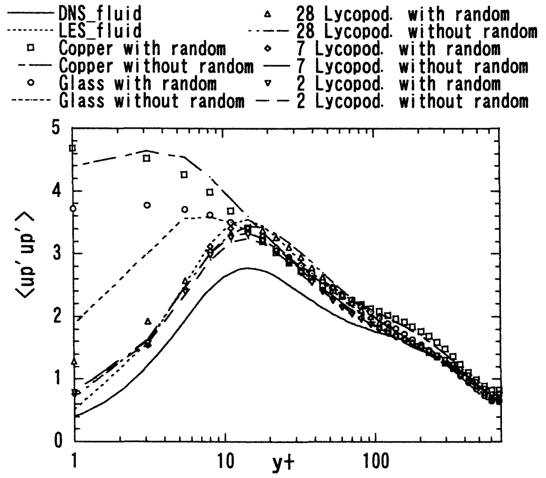


Figure 3: Profile of particles streamwise fluctuation velocity with or without SGS component coupling

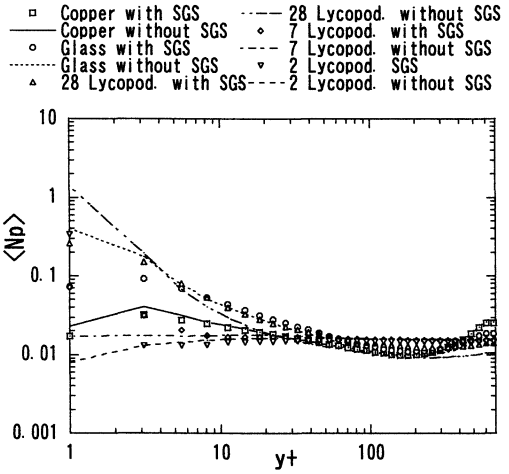


Figure 4: Distribution of particle number density with or without fluid SGS component coupling

SECONDLY, the turbulent channel flow laden with 70 μm copper particles at mass loading ratio 1.0 was studied to verify the efficiency of Dynamic Fluid-Particles SGS Coupling Model. The eddy viscosity model coefficients that were calculated by proposed dynamic SGS model were shown in Fig.5. In the channel buffer region, the dynamic SGS model coefficient of particle-laden flow is smaller than that of particle-unladen flow. In contrast, in the channel center area, the former is higher than the latter. Since effects of two-way coupling of GS and SGS components correspond with the profile of turbulence intensity of fluid in wall normal, the coefficient of proposed dynamic SGS model obtained the correct asymptotic behavior in the near-wall region. In logarithm law region (y+~100), where the 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 Fig.6. In the near-wall region (y+<30), for the effects of SGS component on GS component are relatively small, the distribution of model coefficients corresponds with 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 region.

The cascade profile of GS turbulence energy with or without SGS component coupling is shown in Fig.7, the energy cascade becomes slightly stronger owing to SGS coupling as expected. This indicates that the contribution of SGS component to GS component is expressed as dissipation of GS component. According to this simulation result, the efficiency of presented Dynamic Fluid-Particles Coupling SGS Model is verified. But Intriguingly, contrary to the conjecture of Tanaka et al. (1997), the spatial spectra of fluctuation energy becomes a little stronger with SGS coupling than without it as shown in Fig.8.

THIRDLY, the effects of particle dispersion (70 μm copper particles, at mass loading ratio 0.2) due to the inter-particle collision under the Four Way Coupling simulation with the Dynamic Fluid-Particles SGS Coupling Model above are shown in Fig.9 and Fig.10. Compared with the LES value without collision, the value with it is much closer to experimental measurements (Kulik et al. 1994).

Collision frequencies of five types (2 μm, 7 μm, 28 μm Lycopodium, 50 μm Glass and 70 μm Copper) particle with or without considering SGS component coupling in 60,000 steps of time

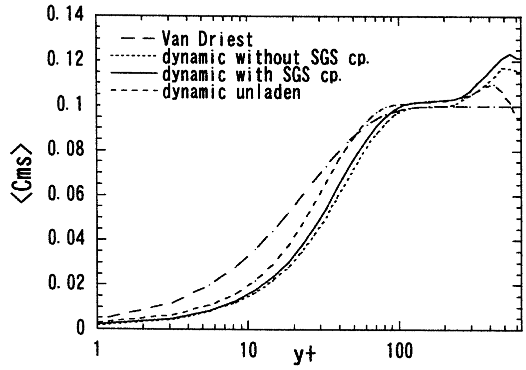


Figure 5: Profile of mean model coefficients with or without SGS component coupling

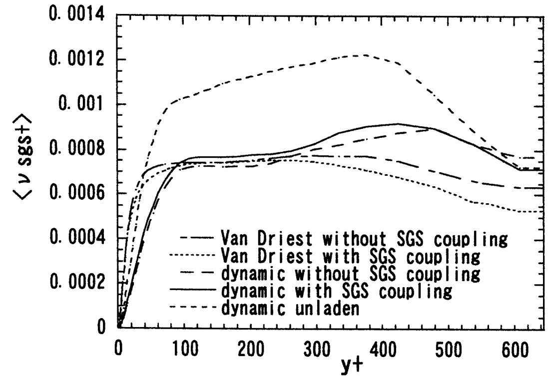


Figure 6: Profile of mean SGS eddy viscosity with or without SGS component coupling

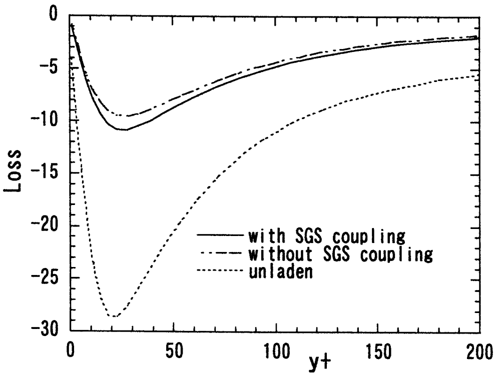


Figure 7: Gascade profile of GS turbulent energy with or without SGS component coupling

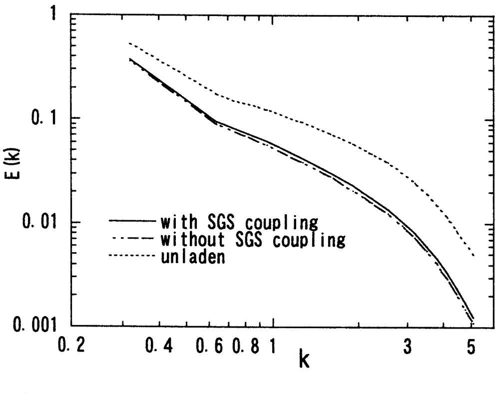


Figure 8: Streamwise spatial spectra of fluctuation energy at y+=5 with or without SGS component

advancement are shown in Fig.11. Collision is hardly observed for 2 μ m and 7 μ m Locopodium. Highest collision frequency of 28 μ m Locopodium is observed when SGS coupling is not considered. However, it is sharply decreased when considering SGS component coupling, while collision frequency of 50 μ m Glass becomes the highest among five particles at this time. So inter-particle collision is affected not only by the local particle number density but also by particle response time. Based on the finding above, the famous map describing the different regimes on a diagram, which was presented by Elghobashi (1994), may be improved and a new proposal about regime of particle-turbulence interaction is shown as Fig.12 using dimensionless coordinates.

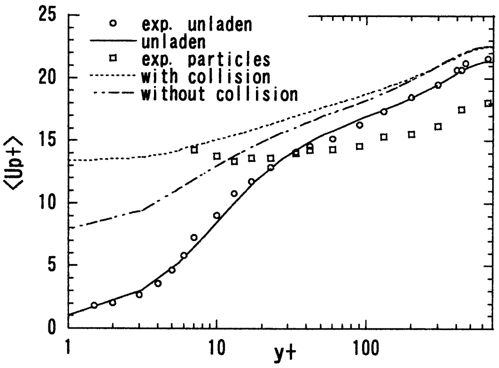


Figure 9: Profile of particles streamwise mean velocity with or without inter-particles collision

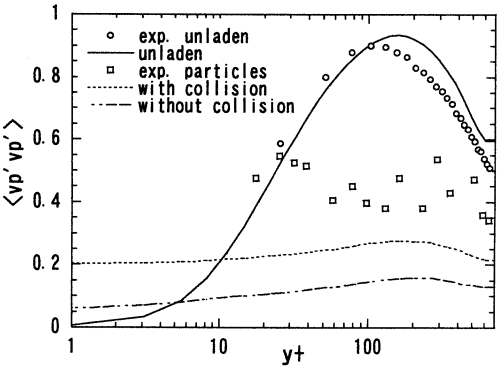


Figure 10: Profile of wall-normal particles fluctuation velocity with or without inter-particle collision

FINALLY, the turbulence modifications of Full Way Coupling simulations, which considered the effects of inter-particle collision and SGS component coupling, are presented as Fig.13 and Fig.14. In the case at mass flow ratio 0.2, the fluid turbulence is attenuated only slightly in Full Way Coupling simulation, whereas, it is significantly attenuated in experiment. It suggests that further study is necessary to explain the quantitative discrepancy between Kulik et al.'s (1994) experiment and numerical simulation.

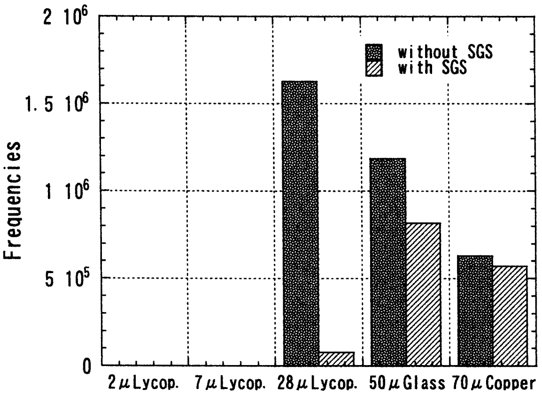


Figure 11: Frequency of collisions for 5 types particles with or without fluid SGS component coupling

CONCLUSIONS

1. Dynamic Random Walk SGS Coupling Model and Dynamic Fluid-Particles SGS Coupling Model were developed. A new method of Full Way Coupling of LES for particle-laden turbulent flow was established with the two models above.
2. As preferred particles were affected by preferred length scale of the eddy structure around, fluid SGS component was indispensable in calculating particles motion with LES.
3. Inter-particle collisions had a strong influence on the statistics of particle velocity even at low mass flow ratio
4. Inter-particle collision was affected not only by the local particle number density but also by particle response time. A new regime (Fig.12) about particle-turbulence interaction was proposed.
5. The LES calculation results were not yet completely consistent with Kulick et al.'s (1994) experimental measurements even though the fluid-particles Full Way Coupling was taken into account.

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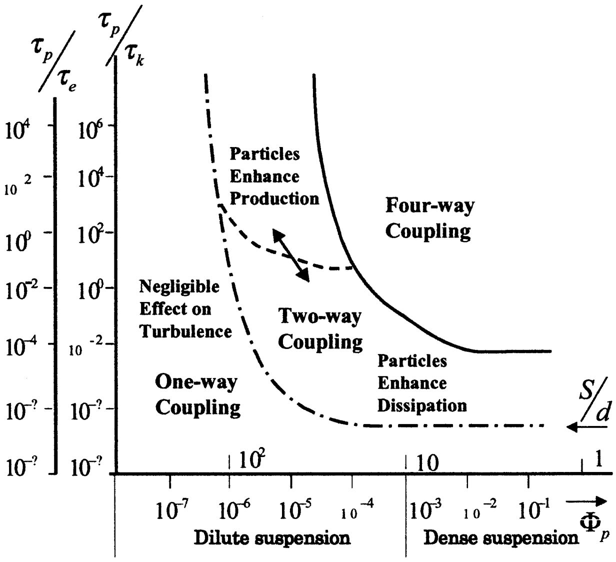

Figure 12: The present concept map for particle-turbulence interaction

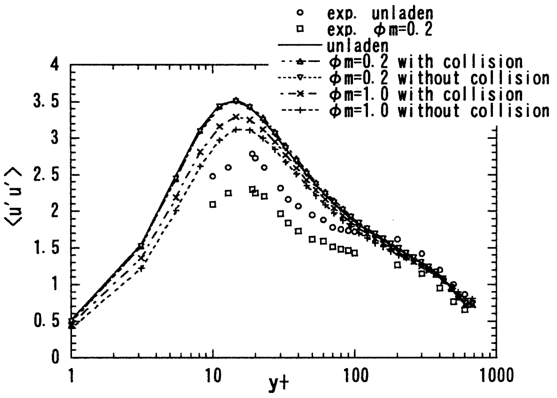

Figure 13 Profile of streamwise turbulent intensity with or without inter-particles collision

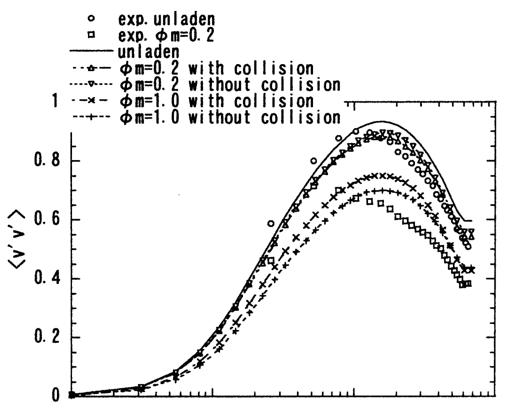

Figure 14: Profile of turbulence intensity in wall normal with or without inter-particles collision