Grid-Averaged Lagrangian Equations of Dispersed Phase in Dilute Two-Phase Flow

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A set of grid-averaged Lagrangian transport equations of the dispersed-phase turbulence kinetic energy $\langle u_{pi}^{k'} u_{pi}^{k'} \rangle$ and the turbulence modulation quantity $\langle u_i' u_{pi}^{k'} \rangle$ is derived and demonstrated through a well-defined test problem of droplet-loading mixing layer. It is shown that accurate predictions of the turbulence kinetic energy of the droplets can be achieved by solving from this set of grid-averaged Lagrangian equations with significantly less computational droplets than those of a purely stochastic model. The information of the turbulence modulation quantity, which is solved from the grid-averaged Lagrangian transport equation of $\langle u_i' u_i^{k'} \rangle$, can also be used to evaluate accurately the source term accounting for the two-phase interaction in the turbulence kinetic energy k transport equation of the carrier fluid, which is important for determining the turbulence characteristics of the carrier fluid.

Nomenclature

 C_D = drag coefficient

 $C_{\varepsilon 3}$ = turbulence model constant; see Eq. (10)

 d_p = droplet diameter

g = gravity

K = history-force kernel k = turbulence kinetic energy

N = turbulence Kinetic energN = number flow rate

P, Q = values of probability density function

 Re_p = particle Reynolds number

 S_p , S_p = instantaneous and mean time source terms due to

turbulence-particle interactions, respectively

T = time

U, u = instantaneous and mean velocities, respectively

 $\langle u'_i u'_{pi} \rangle$ = turbulence modulation quantity

x, y = streamwise and transverse coordinates, respectively

 α_{12} = ratio of velocity slips in two neighboring grid cells

 Δt = time increment

 ε = turbulence energy dissipation rate

 μ = viscosity

 ρ , ρ_r = density and density ratio of dispersed phase

to carrier phase, respectively

 τ_L, τ_P = Lagrangian integral time and dynamic relaxation

time of particle, respectively

 Φ , ϕ = instantaneous and mean quantities of a dependent

variable, respectively

 $\phi(Re_n)$ = factor accounting for deviation from

the Stokesian drag

 Ω_p, ω_p = instantanceous and mean volumetric ratios occupied

by the dispersed phase, respectively

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Subscripts

i = i th component

in = inlet

k = turbulence kinetic energy old = value at the preceding time step

p = dispersed phase s = Stokesian drag

 ε = turbulence energy dissipation rate

Superscripts

k = kth discrete size

= fluctuation

value evaluated with mean quantities

I. Introduction

T WO-PHASE flows can be classified as being dilute or dense. Here the classification defined by Crowe et al. will be used as follows. A dilute flow is a flow in which the particle (or droplet, per se) motion is controlled by the surface and body forces on the particle. In a dense flow, the particle motion is controlled primarily by particle—particle collisions or interactions. In this study, attention is mainly addressed to dilute flows in which the particles are sufficiently dispersed so that particle—particle interactions are deemed negligible.

Two-phase flow models have developed along two parallel paths, that is, Eulerian (or two-fluid) and Eulerian-Lagrangian approaches, depending on the manner in which the dispersed phase is treated.¹⁻⁴ For the dilute two-phase flows, a prerequisite basis of "continuum" on the Eulerian formulation of the dispersed phase is always a stringent challenge for the two-fluid models. In contrast, the dispersedphase field is represented by particle trajectories obtained from integrating the particles motion equation in the Lagrangian models, which is a popular approach for the current simulation of the dilute two-phase flows in engineering practices. Theoretically, every particle in the flowfield has to be tracked in the Lagrangian models. A typical industrial spray, for example, requires tracking 10¹⁰ droplets with sizes of $\mathcal{O}(10^1)$ μ m per cubic meter of mixture, which is obviously well beyond current computer capability. Thus, Lagrangian models identify a parcel of particles as a single computational particle with the same properties as the physical particles. More discussion on the differences between these two formulation approaches for the dispersed phase may be found in Refs. 1–4.

Interactions between turbulence and particles are twofold. One is the turbulent dispersion of the particles, that is, the effects of turbulence on particles. The other is the modulation of the carrier-phase

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turbulence, that is, the effects of the presence of particles on the turbulence structure. An ideal model for two-phase turbulent flows would provide the complete (mean and fluctuating) properties of both the carrier and dispersed phases in the field. Particles dispersion in turbulence is commonly simulated using the stochastic method in which the carrier-phase turbulent field is represented by a random number generator.^{2,4,5} As mentioned in previous studies,^{6,7} there are two fatal defects in most existing stochastic Lagrangian models. One is the quasi-steady assumptions on the interfacial transport processes, such as the drag and heat transfer coefficients of the particle, due to the interaction between the Eulerian and Lagrangian frameworks coupled with the stochastic calculation procedure. The other is neglect of the inlet effects of the dispersed-phase fluctuating information, which was usually made in most existing studies. These two defects are further elaborated as follows.

The stochastic Lagrangian models adopt the stochastic operation, which deals with the Lagrangian equation of "instantaneous" motion for the ith component of velocity described as

$$\frac{\mathrm{d}U_{pi}^k}{\mathrm{d}t} = \frac{U_i - U_{pi}^k}{\tau_n^k} + g_i \tag{1}$$

where τ_p^k is the particle's dynamic relaxation time, which denotes the characteristic time of the particle with the kth discrete size reaching its dynamic equilibrium with the carrier fluid and is defined by

$$\tau_p^k = \frac{4d_p^k \rho_p}{3C_D^k \rho \left| U - U_p^k \right|} \tag{2}$$

The instantaneous velocity of the carrier fluid is determined from the sum of its mean u_i and fluctuating u_i' components, which is given by

$$U_i = u_i + u_i' \tag{3}$$

Note that the dispersed phase is usually split with a number of size groups in the modeling formulation to represent its spectral effect of the polydispersed size characteristic.

In contrast, the Eulerian framework is used to formulate the carrier-phase transport equations. To obtain the solutions of the Eulerian transport equations, the finite volume method, for example, is commonly used in numerical analysis. The basic idea of the discretization process is that the calculation domain is divided into a number of nonoverlapping control volumes (cells), each surrounding a grid node. Uniformly distributed flow properties are usually assumed inside the cell of a grid node. The u_i shown in Eq. (3) is obtained from the solution of its corresponding Reynolds averaged, Eulerian transport equation. Thus, as a particle passes through a grid cell to its neighboring one, it may encounter a remarkable step change in the instantaneous carrier-phase velocity at the interface of these two grid cells, which is caused by the discretization process and, mostly, by the different fluctuating carrier-phase velocities determined in the stochastic calculation procedure at the two neighboring grid cells. It was reported in previous work⁶ that an unsteady drag coefficient has to be used in the modeling formulation to obtain correct, complete information of the dispersed-phase turbulence characteristics including the mean and fluctuating quantities.

Equation (1) can be solved by computing the integrating form of this nonlinear ordinary differential equation to an acceptable tolerance in a given time step, that is,

$$U_{pi}^{k} = U_{i} - \left[U_{i} - \left(U_{pi}^{k}\right)_{\text{old}}\right] \exp\left(-\Delta t / \tau_{p}^{k}\right)$$

$$+ g_{i} \tau_{p}^{k} \left[1 - \exp\left(-\Delta t / \tau_{p}^{k}\right)\right]$$
(4)

where $(U_{pi}^k)_{\mathrm{old}}$ is the value of the instantaneous velocity of the particle at the beginning of the time increment Δt . Let us focus on the first time step as a particle leaves its inlet position. $(U_{pi}^k)_{\mathrm{old}}$ now becomes the inlet value of the particle, $(U_{pi}^k)_{\mathrm{in}}$. However, almost none of the past studies using the stochastic Lagrangian method consider the inlet condition of u'_{pi} in their calculations. Instead, only the mean quantity of particle velocity, determined either from the measured

data or the assumed inlet profile, was used in the calculations. Thus, Eq. (4) becomes

$$U_{pi}^{k} = U_{i} - \left[U_{i} - \left(u_{pi}^{k}\right)_{\text{in}}\right] \exp\left(-\Delta t / \tau_{p}^{k}\right)$$
$$+ g_{i} \tau_{p}^{k} \left[1 - \exp\left(-\Delta t / \tau_{p}^{k}\right)\right] \tag{5}$$

at the first integrating time step. Previous work⁷ showed that the neglect of the inlet u'_{pi} information in the calculations led to significant errors in the predictions of the dispersed-phase turbulence characteristics, particularly when the turbulence intensities of the particles are larger than those of the carrier fluid at the inlet.

A numerical solution procedure accounting for the inlet u'_{pi} information in the stochastic Lagrangian method was developed in previous work⁷ and is briefly described as follows. Without accounting for the inlet u'_{pi} information, the mean value of the particle velocity in a specified grid cell is determined by

$$u_{pi}^{k} = \frac{\sum_{m=1}^{M^{k}} n_{m}^{k} P_{i,m} \left(U_{pi}^{k}\right)_{m}}{\sum_{m=1}^{M^{k}} n_{m}^{k} P_{i,m}}$$
(6)

where P_i is the corresponding value of the probability density function (PDF) for a given u_i' in Eq. (3), which is sampled randomly in the stochastic calculation procedure, and M^k is the total number of the kth computational particles passing through the specified grid cell. The idea embedded in Eq. (6) is as follows. Because each U_{pi}^k is solved from Eqs. (1) and (3) with a randomly sampled u_i' , it is necessary to take into account the corresponding P_i of u_i' as a weighting factor in the ensemble averaging of U_{pi}^k . More information on the numerical solution procedure regarding Eq. (6) may be found in the paper of Chang and Wu. With the inlet u_{pi}' information taken into account in the calculation, the $(U_{pi}^k)_{\text{in}}$ is constructed by the mean quantity $(u_{pi}^k)_{\text{in}}$ and a randomly sampled $(u_{pi}^{k'})_{\text{in}}$. This computational particle, which is numbered as the lth particle issued from the inlet, is always associated with its corresponding PDF value to the $(u_{pi}^{k'})_{\text{in}}$ information, for example, $Q_{i,l}^k$, along its trajectory. With this new information of each computational particle, Eq. (6) has to be reformulated as

$$u_{pi}^{k} = \frac{\sum_{l=1}^{L^{k}} \sum_{m=1}^{M^{k}} \left(n_{l,m}^{k} Q_{i,l}^{k} \right) P_{i,m} \left(U_{pi}^{k} \right)_{m}}{\sum_{l=1}^{L^{k}} \sum_{m=1}^{M^{k}} \left(n_{l,m}^{k} Q_{i,l}^{k} \right) P_{i,m}}$$
(7)

Here L^k is the total number of the kth computational particles that are issued at the inlet.

Taking into consideration the unsteady drag coefficient and the inlet $u_{pi}^{k'}$ condition in the calculation, a correct, complete solution of the dispersed-phase turbulence characteristics including the turbulent dispersion of particles can be then achieved. However, the price to be paid is that a great number of $\mathcal{O}(10^4)$ of the computational particles for each discrete size is required in the calculation to obtain the statistically significant solution.⁷ This is cost ineffective for the two-phase turbulent flow simulation in engineering practices.

It is well-known that presence of particles in the flowfield leads to modulation (either suppression or enhancement) of the turbulence of the carrier fluid. Thus, the effect of the particles on the turbulence of the carrier phase is important in the development of turbulence models for two-phase flows. Elghobashi⁹ proposed a map of regimes of interactions between particles and fluid turbulence. For low values of dispersed-phase volume fraction ($\omega_p < 10^{-6}$), particles have negligible effects on turbulence. In the second regime, $10^{-6} < \omega_p < 10^{-3}$, the existence of particles can augment the turbulence if the ratio of particle response time to the turnover time of a large eddy is greater than unity, or attenuate the turbulence if the ratio is less than unity. This interaction is called two-way coupling. Flows in the two regimes discussed are often referred to as dilute cases. In the third regime, $\omega_p > 10^{-3}$, flows are referred to as dense cases in which particle-particle interactions become important. Elghobashi identifies this effect as four-way coupling. However, current investigation in a two-phase wall jet by Sato et al. 10 revealed that streamwise turbulence intensity was strongly suppressed by the addition of particles in the free shear-layer region, whereas transverse intensity was strongly suppressed in the fully developed region of both the free and wall shear regions. Such local behaviors of the turbulence modification cannot be described simply by the map proposed by Elghobashi.⁹

On the theoretical side, Yuan and Michaelides¹¹ proposed a simple mechanistic model based on wake shedding for turbulence generation. Clearly, this model does not account for the case of turbulence attenuation such as that observed in the experiment of Sato et al.10 Yarin and Hetsroni12 proposed a simplified theory based on the modified mixing-length theory and turbulent kinetic energy balance. However, their model only accounts for the production of turbulence due to velocity gradients in the carrier fluid and turbulent wakes behind the particles. Kenning and Crowe¹³ proposed a simple physical model on modulation of carrier-phase turbulence by taking into account turbulence generation and dissipation due to the addition of particles. Overall, the cited theoretical studies were made using phenomenological modeling rather than the rigorous formulation. Two-equation $k-\varepsilon$ turbulence models have been used over the past two decades as the basis of considerable research on turbulent flow calculation. A complete derivation of the transport equations for the turbulence kinetic energy k and its dissipation rate ε of the carrier phase in two-phase flows can be found in the work of Sato and Hishida.¹⁴ Their usual forms when applied to the dilute two-phase flows are summarized in the current review paper of Gouesbet and Berlemont⁵ and for brevity are not repeated here. Closure of the k equation requires specification of the source term s_{pk} , which accounts for the turbulence-particle interaction as

$$s_{pk} = \sum_{i=1}^{3} \left[\left\langle U_i S_{pu_i} \right\rangle - u_i s_{pu_i} \right] \tag{8}$$

where S_{pu_i} is the momentum source term due to the turbulence-particle interaction. (See the Appendix for its definition.) Equation (8) can be calculated directly along the particle trajectory in the stochastic solution process without introducing additional modeling for $\langle U_i S_{pu_i} \rangle$ (Refs. 15 and 16). In contrast to s_{pk} , the source term s_{pk} accounting for the turbulence-particle interaction, which is defined by

$$s_{p\varepsilon} = 2\nu \sum_{i=1}^{3} \sum_{i=1}^{3} \left\langle \frac{\partial u_i'}{\partial x_j} \frac{\partial s_{pu_i}'}{\partial x_j} \right\rangle \tag{9}$$

in the closure of the ε equation, must be modeled. Various models for $s_{p\varepsilon}$ may be found in the existing literature. ^{15–18} The usual way in modeling $s_{p\varepsilon}$ is parameterized analogously to that of the source term accounting for the single (carrier) phase, ^{15,16} that is,

$$s_{p\varepsilon} = C_{\varepsilon 3}(\varepsilon/k) s_{pk} \tag{10}$$

in which k/ε is a characteristic turbulence timescale. Note that Eq. (10) is an ad hoc parameterization of the effect of particles on ε . There is a wide range of values for $C_{\varepsilon 3}$ currently used in the $k-\varepsilon$ models of two-phase flows. The optimal value of 1.6 calibrated by Sato et al.¹⁰ with their laboratory experiments is adopted in the study. More intensive review on the turbulence modulation topic may be found in Ref. 1.

Clearly, accurate determination of s_{pk} in Eq. (8) depends on a correct simulation of the stochastic Lagrangian model for the particles. This implies that both the correct mean and fluctuating quantities of the dispersed-phase flow properties are required even in the calculation of the carrier-phase transport equations. As mentioned before, the consideration of the unsteady drag coefficient and the inlet $u_{pi}^{k'}$ condition in the theoretical analysis is necessary. Nevertheless, this results in a situation that the calculations incorporated with the stochastic Lagrangian models become cost ineffective.

It was found ⁷ that the need of such many computational particles in the stochastic calculation process is mainly due to an attainment of the statistically stationary solution of turbulence kinetic energy of the dispersed phase k_p , which is defined by ¹⁹

$$k_p = \frac{1}{2} \sum_{i=1}^{3} \langle u'_{pi} u'_{pi} \rangle \tag{11}$$

Different names for the quantity defined in Eq. (11) such as fluctuation energy,²⁰ turbulent fluctuating energy,²¹ and summation of three normal kinetic stresses²² of the dispersed phase, or even granular temperature for dense two-phase flow have been used in the existing literature. We prefer to call it the "turbulence kinetic energy of the dispersed phase" as used in the paper of Abou-Arab and $Roco^{19}$ because the definition of k_p is analogous to k for the carrier phase. Two Lagrangian transport equations of $\langle u'_{pi} u'_{pi} \rangle$ and $\langle u'_i u'_{pi} \rangle$ (the turbulence modulation quantity which is elaborated in detail in the Appendix) on the grid-averaged basis are developed in the work. A new solution procedure that mixes the stochastic Eulerian-Lagrangian method with these two grid-averaged Lagrangian transport equations is proposed mainly for computational efficiency. The new solution procedure is demonstrated through a well-defined twophase flow problem, that of a turbulent mixing-layer flow loaded with polydispersed droplets.

II. Test Problem and Model Formulation

Test Problem

The well-defined experiment of a droplet-loading, planar, mixinglayer flow in a vertical tunnel, 23-25 which provides relatively complete measured data available for the model verification, is selected as the test problem. Details of the test problem and experimental methods may be found in Refs. 24 and 25. Thus, only a brief description of the test problem is given here. The tunnel was divided into two separate flow paths by an upstream central splitting plate. The mean velocities of the high- and low-speed (air) streams were 10.2 and 2.36 m/s, respectively. A Sono-Tek ultrasonic nozzle, located 800 mm upstream of the test section in the high-speed stream, generated polydispersed (2–90- μ m) water droplets. The trailing edge of the splitting plate was extended 150 mm into the test section. The configuration of the test problem in which the droplets were issued at the far upstream (0.95-m) position resulted in $k > k_n$ at the inlet station (x = 5 mm) as shown in Fig. 1. A rectangular coordinate was selected such that the streamwise x coordinate is downward with the origin at the central separation point of the splitting plate and the transverse y coordinate is positive toward the high-speed-stream side.

Measurements of the mean and fluctuating flow properties of the streamwise and transverse components for both phases were made using a two-component phase Doppler particle analyzer (PDPA). Eight sets of data, except for $\langle u_i'u_{pi}'\rangle$, labeled with the mean droplet sizes of 10, 20, 30, 40, 50, 60, 70, and 80 μ m were recorded in the experiment. Only the data of $\langle u_i'u_{pi}'\rangle$ for the droplets with $d_p=10,20$, and 30 μ m were made in the work of Wang and Huang²⁵

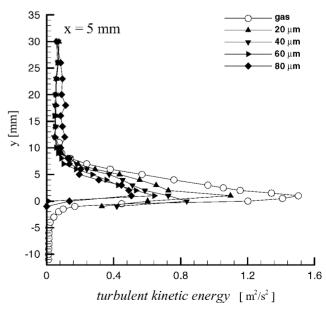


Fig. 1 Measured turbulence kinetic energy 23 of the carrier gas and the droplets with four discrete sizes at the inlet station.

because the number densities for the larger droplets, $d_p \ge 40~\mu m$ (Fig. 2 in Ref. 25), were relatively small and the raw data collected were not sufficient to make statistical quantities of $\langle u_i' u_{pi}' \rangle$ due to the limitation of the memory capacity of the PDPA. Complete measurements at the streamwise station of x = 5~mm were made for the inlet conditions required for the calculations.

Physical Modeling

The boundary-layer approximation, which neglects the diffusion terms along the streamwise direction, is made for the carrier phase in this test problem. The flowfield of the test problem, which is of the simple flow type, is determined using the $k-\varepsilon$ turbulence model. The applicability of the $k-\varepsilon$ model in the simulation of this test problem has been demonstrated by Chang et al.²⁴ Although the volumetric fractions occupied by the droplets, ω_p , are less than 10^{-5} , the effects of turbulence modulation are taken into account in the model formulation through Eqs. (A12) and (10). For details of the carrier-phase modeling, see Ref. 24.

The dispersed phase is treated by tracking individual droplets as they move through the turbulence field of the carrier phase. To account for the effect of the size spectrum, the dispersed phase is represented by eight discrete droplet sizes that conform to the data sets recorded in the experiment. For the case of a stationary droplet where there is a steady fluid flow before t=0 with an impulse at t=0 (i.e., the time when the droplet passes across the interface of a pair of neighboring grid cells), an expression for the unsteady drag coefficient, suggested by Chang and Yang, 6 is given by

$$C_D^k/(C_D)_s^k = (1-\alpha_{12}^k)K^k(t) + \phi^k(Re_p^k), \qquad t > 0$$
 (12)

with

$$Re_{p}^{k} = \rho \left| \mathbf{U} - \mathbf{U}_{p}^{k} \right| d_{p}^{k} / \mu \tag{13}$$

$$\alpha_{12}^{k} = \left| \boldsymbol{U} - \boldsymbol{U}_{p}^{k} \right|_{1} / \left| \boldsymbol{U} - \boldsymbol{U}_{p}^{k} \right|_{2} \tag{14}$$

where ρ and μ are the density and viscosity of the carrier fluid, respectively, and α_{12}^k is the ratio of the slip velocities at the interface

in between the upstream and downstream grid cells. The Stokesian drag coefficient is given by

$$(C_D)_s^k = 24/Re_p^k \tag{15}$$

The history-force kernel K(t) employed in the study of Chang and Yang⁶ was the empirical one developed by Mei and Adrian²⁶ for a stationary droplet subjected to an oscillating fluid:

$$K^{k}(t) = \left\{ \left[\frac{4\pi \mu}{\rho \left(d_{p}^{k} \right)^{2}} t \right]^{\frac{1}{4}} + \left(\frac{\pi \rho}{\mu d_{p}^{k}} \right)^{\frac{1}{2}} t \left[\frac{\left| U - U_{p}^{k} \right|}{f_{H} \left(Re_{p}^{k} \right)} \right]^{\frac{3}{2}} \right\}^{-2}$$
(16)

with

$$f_H(Re_p^k) = 0.75 + 0.105Re_p^k$$
 (17)

However, a more accurate representation of the dispersed-phase motion in the turbulent two-phase flow is freely moving, rather than stationary, droplets traveled in a fluctuating fluid. A history integral accounting for the acceleration/deceleration effects of a moving droplet in the grid cell, therefore, has to be considered in the physical modeling. Kim et al.²⁷ modified the history-force kernel by combining the history integral term in it, which makes its form much more complicated than that of Eq. (16). The study of Kim et al.²⁷ revealed that their history-force kernel can yield more accurate prediction of the unsteady C_D than the kernel expressed in Eq. (16) for the dispersed-phaseto carrier-phase density ratio ρ_r being small, whereas the performances of both the kernels, proposed by Kim et al.²⁷ and by Mei and Adrian,²⁶ differ slightly when ρ_r is as large as 200 (Fig. 5 in Ref. 27). Our preliminary study with the present test problem of $\rho_r \cong 900$ and $Re_p^k < \mathcal{O}(10)$ did corroborate the result reported by Kim et al.²⁷ for the case of very large ρ_r , that is, there was a very minor difference between the two unsteady C_D obtained separately with the use of the history-force kernels developed by Mie and Adrian²⁶ and by Kim et al.²⁷ Therefore, in view of the simpler kernel form and less computational effort required of Mie and Adrian²⁶ as compared to that of Kim et al.,²⁷ Eq. (16) is used in this work.

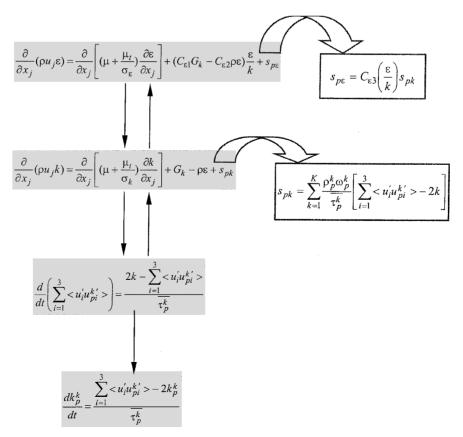


Fig. 2 Relationships among the transport equations of $k, \varepsilon, \langle u_i' u_{pi}^{k'} \rangle$, and k_p^k . (See Appendix H of Ref. 5 for definitions of G_k, μ_t, σ_k , and σ_{ε} .)

x = 40 mm

x = 80 mm

x = 100 mm

x = 20 mm

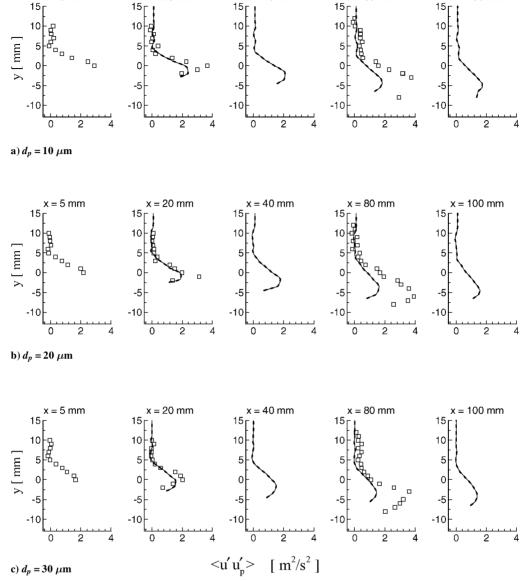


Fig. 3 Evolution of the two predicted (with unsteady and quasi-steady drag coefficients and with the transport equation of $\langle u_i' u_{pi}^{k'} \rangle$ and measured $\langle u' u_p' \rangle$ ($\pm 12\%$) of droplets of various sizes: \Box , measurements²⁵; ——, unsteady drag; and ——, steady drag.

The factor ϕ^k in Eq. (12) accounts for the deviation from the Stokosian drag coefficient at steady state when the condition of $Re_p^k \ll 1$ is not met. One of the best correlations for ϕ^k compiled by Clift et al.²⁸ is used:

$$\begin{aligned} \phi^{k} \left(Re_{p}^{k} \right) &= 1 + (3/16) Re_{p}^{k} & 0 < Re_{p}^{k} \le 0.01 \\ &= 1 + 0.1315 \left(Re_{p}^{k} \right)^{(0.82 - 0.02171} \ln e_{nRe_{p}^{k}} & 0.01 < Re_{p}^{k} \le 20 \\ &= 1 + 0.1935 \left(Re_{p}^{k} \right)^{0.6305} & 20 < Re_{p}^{k} \le 260 \end{aligned}$$

Equation (12) resumes the identical form of the steady-state one for $t\gg 1$ because $K^k(t)$ asymptotically approaches zero value at a sufficiently long time. For the special condition of $\alpha_{12}^k=0$ (starting from the dynamic equilibrium between two phases) and $Re_p^k\leq 1$, Sano's analytical solution,²⁹ which follows, takes over the expression of $C_D^k(t)$ because its performance is better than that in Eq. (12):

$$\frac{C_D^k(t_M^k)}{(C_D)_s^k} = 1 + \frac{3}{16} Re_p^k \left\{ \left[1 + \frac{16}{\left(Re_p^k t_M^k \right)^2} \right] \operatorname{erf} \left(\frac{1}{2} \sqrt{\frac{Re_p^k t_M^k}{2}} \right) \right\}$$

$$+2\sqrt{\frac{2}{\pi Re_p^k t_M^k}} \left(1 - \frac{4}{Re_p^k t_M^k}\right) \exp\left(1 - \frac{Re_p^k t_M^k}{8}\right)$$

$$+\frac{9}{160} \left(Re_p^k\right) \ln\left(\frac{1}{2} Re_p^k\right), \qquad t_M^k > 0$$

$$\tag{19}$$

with the dimensionless time of

$$t_M^k = 2 \left| U - U_p^k \right| \left(t / d_p^k \right) \tag{20}$$

Theoretically, both the correct mean and fluctuating solutions of the dispersed phase can be achieved by using the unsteady drag coefficient and considering the inlet u'_{pi} information provided that an adequate number of computational particles are used in the stochastic calculation process. However, mainly for the sake of computational efficiency at the present scope, two ensemble-averaged Lagrangian transport equations of $\langle u'_{pi} u'_{pi} \rangle$ and $\langle u'_i u'_{pi} \rangle$ are derived as follows:

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{1}{2} \left\langle u_{pi}^{k'} u_{pi}^{k'} \right\rangle \right] = \frac{\left\langle u_i' u_{pi}^{k'} \right\rangle - \left\langle u_{pi}^{k'} u_{pi}^{k'} \right\rangle}{\overline{\tau}_p^k} \tag{A4}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \langle u_i' u_{pi}^{k'} \rangle = \frac{\langle u_i' u_i' \rangle - \langle u_i' u_{pi}^{k'} \rangle}{\overline{\tau_p^k}} \tag{A7}$$

(Details of the derivation are shown in the Appendix.) The ensemble averaging of Eqs. (A4) and (A7) was made on the grid-cell basis, which conforms to the concept of the control volume method³⁰ used as the numerical method in this study. Nadaoka et al.³¹ applied the same ensemble-averaging operation for deriving their grid-averaged equation of motion, but they approximated the $\langle u_i^{k'} u_{pi}^{k'} \rangle$ and $\langle u_i' u_{pi}^{k'} \rangle$ variables using two algebraic relationships with $\langle u_i' u_i' \rangle$, which are different from our work. Obviously, the present work is more theoretically rigorous than that of Nodaoka et al.³¹

The relationships between the two-phase transport equations of k, ε , $\langle u_i'u_{pi}^{k'}\rangle$, and $\langle u_{pi}^{k'}u_{pi}^{k'}\rangle$ are summarized in Fig. 2. It is clearly understood that the $\langle u_i'u_{pi}^{k'}\rangle$ variable is a key quantity affecting k and ε of the carrier phase, which in turn modifies the eddy viscosity μ_t in the $k-\varepsilon$ turbulence model, as well as k_p^k of the dispersed phase. The $\langle u_i'u_{pi}^{k'}\rangle$ variable is, thus, named as the turbulence modulation quantity here. Solving the dispersed-phase flowfield directly from the grid-average dequation of motion (A2) is known as the deterministic separated flow (DSF) model, 4 and its defect, particularly in the

prediction of turbulence dispersion of particles, is well understood. And a Nadaoka et al. Proposed a reallocation process to overcome the defect which stemmed from the DSF model. Nevertheless, the probability distribution of the particle position in a grid cell, which is a key element in the reallocation process, was assumed by a rectangular cloud distribution function for lack of better information. In the present work, the dispersed-phase flowfield is solved from Eq. (1) with the stochastic method. Although the calculation using the stochastic method is more cost ineffective as compared to the one using the reallocation process proposed by Nadaoka et al., It can certainly avoid introducing unexpected errors into the flow-field solution at the present stage of validating the two grid-averaged Lagrangian transport equations for $\langle u_{pi}^{k'} u_{pi}^{k'} \rangle$ and $\langle u_i' u_{pi}^{k'} \rangle$, which are derived in this work.

Numerical Solution Procedure

The carrier-phase flowfield is calculated by the finite volume method using the SIMPLER algorithm and the power law scheme. The dispersed-phase equations are solved using the iterative integration as described for U_{pi}^k , that is, Eq. (4), in the preceding section. The source terms due to two-phase interactions for the transport equations of u_i , k, and ε are obtained using the particle-source-in-cdl

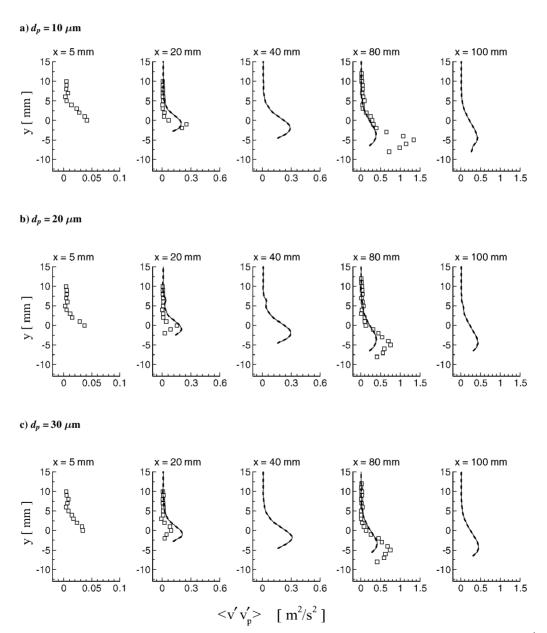


Fig. 4 Evolution of the two predicted (with unsteady and quasi-steady drag coefficients and with the transport equation of $\langle u'_i u^{k'}_{pi} \rangle$ and measured $\langle v'v'_n \rangle$ ($\pm 12\%$) of droplets of various sizes: \Box , measurements²⁵; —, unsteady drag; and ---, steady drag.

method.³² The new solution procedure coupling the stochastic approach for u_{pi} with the two grid-averaged Lagrangian equation for $\langle u_{pi}^{k'} u_{pi}^{k'} \rangle$ and $\langle u_i' u_{pi}^{k'} \rangle$ is summarized as follows:

- 1) Find u_{pi} at each grid cell by means of the stochastic solution procedure as described earlier at each iterate.
- 2) In accord with the revisited u_{pi} at each grid cell, solve $\langle u_{pi}^{k'} u_{pi}^{k'} \rangle$
- and $\langle u'_i u^{k'}_{pi} \rangle$ from Eqs. (A4) and (A7), respectively.

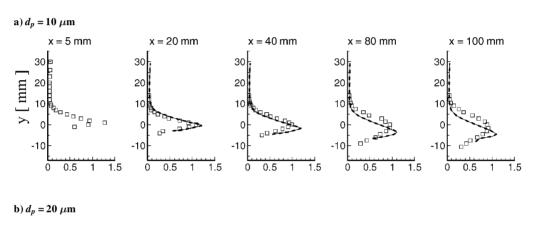
 3) Repeat steps 1 and 2 until all dependent variables converge. More information on the stochastic solution procedure may be found in Refs. 7 and 8.

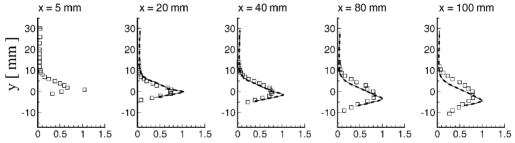
III. Results and Discussion

Together with the Lagrangian transport equation of $\langle u_i' u_{ni}^k \rangle$ [Eq. (A7)], the Lagrangian transport equation of $\langle u_{ni}^{k'} u_{ni}^{k'} \rangle$ [Eq. (A4)] can be solved without using the turbulence modulation model. Note that Eqs. (A4) and (A7) are first-order ordinary differential equations, which require the initial (inlet) conditions in the flowfield to obtain their solutions. The experimental work of Wang and Huang²⁵ provided the measured data of $\langle u'u_p^{k'}\rangle$ and $\langle v'v_p^{k'}\rangle$ for three small droplets with $d_p = 10, 20, \text{ and } 30 \,\mu\text{m}$ at the inlet station ($x = 5 \,\text{mm}$). As a result, only three droplet sizes of 10, 20, and 30 μ m can be

readily solved using Eq. (A7) in association with the measured inlet data. However, the test problem is a very dilute ($\omega_p < 10^{-5}$) twophase flow. A previous study on this test problem conducted by Chang et al.²⁴ revealed that the turbulence modulation effects on the predictions of the carrier-phase flow properties were insignificant. In view of this, only the dispersed-phase equations for these three droplet sizes are considered in the demonstration of the $\langle u'_i u^{k'}_{ni} \rangle$ and $\langle u_{ni}^{k'} \bar{u}_{ni}^{k'} \rangle$ solutions obtained from Eqs. (A4) and (A7) and with the measured inlet data.

The unsteady effect of the drag coefficient on the two-phase flow calculation was speculated to stem primarily from the stochastic process. In the stochastic solution procedure, the mean droplet velocity u_{pi} is calculated from the ensemble-averaging formula of Eq. (7), which accounts for the PDF values as the weighting factors. Previous studies^{6,7} revealed that the differences among the various U_{ni}^k , which correspond to the randomly generated U_i , are evened out in the determination of u_{pi} through the ensemble-averaging formula of Eq. (7). For the new solution procedure described in the subsection of the numerical solution procedure, it is anticipated that this unsteady effect should have little influence on the solution of the grid-averaged equations such as Eqs. (A4) and (A7) because they are independent of the stochastic process. To clarify this issue, two runs with the unsteady





c) $d_p = 30 \ \mu \text{m}$

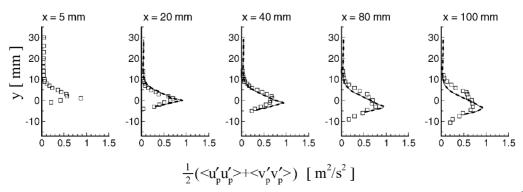


Fig. 5 Evolution of the two predicted (with unsteady and quasi-steady drag coefficients and with the transport equation of $\langle u'_i u^{k'}_{pi} \rangle$ and measured $(\langle u'_p u'_p \rangle + \langle v'_p v'_p \rangle)/2$ of droplets of various sizes: \Box , measurements²⁵; —, unsteady drag; and ---, steady drag.

and quasi-steady drag coefficients were made. Here the quasisteady drag coefficient is obtained from Eq. (12) by setting K(t) = 0. Equation (A7) requires the information of three individual components of $\langle u'_i u'_i \rangle$. A usual assumption for the boundarylayer-type flow, that is, $\langle u'^2 \rangle : \langle v'^2 \rangle : \langle w'^2 \rangle = 2:1:1$, is made for the carrier phase to provide the $\langle u'_i u'_i \rangle$ information required by Eq. (A7) from the k solution obtained with its corresponding transport equation of the carrier phase. Figures 3 and 4 present the evolution of $\langle u'u_p^{k'}\rangle$ and $\langle v'v_p^{k'}\rangle$, respectively, of the droplets with $d_p = 10$, 20, and 30 μ m predicted with the unsteady and quasi-steady drag coefficients in comparison with the measured data of Wang and Huang.25 Note that the measured data of Wang and Huang were available at three streamwise stations (x = 5, 20, and 80 mm) only. Similar comparison for the partial turbulence kinetic energy, $(\langle u_n^{k'} u_n^{k'} \rangle + \langle v_n^{k'} v_n^{k'} \rangle)/2$, is made in Fig. 5. It can be seen that both the predictions using unsteady and quasisteady drag coefficients are almost the same when solved from the grid-averaged Lagrangian transport equations, as anticipated. Agreement between the predicted and measured partial turbulence kinetic energy is generally good. Note that 2500 computational droplets for each discrete size is used in the stochastic calculation process of u_{pi} , whereas only 300 computational droplets for each

discrete size is used for the solution of the grid-averaged Lagrangian equations of Eqs. (A4) and (A7) in the two cases presented in Figs. 3–5. In contrast, a significantly greater number, $\mathcal{O}(10^4)$, of computational droplets for each discrete size was required to obtain correct and statistically stationary prediction of the partial turbulence kinetic energy in the flowfield, as concluded in our previous study.⁷

Remarkable deviations between the predicted and measured $\langle u_i'u_{pi}^{k'}\rangle$ are observed in the shear layer regions (around y=0 and moving to the low-speed-stream side, that is, y<0, in the downstream regions), particularly in the downstream station of x=80 mm. As noted before, theoretical solution of Eq. (A7) requires input of the measured data at the streamwise station of x=5 mm as the initial condition. Accuracy of the $\langle u_{pi}^{k'}u_{pi}^{k'}\rangle$ solution obtained from Eq. (A4) is heavily dependent on the accuracy of the $\langle u_i'u_{pi}^{k'}\rangle$ solution of Eq. (A7). The comparison made for the partial turbulence kinetic energy in Fig. 5 has revealed that the $\langle u_i'u_{pi}^{k'}\rangle$ solution of Eq. (A4) must be correct. Otherwise, the $\langle u_{pi}^{k}u_{pi}^{k'}\rangle$ solution of Eq. (A7), which is incorporated with the $\langle u_i'u_{pi}^{k'}\rangle$ information solved directly from Eq. (A4), would not agree well with the measured $\langle u_{pi}^{k'}u_{pi}^{k'}\rangle$ data as shown in Fig. 5. It is worthwhile to recheck the experimental method for the $\langle u_i'u_{pi}^{k'}\rangle$ data used by Wang and Huang. In view of the measurement process of the PDPA

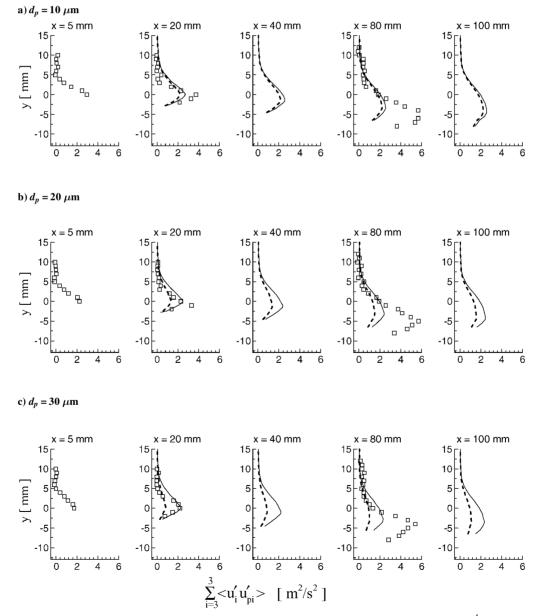


Fig. 6 Evolution of the two predicted [with unsteady and quasi-steady drag coefficients and with the $\langle u'_i u^{k'}_{pi} \rangle$ model of Eq. (22)] and measured $\sum_{i=1}^{3} \langle u'_i u'_{pi} \rangle$ of droplets of various sizes: \square , measurements²⁵; —, unsteady drag; and ---, steady drag.

instrument, $\langle u_i' u_{pi}^{k'} \rangle$ is determined, under a steady-state flow condition for any t, by

$$\left\langle u_i' u_{pi}^{k'} \right\rangle = \lim_{\Delta t \to 0} \left\langle u_i'(t) u_{pi}^{k'}(t + \Delta t) \right\rangle \tag{21}$$

The curve of $\langle u_i'(t)u_{pi}^{k'}(t+\Delta t)\rangle$ (Fig. 4 in Ref. 25) resembles the shape of Frenkiel function, that is, $\langle u_i'u_{pi}^{k'}\rangle\cos(\Delta t/\tau)\exp(-\Delta t/\tau)$, where τ is a Lagrangian timescale. Thus, the $\langle u_i'u_{pi}^{k'}\rangle$ data have to be interpolated from the value at $\Delta t=0$. It was reported²⁵ that maximum errors of 12% were caused by their interpolation scheme in estimating $\langle u_i'u_{pi}^{k'}\rangle$ data. However, their error analysis was made mainly on the data in the freestreamregions, where higher data rates, that is, small Δt in Eq. (17), were achieved in the experiment. In the shear-layer regions to which the droplets immigrate from the high-speed-streamside, the data rates were low and Δt became relatively large. It is then speculated that significant errors could be induced in the evaluation process of Eq. (21) for the data located in the shear layer regions when using the interpolation scheme employed in the work of Wang and Huang. ²⁵

Very few experimental data of $\langle u_i'u_{pi}^{k'}\rangle$ can be found in the literature. Prevost et al.³³ performed the measurements using a phase Doppler anemometer in the far field of a polydispersed

particle-laden tube jet. However, the thorough measured data that could be used as the inlet conditions were made in a single, last downstream axial station (x/D=30) in their test configuration. Therefore, the case investigated by Prevost et al.³³ cannot help demonstrate the application of the two grid-averaged Lagrangian transport equations for $\langle u^k_{pi} u^{k'}_{pi} \rangle$ and $\langle u^i_i u^k_{pi} \rangle$ derived in this work for the simulation of two-phase turbulence.

In contrast to the rigorous formulation of $\langle u_i' u_{pi}^{k'} \rangle$ transport equation proposed, several models for $\langle u_i' u_{pi}^{k'} \rangle$ may be found in the literature.^{34–38} Only the model suggested by Chang et al.,³⁶ which was modified from the one originally developed by Pourahmadi and Humphrey,³⁴ is discussed here for demonstration. It is given by

$$\sum_{i=1}^{3} \left\langle u_i' u_{pi}^{k'} \right\rangle = (k + k_p) \left(\frac{\tau_L}{\overline{\tau_p^k} + \tau_L} \right) \tag{22}$$

where the Lagrangian timescale is estimated by $\tau_L = 0.41k/\varepsilon$. Chang et al.³⁶ showed that their modified $\langle u'_i u^{k'}_{p_i} \rangle$ models perform better than its predecessor developed by Paurahmadi and Humphrey,³⁴ in particular for the two-phase flow with the condition of $k_p > k$. Using the model of Eq. (22) requires information

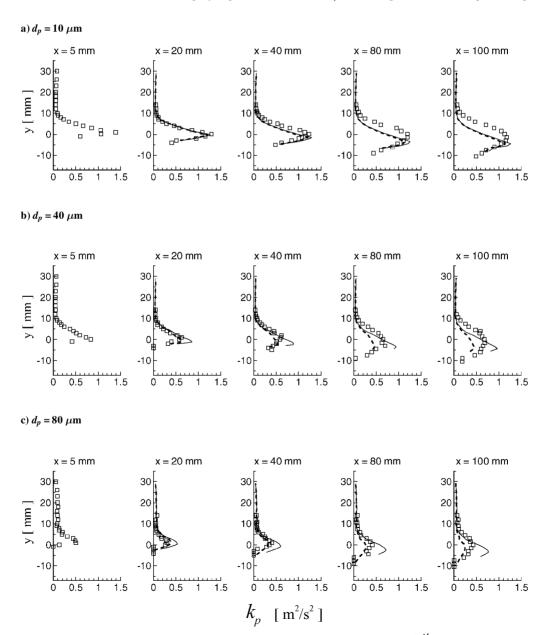


Fig. 7 Evolution of the two predicted [with unsteady and quasi-steady drag coefficients and with the $\langle u'_i u^{k'}_{pi} \rangle$ model of Eq. (22)] and measured k^k_p of droplets of various sizes: \square , measurements²⁵; ——, unsteady drag; and –––, steady drag.

of three components of $\langle u_i'u_{pi}^{k'}\rangle$ and $\langle u_{pi}^{k'}u_{pi}^{k'}\rangle$, whereas the experimental work^{23,25} provided only two-component data. Without better information, the usual assumption of equal distribution made for the two nonpredominant, that is, transverse and spanwise, components of turbulence intensity in a boundary-layer-type flow is extended to the measured data of $\langle u_i'u_{pi}^{k'}\rangle$ and $\langle u_{pi}^{k'}u_{pi}^{k'}\rangle$. Figure 6 presents the evolution of

$$\sum_{i=1}^{3} \left\langle u_i' u_{pi}^{k'} \right\rangle$$

of the droplets with $d_p=10$, 20, and 30 μ m predicted with Eq. (22) and using either the unsteady or quasi-steady drag coefficient in comparison with the measured data. Note that the two predictions with the unsteady and quasi-steady drag coefficients differ and that their deviations become more significant as the droplet size increases. This is because the employed $\langle u'_i u^{k'}_{pi} \rangle$ model includes explicitly the τ^k_p parameter, which is inversely proportional to C^k_D [see Eq. (2)]. As discussed in the study of Chang and Yang, 6 the unsteady effect on C_D becomes stronger for larger droplets, which is consistent with the trend shown in Fig. 6. It is also observed from Fig. 6 that the measured $\langle u'_i u^{k'}_{pi} \rangle$ data of Wang and Huang 25 in the shear layer of the downstream station of x=80 mm are higher than the predicted ones.

Although all measured k_p^k data for the eight discrete droplet sizes used in the simulation are available, only results with $d_p=10$, 40, and 80 μ m, representing small, medium, and large droplets, respectively, are reported here for brevity. Two predicted evolutions of k_p^k with the unsteady and quasi-steady drag coefficients are presented in Fig. 7 and are compared with the measured data.²³ Clearly, the differences in the two predicted $\langle u_i'u_{pi}^{k'}\rangle$, which were obtained by using either the unsteady or quasi-steady drag coefficient in the calculation, are reflected in the k_p^k predictions. Neither performance using the $\langle u_i'u_{pi}^{k'}\rangle$ model of Eq. (22) with the unsteady or quasi-steady drag coefficient is satisfactory as compared with that of the measured data except for the cases of very small droplet sizes such as $d_p=10~\mu\text{m}$. Note that the $\langle u_i'u_{pi}^{k'}\rangle$ model of Chang et al.³⁶ was developed based on the quasi-steady drag coefficient. The poor performance caused by using the $\langle u_i'u_{pi}^{k'}\rangle$ model, as presented in Fig. 7, corroborates a need of the two derived, grid-averaged Lagrangian transport equations for $\langle u_{pi}^{k'}u_{pi}^{k'}\rangle$ and $\langle u_i'u_{pi}^{k'}\rangle$ in the model formulation.

Because the investigated test problem is a very dilute ($\omega_p < 10^{-5}$) case and with small $Re_p^k[<\mathcal{O}(10)]$, that is, close to dynamic equilibrium between two phases, and the s_{pk} and $s_{p\varepsilon}$ terms are directly proportional to ω_p (Fig. 2), it is hard to evaluate the effects of the modulation quantity $\langle u_i^{\prime} u_{ni}^{k^{\prime}} \rangle$ on the carrier-phase turbulence characteristics. A similar conclusion was also made in a previous simulation of this test problem.²⁴ However, in a very recent experimental investigation,³⁹ around 4% of direct rates of dissipation of turbulence by particles was observed as well as a turbulence generation rate sufficient to yield relative turbulence intensities in the range 0.2–5.0% in a monodispersed two-phase flow with $Re_p = 106$ –990 and $\omega_p \simeq 3 \times 10^{-5}$. This reveals that evaluation of s_{pk} and $s_{p\varepsilon}$ accurately in the model of a dilute two-phase flow merits further investigation. The derived grid-averaged Lagrangian equation for $\langle u'_i u^k_{ni} \rangle$ can at least meet one of the requirements, that is, providing accurate evaluation of s_{pk} in the calculation.

IV. Conclusions

A set of the grid-averaged Lagrangian transport equations is derived to obtain the dispersed-phase turbulence kinetic energy, which is an important property for describing the turbulent dispersion ability of particles, accurately and economically, in the calculation. The information of the turbulence modulation quantity solved from the grid-averaged Lagrangian equation of $\langle u'_i u^{k'}_{pi} \rangle$ is not only important in the solution of k_p^k from the grid-averaged Lagrangian equation of $\langle u^k_{pi} u^{k'}_{pi} \rangle$ but also important in accurate evaluation of the source term s_{pk} , accounting for the turbulence-particle interaction for the k equation of the carrier fluid. To avoid additional errors in the determination of the mean flowfield for the dispersed phase, the

stochastic Lagrangian method, which is widely used in the simulation of two-phase turbulent flows, is used in the present work. Using a well-defined test problem of the droplet-loading mixing layer, it is demonstrated that accurate prediction of k_p^k can be achieved by using approximately one-fourth of the computational droplets as usually required in the purely stochastic models, together with another $\mathcal{O}(10^2)$ computational droplets for the grid-averaged Lagrangian transport equations for $\langle u_p^k u_p^k u_p^k u_p^k \rangle$ and $\langle u_p^l u_p^k u_p^k u_p^k u_p^k u_p^k \rangle$. The computational expenditure can be further reduced by solving these two grid-averaged Lagrangian transport equations with the grid-averaged equation of motion, provided that available and reliable information of the PDF of the particle position dispersion can be attained. This part of work remains to be studied further. There is an urgent need for experimental information of $\langle u_p^l u_p$

Appendix: Equation Derivation

When using the stochastic Lagragnian method, it is theoretically necessary to track all particles in the flowfield. Thus, there are usually many trajectories passing through a grid cell. The ensemble averaging for a dispersed-phase flow property $\boldsymbol{\Phi}$ in a grid cell is defined by

$$\langle \Phi
angle = \sum_{m=1}^M \Phi_m \bigg/ M = \phi, \qquad \quad \Phi = \phi + \phi'$$

When the ensemble-averaging process is used for Eq. (1), it yields

$$\frac{\mathrm{d}u_{pi}^k}{\mathrm{d}t} = \left\langle \frac{U_i - U_{pi}^k}{\tau_p^k} \right\rangle + g_i$$

Note that $C_D|U-U_p^k|$, which appeared in the denominator of the definition for τ_p^k [Eq. (2)], is usually a weak nonlinear function of Re_p , which, by its definition, is proportional to $|U-U_p^k|$ for $Re_p \leq \mathcal{O}(10)$. The value of $|U-U_p|$ in a grid cell is determined by three randomly selected u_i' in the stochastic calculation process. An approximation can be reasonably made for the following ensemble-averaging operation of

$$\left\langle \Phi \left[\left(U_i - U_{pi}^k \right) / \tau_p^k \right] \right\rangle \simeq \left\langle \Phi \left(U_i - U_{pi}^k \right) \right\rangle / \overline{\tau_p^k}$$
 (A1)

in which $\overline{\tau_p^k}$ is the value evaluated with the ensemble-averaged quantities of u_i and u_{pi}^k and Φ is a two-phase flow property or unity. With the approximation of Eq. (A1), the ensemble-averaged form of the equation of motion is now expressed by

$$\frac{\mathrm{d}u_{pi}^k}{\mathrm{d}t} = \frac{u_i - u_{pi}^k}{\overline{\tau_p^k}} + g_i \tag{A2}$$

Multiplying Eq. (1) by U_{ni}^k yields

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{2} U_{pi}^{k} U_{pi}^{k} \right) = \frac{U_{i} U_{pi}^{k} - U_{pi}^{k} U_{pi}^{k}}{\tau_{p}^{k}} + U_{pi}^{k} g_{i}$$

Note that the repeated index is not taken as the summation operator here. After decomposing the instantaneous quantities into mean and fluctuating components and taking an ensemble-averaging operation over a grid cell, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{2} u_{pi}^{k} u_{pi}^{k} \right) + \frac{\mathrm{d}}{\mathrm{d}t} \left(\frac{1}{2} \left\langle u_{pi}^{k'} u_{pi}^{k'} \right\rangle \right)$$

$$= \frac{\left[u_{i} u_{pi}^{k} + \left\langle u_{i}^{\prime} u_{pi}^{k'} \right\rangle - u_{pi}^{k} u_{pi}^{k} - \left\langle u_{pi}^{k'} u_{pi}^{k'} \right\rangle \right]}{\overline{\tau_{p}^{k}}} + u_{pi}^{k} g_{i} \tag{A3}$$

Multiplying Eq. (A2) by u_{pi}^k and subtracting it from Eq. (A3) yields the Lagrangian transport equation of the *i*th component of the turbulence kinetic energy of the dispersed phase:

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[\frac{1}{2} \langle u_{pi}^{k'} u_{pi}^{k'} \rangle \right] = \frac{\langle u_i' u_{pi}^{k'} \rangle - \langle u_{pi}^{k'} u_{pi}^{k'} \rangle}{\overline{\tau_p^k}} \tag{A4}$$

There appears one more unknown correlation term $\langle u_i u_{pi}^k \rangle$, which is named the fluid-particle velocity correlation in the two-fluid closure model of Simonin et al.,²² as well as of Hyland and Reeks.⁴⁰ Multiplying Eq. (1) by U_i yields

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(U_i U_{pi}^k \right) - U_{pi}^k \frac{\mathrm{d}U_i}{\mathrm{d}t} = \frac{U_i U_i - U_i U_{pi}^k}{\tau_n^k} + U_i g_i \tag{A5}$$

Note that $\mathrm{d}U_i/\mathrm{d}t$ shown in Eq. (A5) based on the Lagrangian framework is essentially equivalent to $\mathrm{D}U_i/\mathrm{D}t$ (where $\mathrm{D}/\mathrm{D}t$ is a substantial derivative) in the Eulerian framework. With the assumption of the steady-state condition and with the usual assumption of uniform distribution of the carrier-phase flow properties inside a grid cell made for the control volume method,

$$\frac{\mathrm{D}U_i}{\mathrm{D}t} = \Delta U_i \delta(t)$$

where ΔU_i is the velocity difference of the carrier fluid between the upstream and present grid cells and $\delta(t)$ is the Dirac delta function. For t>0 (having entered the present grid cell), $\mathrm{D}U_i/\mathrm{D}t=0$ and the second term shown on the left-hand-side of Eq. (A5) disappear. After decomposing the instantaneous quantities into mean and fluctuating components and taking an ensemble-averaging operation over a grid cell for Eq. (A5), it becomes (for t>0)

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(u_{i}u_{pi}^{k}\right) + \frac{\mathrm{d}}{\mathrm{d}t}\left\langle u_{i}u_{pi}^{k'}\right\rangle = \frac{\left\lfloor u_{i}u_{i} + \left\langle u_{i}'u_{i}'\right\rangle - u_{i}u_{pi}^{k} - \left\langle u_{i}'u_{pi}^{k'}\right\rangle\right\rfloor}{\overline{\tau_{p}^{k}}} + u_{i}g_{i}$$

Multiplying Eq. (A2) by u_i and subtracting it from Eq. (A6) yield the Lagrangian transport equation of $\langle u'_i u^k_{ni} \rangle$ as

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[\left\langle u_i' u_{pi}^{k'} \right\rangle \right] = \frac{\left\langle u_i' u_i' \right\rangle - \left\langle u_i' u_{pi}^{k'} \right\rangle}{\overline{\tau_p^k}} \tag{A7}$$

Note that an argument of $Du_i/Dt = \Delta u_i \delta(t)$ as made earlier has been applied to the derivation of Eq. (A7).

Taking the summation of the three components for Eqs. (A4) and (A7) and introducing the definitions of

$$k\left(=\sum_{i=1}^{3}\langle u_{i}'u_{i}'\rangle\middle/2\right)$$

and k_p [see Eq. (11)] yield the following two equations:

$$\frac{\mathrm{d}}{\mathrm{d}t}k_p^k = \left(\sum_{i=1}^3 \left\langle u_i' u_p^{k'} \right\rangle - 2k_p^k \right) / \overline{\tau_p^k} \tag{A8}$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(\sum_{i=1}^{3} \left\langle u_{i}^{i} u_{pi}^{k^{i}} \right\rangle \right) = \left(2k - \sum_{i=1}^{3} \left\langle u_{i}^{i} u_{pi}^{k^{i}} \right\rangle \right) / \overline{\tau_{p}^{k}} \tag{A9}$$

The source term accounting for the turbulence-particle interaction, which is shown in the U_i momentum equation, S_{pu_i} , under the dilute condition can be expressed by (see Appendix H in Ref. 5)

$$S_{pu_i} = -\sum_{k=1}^{K} \rho_p \Omega_p^k \left(\frac{\mathrm{d}U_{pi}^k}{\mathrm{d}t} - g_i \right)$$

Introducing the relationship of Eq. (1) modifies the preceding equation into

$$S_{pu_i} = -\sum_{k=1}^K \rho_p \Omega_p^k \left(\frac{U_i - U_{pi}^k}{\tau_p^k} \right) \tag{A10}$$

Taking the ensemble-averaging operation for Eq. (A10) and neglecting the correlation terms including $\omega_p^{k'}$ due to the consideration of the dilute two-phase flow⁴¹ here, we obtain

$$s_{pui} = -\sum_{k=1}^{K} \rho_p \omega_p^k \left(\frac{u_i - u_{pi}^k}{\overline{\tau_p^k}} \right) \tag{A11}$$

Substituting Eqs. (A10) and (A11) into Eq. (8) and neglecting all of the correlation terms including $\omega_p^{k'}$, we obtain

$$s_{pk} = -\sum_{k=1}^{K} \frac{\rho_p \omega_p^k}{\overline{\tau_p^k}} \left(2k - \sum_{i=1}^{3} \left\langle u_i' u_{pi}^{k'} \right\rangle \right) \tag{A12}$$

It is clearly seen that the $\langle u'_i u^{k'}_{pi} \rangle$ variable appears in the source term s_{pk} of the carrier-phase transport equation for k, which represents the interaction between the carrier fluid and particles. Through Eq. (10), the influence of the $\langle u'_i u^{k'}_{pi} \rangle$ variable is also brought into the ε transport equation. Details of the relationship between the transport equations of k, ε , $\langle u'_i u^{k'}_{pi} \rangle$, and k_p are shown in Fig. 2. Accordingly, the $\langle u'_i u^{k'}_{pi} \rangle$ variable is related to the ability to modulate the turbulence characteristics of both the carrier fluid and the particles and is, therefore, named the turbulence modulation quantity in this work.

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