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Two-fluid large-eddy simulation approach for particle-laden turbulent flows

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Abstract

In this paper, effects of particles on the subgrid scales of turbulence are properly accounted for during the modeling of subgrid scale stresses in the large-eddy simulation (LES) of fluid phase. In doing so, we propose closed filtered kinetic equations for phase space density of the particle. The various moments of these equations give the 'fluid' equations which can be considered as the LES equations for the particle phase. The influence of subgrid scales motion on the particles is included in these 'fluid' equations.

1. Introduction

In recent years, large-eddy simulation (LES) has emerged as an important predictive technique for fluid turbulence with growing number of models for statistical properties of small scales or subgrid scales which influence the instantaneous flow properties of the large scales or eddies. The pioneering model for subgrid scale stress tensor is due to Smagorinsky [1], followed by other dynamic and similarity models which are reviewed recently by Meneveau and Katz [2]. LES is also emerging in the field of two-phase turbulent flows for accurate prediction of particle or droplet laden flows [3,4].

In these flows, each particle moves under the influence of fluid forces (e.g. fluid drag force, history force), and the instantaneous fluid flow velocity U_i in the vicinity of the particle governs its trajectory. Here, we consider only the fluid drag force and assume the particle to be spherical with time constant $\tau_p = \rho_p d^2/18\mu$, where μ is the fluid viscosity, and ρ_p and d are the particle mass density and diameter, respectively. In this case, the governing Lagrangian equations for the spherical particle's position, X_i, and velocity, V_i, can be written as

$$\frac{dX_i}{dt} = V_i, \tag{1.1}$$

$$\frac{dV_i}{dt} = \beta_v(U_i - V_i), \qquad \beta_v = \frac{1 + 0.15Re_p^{0.687}}{\tau_p}, \tag{1.2}$$

where particle Reynolds number $Re_p = d\rho|\mathbf{V} - \mathbf{U}|/\mu$ and ρ is the fluid density. In this paper, we consider small particles with $Re_p < 1$ and take $\beta_v = 1/\tau_p$. The presence of particles modifies the flow field which is accounted for through the source term S_i in the governing equations for fluid phase velocity u_i, written for incompressible fluid as

$$\frac{\partial u_j}{\partial x_j} = 0, \quad \frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}[u_i u_j] = -\frac{\partial p}{\partial x_i} + \nu\frac{\partial^2 u_i}{\partial x_j \partial x_j} + S_i. \tag{1.3}$$

Here, p represents the fluid pressure divided by ρ at location x_i and time t, ν is the fluid kinematic viscosity, and S_i accounts for the effects of particles on the fluid flow and is given later in this paper. In the case of one-way coupling, $S_i = 0$ and the fluid phase is considered independent of the particle phase. S_i has finite values in the case of two-way coupling. Following the work of Germano et al. [5], we denote the grid filtering operation with filter width Δ on any function f as

$$\tilde{f}(\mathbf{x}) = \int f(\mathbf{x}')\widetilde{G}(\mathbf{x}, \mathbf{x}')d\mathbf{x}', \tag{1.4}$$

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Nomenclature

C	subgrid stress model coefficient
C_*	model coefficient in Eq. (3.9)
d	particle diameter
D	model coefficient in Eq. (3.8)
$\tilde{G}$, $\overline{G}$	filters
G_{jk}	Green's function, Eq. (2.10)
G'_{jk}	Green's function, Eq. (2.17)
G''_{jk}	Green's function, Eq. (2.32)
k, K	subgrid scale kinetic energies per unit mass of fluid
m_p	mass of the particle
n_p	total number of particles
p	fluid pressure divided by fluid density
Re_p	particle Reynolds number
S_i	source term in Eq. (1.3)
S_{ij}	strain rate tensor
$\widetilde{S}_{ij}, \widetilde{\overline{S}}_{ij}$	filtered strain rate tensors
t	time
$T_{b_ib_j}$	Lagrangian integral time scale
u_i	ith component of fluid velocity $\mathbf{u}$
U_i	ith component of fluid velocity $\mathbf{U}$ along the particle path
V_i	ith component of particle velocity $\mathbf{V}$
v_i	phase space variable corresponding to V_i
W	phase space density
x_i	physical space coordinates
X_i	ith component of particle position vector $\mathbf{X}$
Greek symbols	
μ	fluid viscosity
ν	fluid kinematic viscosity
ρ	fluid density
ρ_p	particle mass density
τ_p	particle time constant
Δ, $\overline{\Delta}$	filter widths
Subscript	
p	particle
Symbol	
$\langle\ \rangle$	ensemble average

and the test filtering operation as

$$\overline{f}(\mathbf{x}) = \int f(\mathbf{x}')\overline{G}(\mathbf{x},\mathbf{x}')\mathrm{d}\mathbf{x}', \tag{1.5}$$

and $\overline{\widetilde{G}} = \overline{G}\widetilde{G}$ filter has $\overline{\Delta}$ as filter width.

Now, application of the filter $\widetilde{G}$ to the Navier–Stokes equations gives

$$\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j}[\tilde{u}_i\tilde{u}_j] = -\frac{\partial \tilde{p}}{\partial x_i} + \nu\frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - \frac{\partial}{\partial x_j}\tau(u_i,u_j) + \widetilde{S}_i, \tag{1.6}$$

where the unknown subgrid stress tensor

$$\tau(u_i,u_j) = \widetilde{u_iu_j} - \tilde{u}_i\tilde{u}_j \tag{1.7}$$

and $\widetilde{S}_i$ pose closure problems and need to be modelled. While writing (1.6), and also later in this paper, commutation between filtering and derivative operators is used. In case of a single-phase flow, various models for subgrid stress tensor are suggested and are recently reviewed by Meneveau and Katz [2]. In this paper, we use the framework of dynamic localization model, proposed by Ghosal et al. [6], and derive the model for $\tau(u_i,u_j)$ in case of two-phase flow by incorporating the effects of particles on the subgrid scales. Also, a closed expression for $\widetilde{S}_i$ is derived from the kinetic equation for phase space density of the particle phase.

In the early studies on the LES of two-phase flows with one-way coupling [7,8], particles are tracked by using the LES velocity field, in the Lagrangian Eqs. (1.1) and (1.2), instead of the instantaneous velocity field u_i of the fluid phase. The effect of subgrid scale velocity field $u'_i = u_i - \tilde{u}_i$ on the particle are not taken into account in these studies. Armenio et al. [9] studied these effects in detail by performing and comparing the results from independent direct numerical simulation and LES. The two-way coupling effects are incorporated in LES by Boivin et al. [10] through the source term S_i. Only very recently, the two-way coupling is treated completely by also taking into account the effects of particles in the model for subgrid stress tensor [11]. Yuu et al. [11] modelled subgrid-scale turbulent mass flux of particle by gradient transport using the analogy of the molecular transport.

In all of the existing studies on LES, the particle phase is simulated in Lagrangian framework (see the recent review [3] and references cited therein). Rigorous modeling of the effects of particle phase on the subgrid scales and vice versa, still, remains as an important unfinished task. In this paper, an attempt is made for such modeling and, in doing so, 'fluid' or Eulerian equations are derived for particles which can be considered as LES equations for the dispersed phase.

2. 'Fluid' equations for particle phase

Using the phase space density $W(\mathbf{x},\mathbf{v},t)$, the source term S_i can be written as

$$S_i = -\frac{m_p}{\rho\tau_p}\int (u_i - v_i)W(\mathbf{x},\mathbf{v},t)\mathrm{d}\mathbf{v}, \tag{2.1}$$

where m_p is mass of the particle, $\mathbf{x}$ and $\mathbf{v}$ are phase space variables corresponding to $\mathbf{X}$ and $\mathbf{V}$, and W is governed by [3,12,13]

$$\frac{\partial}{\partial t}W(\mathbf{x},\mathbf{v},t)+\frac{\partial}{\partial x_i}[v_i W]+\frac{\partial}{\partial v_i}[\beta_v(u_i-v_i)W]=0 \qquad (2.2)$$

and is related to the total number of particles n_p by

$$\int W(\mathbf{x},\mathbf{v},t)\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{v}=n_p. \qquad (2.3)$$

Application of the grid filtering process to Eq. (2.1) gives

$$\widetilde{S}_i=-\frac{m_p}{\rho\tau_p}\int(\widetilde{u_iW}-v_i\widetilde{W})\mathrm{d}\mathbf{v}, \qquad (2.4)$$

for which equations are needed for $\widetilde{u_iW}$ and $\widetilde{W}$. Applying the grid filter to (2.2), gives

$$\frac{\partial}{\partial t}\widetilde{W}(\mathbf{x},\mathbf{v},t)+\frac{\partial}{\partial x_i}[v_i\widetilde{W}]+\frac{\partial}{\partial v_i}[\beta_v(\tilde{u}_i-v_i)\widetilde{W}] = -\frac{\partial}{\partial v_i}[\beta_v(\widetilde{u_iW}-\tilde{u}_i\widetilde{W})], \qquad (2.5)$$

which poses closure problem due to the unknown term $\widetilde{u_iW}$ appearing on its right-hand side. The term $(\widetilde{u_iW}-\tilde{u}_i\widetilde{W})$ is of the order of $\widetilde{u_i'W}$ where $u_i'=u_i-\tilde{u}_i$ represents the subgrid scale velocity fluctuations. A similar type of closure problem arising in the ensemble averaged (denoted by $\langle\rangle$) of (2.2) due to $\langle u_iW\rangle-\langle u_i\rangle\langle W\rangle$ was solved by Reeks [12], using Kraichnan's Lagrangian history direct interaction (LHDI). The expression derived by Reeks is

$$\beta_v(\langle u_iW\rangle-\langle u_i\rangle\langle W\rangle)=-\left[\frac{\partial}{\partial x_k}\lambda_{ki}+\frac{\partial}{\partial v_k}\mu_{ki}-\gamma_i\right]\langle W\rangle, \qquad (2.6)$$

where the tensors λ_{ki}, μ_{ki}, and γ_i are given by

$$\lambda_{ki}=\beta_v^2\int_0^t \mathrm{d}t_1[\langle u_i(\mathbf{x},t)u_j(\mathbf{x},\mathbf{v},t|t_1)\rangle-\langle u_i(\mathbf{x},t)\rangle \times\langle u_j(\mathbf{x},\mathbf{v},t|t_1)\rangle]G_{jk}(\mathbf{x}_1,t_1;\mathbf{x},t), \qquad (2.7)$$

$$\mu_{ki}=\beta_v^2\int_0^t \mathrm{d}t_1[\langle u_i(\mathbf{x},t)u_j(\mathbf{x},\mathbf{v},t|t_1)\rangle-\langle u_i(\mathbf{x},t)\rangle \times\langle u_j(\mathbf{x},\mathbf{v},t|t_1)\rangle]\frac{\mathrm{d}}{\mathrm{d}t}G_{jk}(\mathbf{x}_1,t_1;\mathbf{x},t), \qquad (2.8)$$

$$\gamma_i=\beta_v^2\int_0^t \mathrm{d}t_1\left[\left\langle\frac{\partial u_i(\mathbf{x},t)}{\partial x_k}u_j(\mathbf{x},\mathbf{v},t|t_1)\right\rangle \frac{\partial\langle u_i(\mathbf{x},t)\rangle}{\partial x_k}\langle u_j(\mathbf{x},\mathbf{v},t|t_1)\rangle\right]G_{jk}(\mathbf{x}_1,t_1;\mathbf{x},t). \qquad (2.9)$$

Here $u_j(\mathbf{x},\mathbf{v},t|t_1)$ is velocity of fluid in the vicinity of the particle at time t_1 which had (or will have) a velocity $\mathbf{v}$ at position $\mathbf{x}$ at time t. The Green's function $G_{jk}(\mathbf{x}_1,t_1;\mathbf{X},t)$ is defined by the following functional derivative (denoted by $\delta()/\delta()$) of X_k [14]:

$$G_{jk}(\mathbf{x}_1,t_1;\mathbf{X},t)=\frac{\delta X_k(t)}{\beta_v\delta\{u_j(\mathbf{x}_1,t_1)-\langle u_j(\mathbf{x}_1,t_1)\rangle\}\mathrm{d}t_1}. \qquad (2.10)$$

The usual procedure in LES of fluid phase is to assume the model for subgrid scale stress having a form which is similar to a model for Reynolds stress. Adopting this procedure for particle phase also and using (2.6), we propose an analogous expression for $\beta_v[\widetilde{u_iW}-\tilde{u}_i\widetilde{W}]$, written as

$$\beta_v[\widetilde{u_iW}-\tilde{u}_i\widetilde{W}]=-\left[\frac{\partial}{\partial x_k}\lambda'_{ki}+\frac{\partial}{\partial v_k}\mu'_{ki}-\gamma'_i\right]\widetilde{W}, \qquad (2.11)$$

where the tensors λ'_{ki}, μ'_{ki}, and λ'_i are

$$\lambda'_{ki}=\beta_v^2\int_0^t \mathrm{d}t_1\tau\big(u_i(\mathbf{x},t),u_j(\mathbf{x},\mathbf{v},t|t_1)\big)G'_{jk}(\mathbf{x}_1,t_1;\mathbf{x},t), \qquad (2.12)$$

$$\mu'_{ki}=\beta_v^2\int_0^t \mathrm{d}t_1\tau\big(u_i(\mathbf{x},t),u_j(\mathbf{x},\mathbf{v},t|t_1)\big)\frac{\mathrm{d}}{\mathrm{d}t}G'_{jk}(\mathbf{x}_1,t_1;\mathbf{x},t), \qquad (2.13)$$

$$\gamma'_i=\beta_v^2\int_0^t \mathrm{d}t_1\tau\left(\frac{\partial u_i(\mathbf{x},t)}{\partial x_k},u_j(\mathbf{x},\mathbf{v},t|t_1)\right)G'_{jk}(\mathbf{x}_1,t_1;\mathbf{x},t). \qquad (2.14)$$

Here for any variables A and B

$$\tau(A,B)=\widetilde{AB}-\widetilde{A}\widetilde{B} \qquad (2.15)$$

and the correlations of the form $\tau(b_i(\mathbf{x},t),b_j(\mathbf{x},\mathbf{v},t|t_1))$, which appear in (2.12)–(2.14), can be approximated by usual exponential function with Lagrangian integral time scale $T_{b_ib_j}$, written as

$$\tau\big(b_i(\mathbf{x},t),b_j(\mathbf{x},\mathbf{v},t|t_1)\big)=\tau\big(b_i(\mathbf{x},t),b_j(\mathbf{x},t)\big)\mathrm{e}^{(t_1-t)/T_{b_ib_j}}. \qquad (2.16)$$

The Green's function $G'_{jk}(\mathbf{x}_1,t_1;\mathbf{X},t)$ is defined as

$$G'_{jk}(\mathbf{x}_1,t_1;\mathbf{X},t)=\frac{\delta X_k(t)}{\beta_v\delta\{u_j(\mathbf{x}_1,t_1)-\tilde{u}_j(\mathbf{x}_1,t_1)\}\mathrm{d}t_1} \qquad (2.17)$$

and is governed by

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}G'_{jk}(\mathbf{x}_1,t_1;\mathbf{x},t)+\beta_v\frac{\mathrm{d}}{\mathrm{d}t}G'_{jk}-\beta_vG'_{ji}\frac{\partial\tilde{u}_k}{\partial x_i}=\delta_{jk}\delta(t-t_1). \qquad (2.18)$$

Substituting for $\widetilde{u_iW}$ from (2.11) into (2.4) and after integration we obtain

$$\widetilde{S}_i=-\frac{m_p}{\rho\tau_p}\widetilde{N}(\tilde{u}_i-\widetilde{v}_i)+\frac{m_p}{\rho}\left[\frac{\partial}{\partial x_k}(\lambda'_{ki}\widetilde{N})-\gamma'_i\widetilde{N}\right] \qquad (2.19)$$

where

$$\widetilde{N}=\int\widetilde{W}(\mathbf{x},\mathbf{v},t)\mathrm{d}\mathbf{v},\quad \widetilde{v}_i=\frac{1}{\widetilde{N}}\int v_i\widetilde{W}(\mathbf{x},\mathbf{v},t)\mathrm{d}\mathbf{v}, \qquad (2.20)$$

for which equations can be obtained by taking moments of the filtered Eq. (2.5) after substituting for $\widetilde{u_i W}$ from (2.11). These equations are

$$\frac{\partial \widetilde{N}}{\partial t} + \frac{\partial}{\partial x_i}[\tilde{v}_i \widetilde{N}] = 0, \tag{2.21}$$

and

$$\frac{\partial \tilde{v}_j}{\partial t} + \tilde{v}_i \frac{\partial \tilde{v}_j}{\partial x_i} = -\frac{1}{\widetilde{N}}\frac{\partial}{\partial x_i}[(\widetilde{v_i v_j} - \tilde{v}_i\tilde{v}_j)\widetilde{N}] + \beta_v(\tilde{u}_j - \tilde{v}_j) - \lambda'_{kj}\frac{\partial \ln \widetilde{N}}{\partial x_k} - \frac{\partial \lambda'_{kj}}{\partial x_k} + \gamma'_j, \tag{2.22}$$

where

$$\widetilde{v_i v_j} = \frac{1}{\widetilde{N}}\int v_i v_j \widetilde{W}(\mathbf{x}, \mathbf{v}, t)\mathrm{d}\mathbf{v} \tag{2.23}$$

and is governed by

$$\frac{\partial}{\partial t}[\widetilde{N}\widetilde{v_i v_j}] + \frac{\partial}{\partial x_n}\left[\int v_i v_j v_n \widetilde{W}\mathrm{d}\mathbf{v}\right] = \beta_v \widetilde{N}(\tilde{v}_i\tilde{u}_j + \tilde{v}_j\tilde{u}_i - 2\tilde{v}_i\tilde{v}_j) + \widetilde{N}(\mu'_{ij} + \mu'_{ji} + \gamma'_i\tilde{v}_j + \gamma'_j\tilde{v}_i) - \frac{\partial}{\partial x_k}[\lambda'_{kj}\tilde{v}_i\widetilde{N}] - \frac{\partial}{\partial x_k}[\lambda'_{ki}\tilde{v}_j\widetilde{N}]. \tag{2.24}$$

If we now write an equation for $\int v_i v_j v_n \widetilde{W}\mathrm{d}\mathbf{v}$, it would contain the higher order term $\int v_i v_j v_n v_m \widetilde{W}\mathrm{d}\mathbf{v}$ posing closure problem and so on. We close the set of equations (2.21)–(2.24) by considering third-order correlations of particle velocity fluctuation over $\tilde{v}_i$, to be approximately equal to zero, that is

$$\int (v_i - \tilde{v}_i)(v_j - \tilde{v}_j)(v_n - \tilde{v}_n)\widetilde{W}(\mathbf{x}, \mathbf{v}, t)\mathrm{d}\mathbf{v} \simeq 0 \tag{2.25}$$

and thus

$$\int v_i v_j v_n \widetilde{W}\mathrm{d}\mathbf{v} \simeq \widetilde{N}[\tilde{v}_i\widetilde{v_j v_n} + \tilde{v}_j\widetilde{v_i v_n} + \tilde{v}_n\widetilde{v_i v_j} - 2\tilde{v}_i\tilde{v}_j\tilde{v}_n]. \tag{2.26}$$

Eqs. (2.21), (2.22), and (2.24) along with (2.26) are in the Eulerian framework and can be considered as the LES 'fluid' equations for the particle phase.

In the framework of dynamic localization model, we also need expression for $\widetilde{\widetilde{S}}_i$. Now, application of filter $\widetilde{\widetilde{G}}$ to (2.2) produces equation for $\widetilde{\widetilde{W}}$ with unknown terms $\widetilde{\widetilde{u_i W}}$. Following a procedure similar to that described above to obtain $\widetilde{u_i W}$ and equations for $\widetilde{N}$ and $\tilde{v}_i$, we can write

$$\beta_v\left[\widetilde{\widetilde{u_i W}} - \tilde{\tilde{u}}_i\widetilde{\widetilde{W}}\right] = -\left[\frac{\partial}{\partial x_k}\lambda''_{ki} + \frac{\partial}{\partial v_k}\mu''_{ki} - \gamma''_i\right]\widetilde{\widetilde{W}}, \tag{2.27}$$

where the tensors λ''_{ki}, μ''_{ki}, and λ''_i are

$$\lambda''_{ki} = \beta_v^2\int_0^t \mathrm{d}t_1 T\big(u_i(\mathbf{x}, t), u_j(\mathbf{x}, \mathbf{v}, t|t_1)\big)G''_{jk}(\mathbf{x}_1, t_1; \mathbf{x}, t), \tag{2.28}$$

$$\mu''_{ki} = \beta_v^2\int_0^t \mathrm{d}t_1 T\big(u_i(\mathbf{x}, t), u_j(\mathbf{x}, \mathbf{v}, t|t_1)\big)\frac{\mathrm{d}}{\mathrm{d}t}G''_{jk}(\mathbf{x}_1, t_1; \mathbf{x}, t), \tag{2.29}$$

$$\gamma''_i = \beta_v^2\int_0^t \mathrm{d}t_1 T\left(\frac{\partial u_i(\mathbf{x}, t)}{\partial x_k}, u_j(\mathbf{x}, \mathbf{v}, t|t_1)\right)G''_{jk}(\mathbf{x}_1, t_1; \mathbf{x}, t). \tag{2.30}$$

Here for any variables A and B

$$T(A, B) = \widetilde{\widetilde{AB}} - \tilde{\tilde{A}}\tilde{\tilde{B}}. \tag{2.31}$$

Green's function

$$G''_{jk}(\mathbf{x}_1, t_1; \mathbf{X}, t) = \frac{\delta X_k(t)}{\beta_v \delta\{u_j(\mathbf{x}_1, t_1) - \tilde{\tilde{u}}_j(\mathbf{x}_1, t_1)\}\mathrm{d}t_1}, \tag{2.32}$$

is governed by

$$\frac{\mathrm{d}^2}{\mathrm{d}t^2}G''_{jk}(\mathbf{x}_1, t_1; \mathbf{x}, t) + \beta_v\frac{\mathrm{d}}{\mathrm{d}t}G''_{jk} - \beta_v G''_{ji}\frac{\partial \tilde{\tilde{u}}_k}{\partial x_i} = \delta_{jk}\delta(t - t_1). \tag{2.33}$$

The expression for $\widetilde{\widetilde{S}}_i$ is

$$\widetilde{\widetilde{S}}_i = -\frac{m_\mathrm{p}}{\rho\tau_\mathrm{p}}\widetilde{\widetilde{N}}(\tilde{\tilde{u}}_i - \tilde{\tilde{v}}_i) + \frac{m_\mathrm{p}}{\rho}\left[\frac{\partial}{\partial x_k}\left(\lambda''_{ki}\widetilde{\widetilde{N}}\right) - \gamma''_i\widetilde{\widetilde{N}}\right] \tag{2.34}$$

and equations for

$$\widetilde{\widetilde{N}} = \int \widetilde{\widetilde{W}}(\mathbf{x}, \mathbf{v}, t)\mathrm{d}\mathbf{v}, \quad \tilde{\tilde{v}}_i = \frac{1}{\widetilde{\widetilde{N}}}\int v_i\widetilde{\widetilde{W}}(\mathbf{x}, \mathbf{v}, t)\mathrm{d}\mathbf{v},$$
$$\widetilde{\widetilde{v_i v_j}} = \frac{1}{\widetilde{\widetilde{N}}}\int v_i v_j\widetilde{\widetilde{W}}(\mathbf{x}, \mathbf{v}, t)\mathrm{d}\mathbf{v} \tag{2.35}$$

and

$$\int v_i v_j v_n\widetilde{\widetilde{W}}(\mathbf{x}, \mathbf{v}, t)\mathrm{d}\mathbf{v}, \tag{2.36}$$

have the forms similar to the Eqs. (2.21), (2.22), (2.24), and (2.26) and can be obtained by changing $\widetilde{\ }$, λ'_{ij}, μ'_{ij}, and γ'_i to $\widetilde{\widetilde{\ }}$, λ''_{ij}, μ''_{ij}, and γ''_i, respectively, in these equations.

3. Dynamic subgrid scale model for fluid

In this section, we use the framework of dynamic localization model [6] and derive the model for $\tau(u_i, u_j)$ which accounts for the effects of particles on the subgrid scale turbulent motion. The model for $\tau(u_i, u_j)$ is written as

$$\tau(u_i, u_j) - \frac{\delta_{ij}}{3}\tau(u_l, u_l) = -2C\Delta k^{1/2}\widetilde{S}_{ij}, \tag{3.1}$$

where $\widetilde{S}_{ij} = \frac{1}{2}[\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}]$ and $k = \frac{1}{2}\tau(u_l, u_l)$ is governed by

$$\frac{\partial k}{\partial t} + \frac{\partial}{\partial x_j}[\tilde{u}_j k] = -\frac{\partial}{\partial x_j}\left[\frac{1}{2}\tau(u_i, u_i, u_j) + \tau(p, u_j) - \nu\frac{\partial k}{\partial x_j}\right] - \tau(u_i, u_j)\widetilde{S}_{ij} - \nu\tau\left(\frac{\partial u_i}{\partial x_j}, \frac{\partial u_i}{\partial x_j}\right) + \tau(u_i, S_i). \tag{3.2}$$

Here, $\tau(f,g,h)$ for any variables f, g, and h is defined as [15]

$$\tau(f,g,h) = \widetilde{fgh} - \tilde{f}\tau(g,h) - \tilde{g}\tau(f,h) - \tilde{h}\tau(f,g) - \tilde{f}\tilde{g}\tilde{h}. \tag{3.3}$$

Also, $\tau(u_i, S_i)$ is source/sink term arising due to the presence of particles and is given by

$$\tau(u_i, S_i) = \widetilde{u_i S_i} - \tilde{u}_i \widetilde{S}_i, \tag{3.4}$$

where

$$\widetilde{u_i S_i} = -\frac{m_\mathrm{p}}{\rho\tau_\mathrm{p}} \int [\widetilde{u_i^2 W}(\mathbf{x},\mathbf{v},t) - v_i \widetilde{u_i W}(\mathbf{x},\mathbf{v},t)]\mathrm{d}\mathbf{v},$$
$$u_i^2 = u_i u_i \tag{3.5}$$

is written using the expression for S_i from (2.1). Using the definition of $\tau(f,g,h)$ from (3.3), $\widetilde{u_i^2 W}$ can be written as

$$\widetilde{u_i^2 W} = 2\tau(u_i, W)\tilde{u}_i + \tau(u_i,u_i)\widetilde{W} + \tilde{u}_i\tilde{u}_i\widetilde{W} + \tau(u_i,u_i,W). \tag{3.6}$$

The unknown term $\tau(u_i,u_i,W)$ is of the order of third-order correlation $\widetilde{u_i'^2 W'}$ with $W' = W - \widetilde{W}$. The correlation $\tau(u_i,u_i,W)$ is small in comparison to other second-order correlations in (3.6) and is not taken into account now onwards. Thus, from (2.11), (3.5), and (3.6)

$$\begin{aligned}\widetilde{u_i S_i} = &-\frac{m_\mathrm{p}\widetilde{N}}{\rho\tau_\mathrm{p}}\left[\tau(u_i,u_i) + \tilde{u}_i\tilde{u}_i - \tilde{u}_i\tilde{v}_i\right] \\ &-\frac{2m_\mathrm{p}}{\rho}\left[\tilde{u}_i\gamma_i'\widetilde{N} - \tilde{u}_i\frac{\partial}{\partial x_k}\lambda_{ki}'\widetilde{N}\right] \\ &-\frac{m_\mathrm{p}}{\rho}\left[\frac{\partial}{\partial x_k}\lambda_{ki}'\tilde{v}_i\widetilde{N} - \mu_{ii}'\widetilde{N} - \gamma_i'\tilde{v}_i\widetilde{N}\right].\end{aligned} \tag{3.7}$$

Introducing the models for different terms,

$$\frac{1}{2}\tau(u_i,u_i,u_j) + \tau(p,u_j) = -D\Delta k^{1/2}\frac{\partial k}{\partial x_j} \tag{3.8}$$

and

$$\epsilon_g = v\tau\left(\frac{\partial u_i}{\partial x_j},\frac{\partial u_i}{\partial x_j}\right) = C_*\frac{k^{3/2}}{\Delta}, \tag{3.9}$$

the modelled equation for k is

$$\frac{\partial k}{\partial t} + \frac{\partial}{\partial x_j}[\tilde{u}_j k] = \frac{\partial}{\partial x_j}\left[D\Delta k^{1/2}\frac{\partial k}{\partial x_j}\right] + \frac{\partial}{\partial x_j}\left[v\frac{\partial k}{\partial x_j}\right] - \tau(u_i,u_j)\widetilde{S}_{ij} - C_*\frac{k^{3/2}}{\Delta} + \tau(u_i,S_i). \tag{3.10}$$

Now we discuss the method to find the model coefficients C, D, and C_* appearing in (3.1), (3.8) and (3.9). Application of filter $\overline{\widetilde{G}}$ to (1.3) produces subgrid scale stress

$$T(u_i,u_j) = \overline{\widetilde{u_i u_j}} - \bar{\tilde{u}}_i\bar{\tilde{u}}_j, \tag{3.11}$$

which is modelled as [6]

$$T(u_i,u_j) - \frac{\delta_{ij}}{3}T(u_l,u_l) = -2C\overline{\Delta}K^{1/2}\overline{\widetilde{S}}_{ij}. \tag{3.12}$$

The coefficient C is assumed to be independent of filter width while writing (3.12). A recent work by Meneveau and Lund [16] suggests that the coefficient appearing in the dynamic Smagorinsky model is scale-dependent, which could also be the case for model coefficients C, D, and C_*. Here we do not consider the scale-dependency and take all the coefficients independent of filter width. Similar to (3.2), equation for $K = T(u_l,u_l)/2$ is written as

$$\begin{aligned}\frac{\partial K}{\partial t} + \frac{\partial}{\partial x_j}[\bar{\tilde{u}}_j K] = &-\frac{\partial}{\partial x_j}\left[\frac{1}{2}T(u_i,u_i,u_j) + T(p,u_j) - v\frac{\partial K}{\partial x_j}\right] \\ &- T(u_i,u_j)\overline{\widetilde{S}}_{ij} - vT\left(\frac{\partial u_i}{\partial x_j},\frac{\partial u_i}{\partial x_j}\right) + T(u_i,S_i).\end{aligned} \tag{3.13}$$

Here, for any variables f, g, and h

$$\begin{aligned}T(f,g,h) = &\overline{\widetilde{fgh}} - \bar{\tilde{f}}T(g,h) - \bar{\tilde{g}}T(f,h) \\ &- \bar{\tilde{h}}T(f,g) - \bar{\tilde{f}}\bar{\tilde{g}}\bar{\tilde{h}},\end{aligned} \tag{3.14}$$

$$T(u_i,S_i) = \overline{\widetilde{u_i S_i}} - \bar{\tilde{u}}_i\overline{\widetilde{S}}_i, \tag{3.15}$$

and

$$\overline{\widetilde{u_i S_i}} = -\frac{m_\mathrm{p}}{\rho\tau_\mathrm{p}}\int\left[\overline{\widetilde{u_i^2 W}}(\mathbf{x},\mathbf{v},t) - v_i\overline{\widetilde{u_i W}}(\mathbf{x},\mathbf{v},t)\right]\mathrm{d}\mathbf{v},$$
$$u_i^2 = u_i u_i. \tag{3.16}$$

Introducing the models for different terms,

$$\frac{1}{2}T(u_i,u_i,u_j) + T(p,u_j) = -D\overline{\Delta}K^{1/2}\frac{\partial K}{\partial x_j} \tag{3.17}$$

and

$$\epsilon_t = vT\left(\frac{\partial u_i}{\partial x_j},\frac{\partial u_i}{\partial x_j}\right) = C_*\frac{K^{3/2}}{\overline{\Delta}}, \tag{3.18}$$

the modelled equation for K can be written in the form

$$\begin{aligned}\frac{\partial K}{\partial t} + \frac{\partial}{\partial x_j}[\bar{\tilde{u}}_j K] = &\frac{\partial}{\partial x_j}\left[D\Delta K^{1/2}\frac{\partial K}{\partial x_j}\right] + \frac{\partial}{\partial x_j}\left[v\frac{\partial K}{\partial x_j}\right] \\ &- T(u_i,u_j)\overline{\widetilde{S}}_{ij} - C_*\frac{K^{3/2}}{\overline{\Delta}} + T(u_i,S_i).\end{aligned} \tag{3.19}$$

3.1. Determination of coefficient C

Eqs. (1.7) and (3.11) give the Germano identity

$$L_{ij} = T(u_i,u_j) - \bar{\tau}(u_i,u_j) = \overline{\tilde{u}_i\tilde{u}_j} - \bar{\tilde{u}}_i\bar{\tilde{u}}_j, \tag{3.20}$$

where $\overline{\tau}(u_i, u_j)$ is obtained by applying the filter $\overline{G}$ to τ. Now, from (3.1) and (3.12)

$$L_{ij} - \frac{\delta_{ij}}{3} L_{ll} = \alpha_{ij} C - \overline{C\beta}_{ij}, \tag{3.21}$$

where

$$\alpha_{ij} = -2\overline{\Delta} K^{1/2} \overline{\widetilde{S}}_{ij}, \quad \beta_{ij} = -2\Delta k^{1/2} \widetilde{S}_{ij}. \tag{3.22}$$

Ghosal et al. [6] have proposed a variational formulation which obtains C such that it minimizes integral $\mathscr{F}[C]$, over the entire flow domain $\mathbf{x}$, of the squares of the error

$$E_{ij}(\mathbf{x}) = L_{ij} - \frac{\delta_{ij}}{3} L_{ll} - \alpha_{ij} C + \overline{C\beta}_{ij}, \tag{3.23}$$

that is

$$\delta \mathscr{F} = 2 \int E_{ij}(\mathbf{x}) \delta E_{ij}(\mathbf{x}) \mathrm{d}\mathbf{x} = 0, \tag{3.24}$$

under the conditions when L_{ij}, α_{ij}, and β_{ij} are known. In general, L_{ij}, α_{ij}, and β_{ij} are not known prior to the calculations of $\tilde{u}_i$ and $\overline{\tilde{u}}_i$, and their values can be computed by using LES equations. In view of this, any change in C would cause a change in L_{ij}, α_{ij}, and β_{ij} as the governing equations for the velocity field $\tilde{u}_i$ and $\overline{\tilde{u}}_i$ depend on C. This dependency makes it difficult to solve the variational problem posed by (3.24) when $\tilde{u}_i$ and $\overline{\tilde{u}}_i$ are not known. Thus the solution given by Ghosal et al. [6] can be considered as a first approximation as it does not include the terms accounting for the dependency. Then the approximate equation obtained from (3.24) is [6]

$$\int \left[-\alpha_{ij} E_{ij} \delta C + E_{ij} \overline{\delta C \beta_{ij}} \right] \mathrm{d}\mathbf{x} = 0 \tag{3.25}$$

and for the condition $C \geqslant 0$ it gives

$$\begin{aligned} C(\mathbf{x}) = H^{-1} \Big[& \alpha_{ij}(\mathbf{x}) L_{ij}(\mathbf{x}) - \beta_{ij}(\mathbf{x}) \int L_{ij}(\mathbf{y}) \overline{G}(\mathbf{y}, \mathbf{x}) \mathrm{d}\mathbf{y} \\ & + \alpha_{ij}(\mathbf{x}) \int \beta_{ij}(\mathbf{y}) C(\mathbf{y}) \overline{G}(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y} \\ & + \beta_{ij}(\mathbf{x}) \int \alpha_{ij}(\mathbf{y}) C(\mathbf{y}) \overline{G}(\mathbf{y}, \mathbf{x}) \mathrm{d}\mathbf{y} \\ & - \beta_{ij}(\mathbf{x}) \int \mathrm{d}\mathbf{y} \Big\{ \beta_{ij}(\mathbf{y}) C(\mathbf{y}) \int \mathrm{d}\mathbf{z} \overline{G}(\mathbf{z}, \mathbf{y}) \overline{G}(\mathbf{z}, \mathbf{x}) \Big\} \Big], \end{aligned} \tag{3.26}$$

with $H = \alpha_{ij}(\mathbf{x}) \alpha_{ij}(\mathbf{x})$ and $C(\mathbf{x}) = 0$ when (3.26) gives negative values for C. While writing (3.26), condition of incompressibility is used.

3.2. Determination of coefficient D

Applying filter $\overline{G}$ to (3.8) and then subtracting from (3.17), we obtain

$$\begin{aligned} & D\overline{\Delta} K^{1/2} \frac{\partial K}{\partial x_j} - \overline{D\Delta k^{1/2} \frac{\partial k}{\partial x_j}} \\ & = \overline{\overline{\tilde{u}}_j \left(\tilde{p} + k + \frac{\tilde{u}_i \tilde{u}_i}{2} \right)} - \overline{\tilde{u}_j \left(\tilde{p} + k + \frac{\tilde{u}_i \tilde{u}_i}{2} \right)} \\ & \quad - \overline{\tilde{u}_i \tau(u_i, u_j)} + \overline{\tilde{u}}_i [L_{ij} + \overline{\tau}(u_i, u_j)] \equiv L_j. \end{aligned} \tag{3.27}$$

To obtain D, the integral

$$\begin{aligned} \mathscr{D}[D] = \int & \left[L_j - D\overline{\Delta} K^{1/2} \frac{\partial K}{\partial x_j} + \overline{D\Delta k^{1/2} \frac{\partial k}{\partial x_j}} \right] \\ & \times \left[L_j - D\overline{\Delta} K^{1/2} \frac{\partial K}{\partial x_j} + \overline{D\Delta k^{1/2} \frac{\partial k}{\partial x_j}} \right] \mathrm{d}\mathbf{y}, \end{aligned} \tag{3.28}$$

is to be minimized. A δD change in D would also cause changes in K, k, and L_j. Neglecting these changes, an approximate solution for D with the constraint $D \geqslant 0$ can be written as

$$\begin{aligned} D(\mathbf{x}) = J^{-1} \Big[& \alpha_j(\mathbf{x}) L_j(\mathbf{x}) - \beta_j(\mathbf{x}) \int L_j(\mathbf{y}) \overline{G}(\mathbf{y}, \mathbf{x}) \mathrm{d}\mathbf{y} \\ & + \alpha_j(\mathbf{x}) \int \beta_j(\mathbf{y}) D(\mathbf{y}) \overline{G}(\mathbf{x}, \mathbf{y}) \mathrm{d}\mathbf{y} \\ & + \beta_j(\mathbf{x}) \int \alpha_j(\mathbf{y}) D(\mathbf{y}) \overline{G}(\mathbf{y}, \mathbf{x}) \mathrm{d}\mathbf{y} \\ & - \beta_j(\mathbf{x}) \int \mathrm{d}\mathbf{y} \Big\{ \beta_j(\mathbf{y}) D(\mathbf{y}) \int \mathrm{d}\mathbf{z} \overline{G}(\mathbf{z}, \mathbf{y}) \overline{G}(\mathbf{z}, \mathbf{x}) \Big\} \Big] \end{aligned} \tag{3.29}$$

and $D = 0$ when (3.29) gives negative value for D. Here, $J = \alpha_l(\mathbf{x}) \alpha_l(\mathbf{x})$, $\alpha_j = \overline{\Delta} K^{1/2} \partial K / \partial x_j$, $\beta_j = \Delta k^{1/2} \partial k / \partial x_j$, and the result given by (3.29) is identical to that given by Ghosal et al. [6,17] with some difference in notations.

3.3. Determination of coefficient C_*

To determine C_* following the procedure given by Ghosal et al. [6], we obtain

$$\frac{C_* K^{3/2}}{\overline{\Delta}} - \frac{\overline{C_* k^{3/2}}}{\Delta} = \chi, \tag{3.30}$$

where

$$\begin{aligned} \chi = & -\frac{1}{2} \left[\frac{\partial L_{ii}}{\partial t} + \frac{\partial}{\partial x_j} (\overline{\tilde{u}}_j L_{ii}) \right] + \frac{1}{2} \frac{\partial}{\partial x_j} \left[\nu \frac{\partial L_{ii}}{\partial x_j} \right] \\ & - L_{ij} \overline{\widetilde{S}}_{ij} + \overline{\tau(u_i, u_j) \widetilde{S}_{ij}} - \overline{\tau}(u_i, u_j) \overline{\widetilde{S}}_{ij} \\ & + \frac{\partial}{\partial x_j} \left[\overline{\overline{\tilde{u}}_j \left(\tilde{p} + \frac{\tilde{u}_i \tilde{u}_i}{2} \right)} - \overline{\tilde{u}_j \left(\tilde{p} + \frac{\tilde{u}_i \tilde{u}_i}{2} \right)} \right. \\ & \left. + \overline{\tilde{u}}_i (L_{ij} + \overline{\tau}(u_i, u_j)) - \overline{\tilde{u}_i \tau(u_i, u_j)} \right] + \left[\overline{\tilde{u}_i \widetilde{S}_i} - \overline{\tilde{u}}_i \overline{\widetilde{S}}_i \right]. \end{aligned} \tag{3.31}$$

It should be noted that the last term in the square bracket on the right-hand side of (3.31) accounts for the effect of particles and appears explicitly in the determination of coefficient C_*. Whereas, the form of the expressions for C and D are identical to that obtained by Ghosal et al. [6,17]. And the effect of particles appears in coefficients C and D only through the modification of LES flow fields due to the presence of the source term S_i.

The variational problem of minimizing the integral

$$\mathscr{H}[C_*] = \int \left[\chi - \frac{C_* K^{3/2}}{\overline{\Delta}} + \frac{\overline{C_* k^{3/2}}}{\Delta}\right]^2 \mathbf{dy}, \tag{3.32}$$

gives an approximate solution for C_* when the changes in K, k, and χ due to the change δC_* in C_* are neglected. The approximate solution with constraint $C_* \geqslant 0$ can be written in the form

$$\begin{aligned} C_*(\mathbf{x}) = \frac{1}{\alpha(\mathbf{x})\alpha(\mathbf{x})} \Bigg[& \alpha(\mathbf{x})\chi(\mathbf{x}) - \beta(\mathbf{x}) \int \chi(\mathbf{y})\overline{G}(\mathbf{y},\mathbf{x})\mathbf{dy} \\ & + \alpha(\mathbf{x}) \int \beta(\mathbf{y}) C_*(\mathbf{y})\overline{G}(\mathbf{x},\mathbf{y})\mathbf{dy} \\ & + \beta(\mathbf{x}) \int \alpha(\mathbf{y}) C_*(\mathbf{y})\overline{G}(\mathbf{y},\mathbf{x})\mathbf{dy} \\ & - \beta(\mathbf{x}) \int \mathbf{dy} \left\{ \beta(\mathbf{y}) C_*(\mathbf{y}) \int \mathbf{dz}\overline{G}(\mathbf{z},\mathbf{y})\overline{G}(\mathbf{z},\mathbf{x}) \right\} \Bigg] \end{aligned} \tag{3.33}$$

and $C_* = 0$ when (3.33) gives negative value for C_*. Here $\alpha = K^{3/2}/\overline{\Delta}$ and $\beta = k^{3/2}/\Delta$.

4. Concluding remarks

The LES 'fluid' equations for particles have been derived which govern the large scale structure of particle phase concentration and velocity field arising due to the LES flow and subgrid scale field of fluid phase. The subgrid scales contributions in these equations appear through statistical properties of the form $\tau(u_i(\mathbf{x},t), u_j(\mathbf{x},\mathbf{v},t|t_1))$, $\tau(\partial u_i(\mathbf{x},t)/\partial x_k, u_j(\mathbf{x},\mathbf{v},t|t_1))$, $T(u_i(\mathbf{x},t), u_j(\mathbf{x},\mathbf{v},t|t_1))$, and $T(\partial u_i(\mathbf{x},t)/\partial x_k, u_j(\mathbf{x},\mathbf{v},t|t_1))$. The presence of particles influence the subgrid scale motions and their influence has been properly accounted for during the subgrid-scale stress modeling in the dynamic localization model framework. The variational method, due to Ghosal et al. [6], has been used to obtain model coefficients C, D, and C_* and it has been pointed out that the method gives approximate expressions due to the neglect of the dependency of various LES flow fields on these coefficients.

The main objective has been to propose a new approach of LES for two-phase flows where the particle phase can also be described by the 'fluid' equations. Further simplifications and reduction in the number of 'fluid' equations by deriving constitutive relations for $(\widetilde{v_i v_j} - \tilde{v}_i\tilde{v}_j)$ are possible. This remains as a part of future work on the detailed assessments of the present model equations.

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