A Lagrangian filtering approach for large-eddy simulation of particle-laden turbulence

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We develop a Lagrangian filtering approach for large-eddy simulation of particle-laden turbulence. A Lagrangian filter is introduced to extract large-scale motions from particle dynamics. Its second-order de-filtering approximation is made to construct a Lagrangian gradient SGS model for the fluid velocities seen by particles. We further propose the algebraic identities at different filter widths which can be used to dynamically determine the coefficient in the Lagrangian gradient SGS model. The preliminary numerical results validate the capability of the Lagrangian gradient SGS model and the dynamic scheme.

1. Introduction

Large-eddy simulation (LES) coupled with discrete particle dynamics (DPS) has been developed to numerically predict the interactions of particles and turbulence. In LES of turbulent flows, large-scale parts of velocity fields are numerically computed from Navier-Stokes equations and small-scale (or subgrid scale) ones are ignored, but their effects on large-scale parts are represented using a subgrid scale (SGS) velocity model. Meanwhile, particle dynamics is simulated using the large-scale velocity obtained from the LES of Navier-Stokes equations (Wang & Squires 1996; Armenio *et al.* 1999). Previous research has shown that the particle-pair and collision-related statistics are significantly affected by the SGS velocity fields (Yang *et al.* 2008; Fede & Simonin 2006; Jin *et al.* 2010*a*; Ray & Collins 2011). A new challenge for LES is how to represent the effects of SGS fluid velocity on particle dynamics.

We consider a simple case: particles suspended in isotropic turbulence, where the particle size is much smaller than the Kolmogorov length scales and the particle density is much larger than the surrounding fluids. In this case, the equations of motion for particles can be described as follows (Maxey 1987):

$$\frac{d\mathbf{Y}_p(t)}{dt} = \mathbf{V}_p(t), \tag{1.1}$$

$$\frac{d\mathbf{V}_p(t)}{dt} = \frac{\mathbf{u}[\mathbf{Y}_p(t), t] - \mathbf{V}_p(t)}{\tau_p}, \tag{1.2}$$

where $\mathbf{Y}_p(t)$ and $\mathbf{V}_p(t)$ are the particle location and velocity, respectively. τ_p is the particle response time. $\mathbf{u}[\mathbf{Y}_p(t), t]$ is the fluid velocity seen by the particle $(\mathbf{Y}_p(t), \mathbf{V}_p(t))$ at time t and $\mathbf{u}(\mathbf{x}, t)$ is the Eulerian velocity at location $\mathbf{x}$ and time t, which satisfy the Navier-Stokes equation.

Two problems immediately arise in the application of LES to particle dynamics. The first one is how to find an appropriate filter to extract large-scale motions of particles, since a spatial filter is only valid for the field variables (Pozorski & Apte 2009) and is not applied to any one-dimensional particle trajectory (curve). Deconvolution SGS models

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based on Eulerian filtering have been developed for different purposes (Kuerten & Vreman 2005; Shotorban & Mashayek 2005). The second problem is how to model small-scale parts of velocity fields to recover their effects on particle dynamics. This type of model is referred to as the SGS particle model. For example, Langevin equations (Pozorski & Apte 2009; Pope 1994) and stochastic Lagrangian equations have been introduced to mimic the small-scale fluid velocity (Fede *et al.* 2006; Jin *et al.* 2010*b*). Stochastic differential equations could improve LES predictions on single-particle statistics but have the limitation on pair-particle statistics. Pair-particle statistics are mainly determined by two-particle, two-time correlations, which are involved in the Lagrangian time scales. Conventional SGS models are based on energy balance equations so that they are able to predict the energy spectra, but they may not be able to accurately predict time scales (He *et al.* 2002), since the Lagrangian time scales cannot be determined by energy spectra alone (He *et al.* 2009). The Lagrangian time accuracy presents a new topic for LES of multiphase turbulent flows.

In this paper, we will develop the Lagrangian filter approach for particle dynamics coupled with LES. The new development is that a Lagrangian filter is introduced to particle trajectory, while the conventional spatial filter is applied to fluid velocity fields. This paper is organized as follows: In section 2, we will introduce a Lagrangian filter and develop a Lagrangian de-filtering model. It follows that we will develop a dynamic scheme for the de-filtering model. Section 3 will be used to present the numerical results. Finally, in section 4, we will give a summary and conclusion.

2. A Lagrangian filtering approach

2.1. *Lagrangian filtering*

A filtering operator must be introduced at first to derive the governing equations for large-scale motions. A spatial or temporal filter in the Eulerian frame has been defined to derive the governing equations for large-scale eddies from Navier-Stokes equations. However, neither a spatial nor a temporal filter in the Eulerian frame can be used to particle dynamics, since Eulerian spatial filter is only applied to field variables and Eulerian temporal one is applied only to time signals at a fixed point. A possible way to extract large-scale motions from particle dynamics is to perform local averaging along a particle trajectory in the Lagrangian frame.

We introduce the Lagrangian time filter for particle motions as follows:

$$\overline{\mathbf{Y}}_p(t) = \int_{\infty}^{t} G(\tau - t, \delta_t)\mathbf{Y}_p(\tau)d\tau, \tag{2.1}$$

$$\overline{\mathbf{V}}_p(t) = \int_{\infty}^{t} G(\tau - t, \delta_t)\mathbf{V}_p(\tau)d\tau. \tag{2.2}$$

Here $\mathbf{V}_p(t)$ and $\mathbf{Y}_p(t)$ are the particle velocity and location, respectively. They could be any other physical quantities related to particle motions. $G(t, \delta_t)$ is a Lagrangian filter function of filter width δ_t. The filter function has the general form of

$$G(t, \delta_t) \equiv \frac{1}{\delta_t} g(\frac{t}{\delta_t}), \tag{2.3}$$

and g satisfies

$$g(t) \geq 0, \int_{-\infty}^{0} g(t)dt = 1, g(0) = 1. \tag{2.4}$$

A Lagrangian time filter should be caustic in real time since a present state is only dependent on past events. Causality requires that the integral limit of the Lagrangian filter is ranged from the past to the present. The Lagrangian filter provides a mathematic tool to perform local averaging along a Lagrangian trajectory. In this case, particle dynamics can be used in combination with Eulerian filters for Navier-Stokes equations provided that their truncation errors are consistent.

2.2. *Lagrangian filtered equations of motion for particles*

We apply a Lagrangian filter to the equations of motion for particles, which generates the Lagrangian filtered equations for large-scale motions of particles

$$\frac{d\overline{\mathbf{Y}}_p(t)}{dt} = \overline{\mathbf{V}}_p(t), \tag{2.5}$$

$$\frac{d\overline{\mathbf{V}}_p(t)}{dt} = \frac{\overline{\mathbf{u}[\mathbf{Y}_p(t),t]} - \overline{\mathbf{V}}_p(t)}{\tau_p}. \tag{2.6}$$

In the filtered equations, the filtered velocities $\overline{\mathbf{V}}_p(t)$ and the filtered trajectories $\overline{\mathbf{Y}}_p(t)$ for particles are explicitly calculated. However, the filtered fluid velocities at the unfiltered trajectories, $\overline{\mathbf{u}[\mathbf{Y}_p(t),t]}$, are not available. To further clarify this problem, we recall

$$\overline{\mathbf{u}[\mathbf{Y}_p(t),t]} = \int_{-\infty}^{t} G(t-\tau,\delta_t)\mathbf{u}[\mathbf{Y}_p(\tau),\tau]d\tau, \tag{2.7}$$

$$\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t),t] = \int_{-\infty}^{t} G(t-\tau,\delta_t)\mathbf{u}[\overline{\mathbf{Y}}_p(\tau),\tau]d\tau. \tag{2.8}$$

It is easy to find

$$\overline{\mathbf{u}[\mathbf{Y}_p(t),t]} \neq \overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t),t]. \tag{2.9}$$

This closure problem is central to LES of particle-laden turbulence. It comes from the nonlinearity where the fluid velocity seen by particles and particle location are not the linear function of time t in general. Another difficult problem is that the chaotic motions of particles induce the divergence of particle trajectories $\mathbf{Y}_p(t)$ and $\overline{\mathbf{Y}}_p(t)$.

2.3. *A Lagrangian gradient SGS model*

A Lagrangian filtering generates the filtered fluid velocity seen by particles, which is given by

$$\overline{\mathbf{u}[\mathbf{Y}_p(t),t]} = \overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t),t] + \mathbf{u}_p^{'}, \tag{2.10}$$

where $\mathbf{u}_p^{'}$ is the unresolved fluid velocity along the particle trajectory. The unresolved fluid velocity $\mathbf{u}_p^{'}$ can be reconstructed using the defiltering method. In the following, we will use the defiltering method to construct a second-order approximation with the specific Lagrangian filtering function $g(t) = \exp(t)$ or $G(t,\delta_t) = \exp(t/\delta_t)/\delta_t$.

We use the Taylor series expansion for $\overline{\mathbf{u}[\mathbf{Y}_p(t),t]}$ and $\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t),t]$,

$$\overline{\mathbf{u}[\mathbf{Y}_p(t),t]} = \mathbf{u}[\mathbf{Y}_p(t),t] + a_1\left(\nabla_{\mathbf{Y}_p}\mathbf{u}[\mathbf{Y}_p,t]\frac{\partial \mathbf{Y}_p(t)}{\partial t} + \frac{\partial \mathbf{u}(\mathbf{Y}_p,t)}{\partial t}\right)\delta_t + o(\delta_t^2), \tag{2.11}$$

$$\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t),t] = \mathbf{u}[\mathbf{Y}_p(t),t] + a_1\left(2\nabla_{\mathbf{Y}_p}\mathbf{u}[\mathbf{Y}_p,t]\frac{\partial \mathbf{Y}_p(t)}{\partial t} + \frac{\partial \mathbf{u}(\mathbf{Y}_p,t)}{\partial t}\right)\delta_t + o(\delta_t^2). \tag{2.12}$$

The difference between the above two equations leads to

$$\overline{\mathbf{u}[\mathbf{Y}_p(t),t]} - \overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t),t] = -a_1\mathbf{V}_p(t)\nabla_{\mathbf{Y}_p}\mathbf{u}[\mathbf{Y}_p,t]\delta_t + o(\delta_t^2). \tag{2.13}$$

It is easy to show

$$\mathbf{V}_p(t)\nabla_{\mathbf{Y}_p}\mathbf{u}[\mathbf{Y}_p, t] = \overline{\mathbf{V}}_p(t)\nabla_{\overline{\mathbf{Y}}_p}\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p, t] + o(\delta_t), \tag{2.14}$$

which generates the following expression

$$\overline{\mathbf{u}[\mathbf{Y}_p(t), t]} - \overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t), t] = -a_1\delta_t\overline{\mathbf{V}}_p(t)\nabla_{\overline{\mathbf{Y}}_p}\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p, t] + o(\delta_t^2). \tag{2.15}$$

Therefore, we propose a Lagrangian gradient SGS model

$$\overline{\mathbf{u}[\mathbf{Y}_p(t), t]} = \overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t), t] + C\delta_t\overline{\mathbf{V}}_p(t)\nabla_{\overline{\mathbf{Y}}_p}\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p, t]. \tag{2.16}$$

Here C is a constant which will be dynamically determined in the next subsection. Note that $\delta_t\overline{\mathbf{V}}_p(t)$ gives the length scale over which a particle travels and $\nabla_{\overline{\mathbf{Y}}_p}\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p, t]$ gives the gradient of fluid velocity along particle trajectory. Therefore, the gradient term provides the variation of fluid velocity along the particle trajectory at the characteristic time scale δ_t. It should be noted that the gradient SGS model (Eq. 2.16) is not a Galilean invariant. This drawback can be removed by using the Taylor series expansion around the filtered velocity, which gives

$$\overline{\mathbf{u}[\mathbf{Y}_p(t), t]} = \overline{\mathbf{u}}[\overline{\mathbf{Y}}_p(t), t] + C\delta_t\left(\overline{\mathbf{V}}_p(t) - \overline{\overline{\mathbf{V}}}_p(t)\right)\nabla_{\overline{\mathbf{Y}}_p}\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p, t]. \tag{2.17}$$

2.4. *A dynamic scheme for SGS particle motions*

In this subsection, we will propose an algebraic identity to determine the coefficient in the Lagrangian gradient SGS model. The proposed identity is given for the fluid velocity seen by particles at different filter widths

$$\overline{\overline{\mathbf{u}}(\overline{\mathbf{Y}}(t), t)} - \overline{\overline{\mathbf{u}}}(\overline{\overline{\mathbf{Y}}}(t), t) = \left(\overline{\overline{\mathbf{u}[\mathbf{Y}(t), t]}} - \overline{\overline{\mathbf{u}}}[\overline{\overline{\mathbf{Y}}}(t), t]\right) - \left(\overline{\overline{\mathbf{u}[\mathbf{Y}(t), t]}} - \overline{\overline{\mathbf{u}}[\overline{\mathbf{Y}}(t), t]}\right). \tag{2.18}$$

Here, the left-hand side is the resolved fluid velocity seen by particles, denoted by

$$\mathbf{L} \equiv \overline{\overline{\mathbf{u}}(\overline{\mathbf{Y}}(t), t)} - \overline{\overline{\mathbf{u}}}(\overline{\overline{\mathbf{Y}}}(t), t). \tag{2.19}$$

The first term on the right-hand side is the fluid velocity on the test grids and the second term on the right-hand side is the one on the filter grids. Using the Lagrangian gradient SGS model, we can represent the first and second terms on the right-hand side as follows:

$$\mathbf{u}_p{}'[\overline{\overline{\mathbf{Y}}}_p(t), t] \equiv \overline{\overline{\mathbf{u}[\mathbf{Y}_p(t), t]}} - \overline{\overline{\mathbf{u}}}[\overline{\overline{\mathbf{Y}}}_p(t), t] = C\overline{\overline{\delta}}_t\overline{\overline{\mathbf{V}}}_p(t)\nabla_{\overline{\overline{\mathbf{Y}}}_p}\overline{\overline{\mathbf{u}}}[\overline{\overline{\mathbf{Y}}}_p, t], \tag{2.20}$$

$$\overline{\mathbf{u}_p{}'[\overline{\mathbf{Y}}_p(t), t]} \equiv \overline{\overline{\mathbf{u}[\mathbf{Y}(t), t]}} - \overline{\overline{\mathbf{u}}[\overline{\mathbf{Y}}(t), t]} = C\overline{\delta}_t\overline{\overline{\mathbf{V}}_p(t)\nabla_{\overline{\mathbf{Y}}_p}\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p, t]}. \tag{2.21}$$

Their difference can be given by

$$\mathbf{M} \equiv \mathbf{u}_p{}'[\overline{\overline{\mathbf{Y}}}_p(t), t] - \overline{\mathbf{u}_p{}'[\overline{\mathbf{Y}}_p(t), t]} = C\left(\overline{\overline{\delta}}_t\overline{\overline{\mathbf{V}}}_p(t)\nabla_{\overline{\overline{\mathbf{Y}}}_p}\overline{\overline{\mathbf{u}}}[\overline{\overline{\mathbf{Y}}}_p, t] - \overline{\delta}_t\overline{\overline{\mathbf{V}}_p(t)\nabla_{\overline{\mathbf{Y}}_p}\overline{\mathbf{u}}[\overline{\mathbf{Y}}_p, t]}\right). \tag{2.22}$$

Here, both $\mathbf{M}$ and $\mathbf{L}$ can be obtained from the LES. The algebraic identity requires minimizing the residual $\epsilon = \|\mathbf{L} - C\mathbf{M}\|$. The least-mean-squares method is used to minimize ϵ, which gives

$$C = \frac{\langle \mathbf{ML} \rangle}{\langle \mathbf{MM} \rangle}. \tag{2.23}$$

The expression can be used to dynamically determine the coefficient in the Lagrangian gradient SGS model as the calculation progresses. Note that we can use $-C$ to replace C

in our derivation to obtain formulations consistent with the dynamic Smagorinsky SGS model.

The algebraic identity can be extended to a general form. We can further introduce a functional $\mathbf{Q}$ of fluid velocity $\mathbf{u}(\mathbf{Y}, t)$ and particle velocity $\mathbf{V}(t)$, such as $\mathbf{Q}(\mathbf{u}, \mathbf{v})$, and construct a family of algebraic identities

$$\overline{\mathbf{Q}(\overline{\mathbf{u}}, \overline{\mathbf{v}})} - \overline{\overline{\mathbf{Q}}}(\overline{\overline{\mathbf{u}}}, \overline{\overline{\mathbf{v}}}) = \{\overline{\mathbf{Q}(\overline{\mathbf{u}}, \overline{\mathbf{v}})} - \overline{\overline{\mathbf{Q}(\mathbf{u}, \mathbf{v})}}\} - \{\overline{\overline{\mathbf{Q}}}(\overline{\overline{\mathbf{u}}}, \overline{\overline{\mathbf{v}}}) - \overline{\overline{\mathbf{Q}(\mathbf{u}, \mathbf{v})}}\}. \tag{2.24}$$

The identity relates the fluid velocities with particle velocities at different scales. The choice of functional $\mathbf{Q}$ offers possibilities for the relationship between filtered fluid and particle velocities.

3. Numerical results

The direct numerical simulation (DNS) of isotropic turbulence is performed using a standard pseudospectral method on a periodic box of side length $L = 2\pi$, where the flow is driven and maintained by a random forcing. Aliasing errors are removed using the two-thirds truncation method. A second-order Adams-Bashforth method is used for time integration. The box is covered by 256^3 grids. The spatial resolution is monitored by the value of $k_{\max}\eta$, where k_{max} is the maximum wavenumber and η the Kolmogorov length scale. The typical value of $k_{\max}\eta$ is larger than the unit in the present simulation. The filtered DNS (FDNS) velocity field is obtained from the DNS velocity field by truncating the Fourier modes larger than the cutoff wavenumber k_{cf}, where k_{cf} is chosen so that the corresponding grids in the FDNS are 64^3. The FDNS can be regarded as an ideal LES to study the SGS particle models since the FDNS has no any error from the SGS velocity models. The Stokes number S_t is defined as the ratio of particle response time to flow Kolmogorov time.

Two statistical quantities will be used to evaluate the performance of the Lagrangian gradient SGS model in combination with the algebraic identity. The first one is the relative separation of particle pairs. The relative separation vector $\mathbf{R}$ of two particles at the locations $\mathbf{Y}_{p1}(t)$ and $\mathbf{Y}_{p2}(t)$) is defined by

$$\mathbf{R}(t) = \mathbf{Y}_{p1}(t) - \mathbf{Y}_{p2}(t). \tag{3.1}$$

Thus, its relative separation can be calculated from

$$R(t) = \sqrt{\mathbf{R}(t) \cdot \mathbf{R}(t)}. \tag{3.2}$$

The second one is the PDF difference given by

$$Pc = \sum_{i=0}^{N_c} \left[P_t(i) - P_0(i)\right]^2, \tag{3.3}$$

where $P_t(i)$ denotes the probability of finding the cells where the particle number is "i" at time t and N_C is the total particle number under consideration. The PDF difference defines the difference between an instantaneous and an initial PDF.

Figure 1 and Figure 2 compare the relative separations obtained from DNS with the ones obtained from FDNS in combination with those Lagrangian gradient SGS models. The various values of the coefficient C, such as $C = -2, -1, 1, 2$, are taken in order to study the capability of the proposed model. It is observed that the FDNS lines with the chosen coefficients shift around the FDNS line alone. The FDNS lines for negative coefficients are a better approximation to the DNS line than those for positive coefficients.

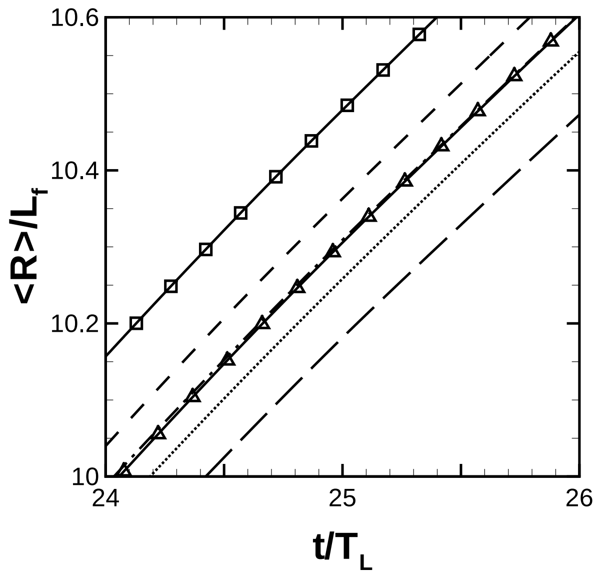

FIGURE 1. Means of relative separation distances of particle pairs for initial separation distance 0.25η and St=0.1. T_L is the Lagrangian integral time scale, L_f is the integral length scale, η denotes the Kolmogorov length scale. Solid line with squares, DNS; solid line with deltas, FDNS; dashed line, C=-2; dashdotted line, C=-1; dotted line, C=1; longdashed line, C=2.

The choice $C = -2$ yields the best results. This implies that the Lagrangian gradient SGS model is able to improve the LES prediction on particle dispersion. Two smaller initial separations are taken as $R(0) = \eta/4$ and $R(0) = 4\eta$. The Lagrangian gradient SGS model becomes effective at a later stage where the relative separations are comparable with resolved eddies in size.

Figure 3 and Figure 4 plot the temporal evolutions of the PDF differences obtained from DNS, FDNS and FDNS with the Lagrangian gradient SGS model. The coefficient in the SGS model is dynamically determined using the algebraic identity. Two Stokes numbers $St = 0.5$ and 1.0 are taken into account with the rescaled response time. The lines from FDNS with the SGS particle model are located between two lines from DNS and provide better approximation to the DNS lines than the FDNS ones. In this report, we only consider the case of the PDF difference. Further studies are needed to use the algebraic identity to dynamically search the coefficient in the Lagrangian gradient models for other statistical quantities.

4. Discussion and summary

We develop a Lagrangian filtering approach for LES of particle-laden turbulence. The Lagrangian filters can be used to extract large-scale motions from particle dynamics. A second-order de-filtering in terms of the Lagrangian filter is made to construct a Lagrangian gradient SGS model for the fluid velocity seen by particles. We further propose an algebraic identity to dynamically determine the coefficient in the Lagrangian gradient SGS model.

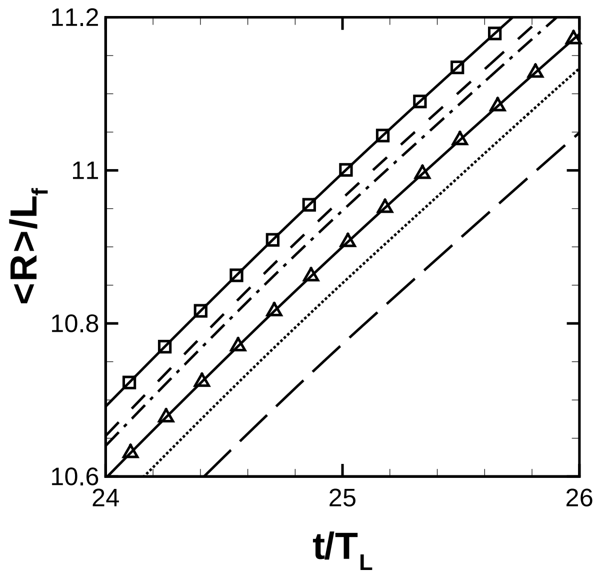

FIGURE 2. Means of relative separation distances of particle pairs for initial separation distance 4η and St=0.1. T_L is the Lagrangian integral time scale, L_f is the integral length scale, η denotes the Kolmogorov length scale. Solid line with squares, DNS; solid line with deltas, FDNS; dashed line, C=-2; dashdotted line, C=-1; dotted line, C=1; longdashed line, C=2.

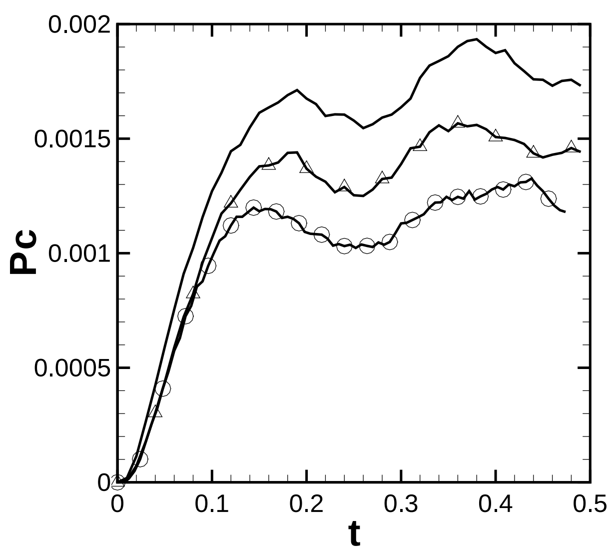

FIGURE 3. Temporal evolutions of the square of PDF differences at St=0.5. Solid line, DNS; solid line with circles, FDNS; solid line with deltas, the proposed dynamic model.

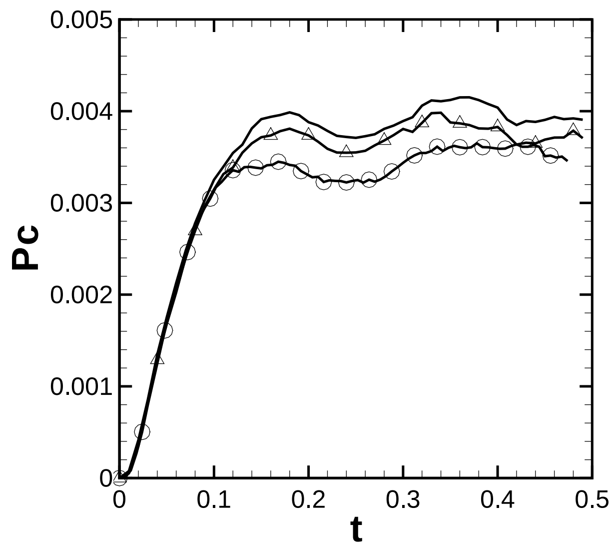

FIGURE 4. Temporal evolutions of the square of PDF differences at St=1.0. Solid line, DNS; solid line with circles, FDNS; solid line with deltas, the proposed dynamic model.

Elementary numerical evaluation on a dynamic Lagrangian gradient SGS model has been performed. Numerical simulations indicate that this model is able to improve LES prediction on relative dispersions, and the dynamic scheme based on the algebraic identity could select the unknown coefficient in the gradient model. Future work will be directed to (1) high-order Lagrangian de-filtering for chaotic trajectories of particles; (2) the algebraic identity for the fluid velocities seen by particles used to dynamically determine the free coefficients in the Lagrangian de-filtering models.

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