A GENERAL PARTICLE DISPERSION MODEL FOR LAGRANGIAN TRAJECTORY SIMULATION OF TWO-PHASE FLOWS IN CURVILINEAR COORDINATES

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ABSTRACT

An efficient particle dispersion model (SPEED) was described for predicting dilute turbulent two-phase flows in non-orthogonal grids. The continuous-phase flow field was modeled using the Reynolds-stress transport model whereas the particular flow field was modeled using the Lagrangian trajectory model. The two phases are linked with each other via two-way coupling sources. A robust numerical algorithm was developed to determine the spatial distribution of physical particles in irregular Eulerian control volumes. The SPEED model requires tracking a small number of particle trajectories to achieve a stochastically significant solution. The present paper has focussed on how to implement the SPEED model in body-fitted coordinates. To validate the model, some demonstrative results are presented and compared with the experimental measurements for a particle-laden turbulent gas flow.

INTRODUCTION

When used to predict dilute steady turbulent two-phase flows, the Lagrangian trajectory model is often associated with a stochastic model to account for particle dispersion induced by the carrier-phase turbulence. The conventional Lagrangian stochastic model (Gosman and Ioannides, 1981) assumes that discrete particles or droplets are interacting with a series of turbulent eddies along their trajectories. The period of time, over which a particle is interacting with a randomly sampled eddy, is determined by minimizing an eddy lifetime and an eddy transit time. The drawback of these conventional models is that a relatively large number of particle trajectories are often necessarily tracked to achieve a stochastically significant solution. As a result, much computer CPU time is often required for the Lagrangian solver.

To avoid tracking too many particle trajectories, Chen and Pereira (1996a; 1997a) developed a Stochastic-Probabilistic Efficiency Enhanced Dispersion (SPEED) model. Different from the conventional Lagrangian stochastic model, the SPEED model uses the additional probabilistic computation to account for the probabilistic distribution of physical particles in space. A trajectory-variance equation was derived to govern the variance of particle trajectories induced by gas turbulence. The SPEED model has the characteristics of simplicity in physical background and ease in numerical implementations, and has insofar been validated against various dilute turbulent two-phase flows with simple flow geomtries, where the orthogonal Cartesian coordinates are employed; see Chen and Pereira (1998a; 1998b).

Most two-phase flows in industrial applications, nevertheless, are often characterized by the complexity of flow geometry. For example, dust particles are moving in an ultrasonic gas flow meter (Chen and Pereira, 1997b). To predict such two-phase flows, non-orthogonal coordinates with Cartesian velocity vectors, so-called partial-transformation approach, are often used to deal with complex flow geometry. It is known that the hybrid Eulerian-Lagrangian modeling of two-phase flows requires knowing, for the flow-field interpolation, the information of the Eulerian control volume where a particle moves after an advancing time step, regardless of one-way or two-way coupling considered.

The objective of the present work is to extend the SPEED model to curvilinear coordinates in order to predict two-phase flows with complex geometry. An efficient numerical algorithm is described for detecting arbitrary Eulerian control volumes, thus greatly improving computational efficiency. In addition, a robust numerical algorithm is developed for integrating the probability density function (pdf) over irregular Eulerian control volumes, as required by the SPEED model. Such a robust numerical algorithm makes it possible that the SPEED model be able to efficiently predict dispersed turbulent two-phase flows using curvilinear coordinates.

MODELING OF THE FLUID FLOW

For steady, dilute, turbulent two-phase flows, the time-averaged Navier-Stokes equations for the continuous phase are similar in form to those for single-phase flows. The exchanges in momentum and energy between the two phases, so-called two-way coupling sources, are accounted for in the continuous-phase equations. The final time-averaged transport equations for continuity and momentum can be written tensorially in curvilinear coordinates as:

$$\frac{\partial \rho U_m \beta^j_m}{\partial \xi_j} = 0 \tag{1}$$

$$\frac{\partial \rho U_m \beta^j_m U_i}{\partial \xi_j} = -\frac{\partial P}{\partial \xi_j}\beta^j_i + \frac{\partial}{\partial \xi_j}\left(-\rho \overline{u_i u_j}\beta^j_k\right) + S^p_{U_i} \tag{2}$$

where β's denote the cofactors of the coordinate transformations, J the Jacobean determinant, and $S^p_{U_i}$ the two-phase momentum exchange. Note that the Cartesian velocity vectors are used in the above equations, and that x_i and ξ_i represent the Cartesian and curvilinear coordinate systems, respectively. The Reynolds stresses are governed by

$$\frac{\partial \rho U_k \beta^m_k \overline{u_i u_j}}{\partial \xi_m} = \frac{\partial}{\partial \xi_n}\left(\frac{1}{J}\beta^n_k \rho C_s \frac{k}{\varepsilon}\overline{u_k u_m}\beta^l_m \frac{\partial \overline{u_i u_j}}{\partial \xi_l}\right) + J\left(P_{ij} - \frac{2}{3}\rho\varepsilon\delta_{ij} + \phi_{ij}\right) + S^p_{ij} \tag{3}$$

where P_{ij}, ϕ_{ij} and S^p_{ij} represent, respectively, the generation, pressure-strain processes, and two-way coupling sources between the continuous and dispersed phases. The generation term is given by

$$P_{ij} = -\rho\left(\overline{u_j u_k}\frac{1}{J}\frac{\partial U_i}{\partial \xi_m}\beta^m_k + \overline{u_i u_k}\frac{1}{J}\frac{\partial U_j}{\partial \xi_n}\beta^n_k\right) \tag{4}$$

The pressure-strain terms are modeled using the wall-reflection modifications; see Chen and Pereira (1995) for details. The transport equation for the dissipation rate of the turbulent kinetic energy, ε, is governed by

$$\frac{\partial \rho \beta^m_k U_k \varepsilon}{\partial \xi_m} = \frac{\partial}{\partial \xi_n}\left(\frac{1}{J}\beta^n_k \rho C_\varepsilon \frac{k}{\varepsilon}\overline{u_k u_m}\beta^l_m \frac{\partial \varepsilon}{\partial \xi_l}\right) + J\frac{\varepsilon}{k}\left(C_{\varepsilon 1}G - C_{\varepsilon 2}\rho\varepsilon\right) + C_{p\varepsilon}\rho\frac{\varepsilon}{2k}S^p_{mm} \tag{5}$$

where S^p_{mm} accounts for the turbulence modulation by the dispersed phase. The production term of the turbulent kinetic energy is given by $G = 0.5P_{kk}$. The foregoing model constants are given as follows: (C_s, C_ε, $C_{\varepsilon 1}$, $C_{\varepsilon 2}$, $C_{p\varepsilon}$) = (0.22, 0.18, 0.18, 1.45, 1.6).

MODELING OF THE PARTICULATE FLOW

The Lagrangian equation of motion for each of representative particle sizes can be written as

$$\frac{dU_{pi}}{dt} = \frac{\tilde{U}_i - U_{pi}}{\tau_p}f_p + F_{pi} \tag{6}$$

where the subscript p represents the particle phase, i the Cartesian component, t time, $\tilde{U}_i$ the fluid-phase instantaneous Cartesian velocity, τ_p the particle relaxation time, f_p the drag correction coefficient, and F_{pi} an extra force, such as the lift force or gravity force. The fluid instantaneous velocity is obtained using a modified particle dispersion model (Chen and Pereira, 1995; 1998b) to account for the effect of the turbulence anisotropy. The relaxation time constant and the drag correction coefficient are determined by

$$\tau_p = \frac{\rho_p D_p^2}{18\mu},\quad f_p = 1 + 0.15\mathrm{Re}_p^{0.687},\quad \left(\mathrm{Re}_p < 1000\right) \tag{7}$$

where ρ_p is the particle density, D_p the particle diameter, and Re_p the relative Reynolds number. The particle trajectories in the computational domain are obtained by integrating the available particle velocities, that is,

$$\frac{dx_{pi}}{dt} = \tilde{U}_{pi} \tag{8}$$

TWO-PHASE COUPLING SOURCES

The two-way coupling effect requires accounting for the sources in the Eulerian equations. The computations of the exchanges in momentum and energy between the gas and particle phases can be found in Chen and Pereira (1998b).

PARTICLE DISPERSION MODEL

Following Chen and Pereira (1997a), the evolution of the particle trajectory variance σ_{pi} is governed by

$$\frac{d\sigma^2_{pi}}{dt} = 2\int_0^t \langle u_{pi}(t)u_{pi}(t_1)\rangle dt_1 = 2\Omega_{pi}\overline{u_i^2}\int_0^t R_{Li}(\tau)d\tau \tag{9}$$

where the angular bracket represents the ensemble averaging and Ω_{pi} denotes the correlation between the two-phase fluctuating velocities, given by

$$\Omega_{pi} = \frac{1}{1 + St_i} \tag{10}$$

where $St_i = \tau_p / T_{Li}$ is a Stokes number, defined as the ratio of a particle relaxation time to a characteristic flow time. Such a simulation of Ω_{pi} is aimed at correctly predicting the limiting behavior for fluid particles and large heavy particles. The Lagrangian autocorrelation function of $R_{Li}(\tau)$ can be obtained using a Frenkiel function

$$R_{Li}(\tau) = \cos\left(\frac{\tau}{2T_{Li}}\right)\exp\left(-\frac{\tau}{2T_{Li}}\right)\quad \left(\text{no summation}\right) \tag{11}$$

where T_{Li} is the integral time scale. For the SPEED model, the trajectory determined with Eq. (8) represents the locus of the trajectory center at each Lagrangian advance step. Simultaneously, particle trajectory variances are determined with Eq. (9) to account for the dispersive effect induced by

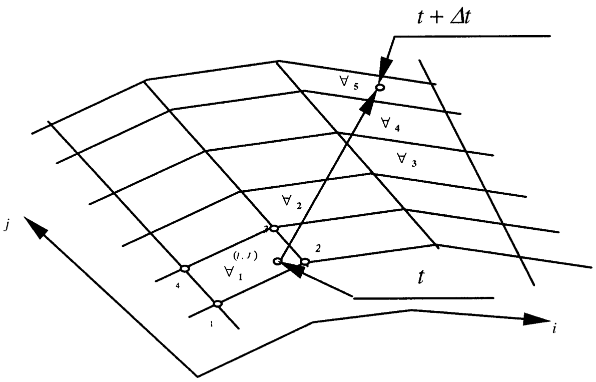

Figure 1. Particle Motion in Non-orthogonal Grids

turbulence. Given a probability density function (pdf), $f(x,y)$, an ensemble-averaged particle property in a Eulerian control volume $\forall(x,y)$ can be obtained (Chen and Pereira, 1997a) by

$$\langle\Phi\rangle = \frac{\sum \dot{N}_k \Delta t_k \iint_{\forall(x,y)} \Phi_k(x_p, y_p) f_k(x,y)\,dxdy}{\sum \dot{N}_k \Delta t_k \iint_{\forall(x,y)} f_k(x,y)\,dxdy} \qquad (12)$$

where the integral is performed over a Eulerian control volume, $\forall(x,y)$. The summation over k represents all the particle sizes crossing the Eulerian control volume, with $\dot{N}_k$ being the particle number flowrate of the *k-th* particle. Here Δt_k stands for the residence time of the particle in the Eulerian control volume in question. Similarly, the two-way coupling source can be distributed over a Eulerian control volume. The two-dimensional pdf $f(x,y)$ can be expressed as,

$$f(x,y) = \frac{1}{2\pi\sigma_{px}\sigma_{py}} \exp\left[-\frac{(x-x_p)^2}{2\sigma_{px}^2} - \frac{(y-y_p)^2}{2\sigma_{py}^2}\right] \qquad (13)$$

where σ_{px} and σ_{py} are the deviations of the particle trajectory fluctuations in x and y directions, respectively.

CONTROL-VOLUME DETECTION

To detect which control volume is holding a particle, it requires completing two tasks: 1) to judge whether a particle lies inside a Eulerian control volume, and/or 2) to determine an optimal search path towards the control volume holding the particle, if the control volume being detected does not hold the particle. Figure 1 illustrates a typical movement of a particle in non-orthogonal grids during one time step Δt.

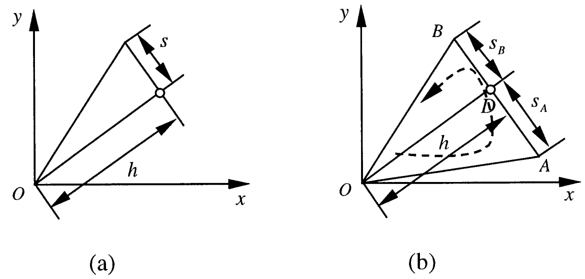

Figure 2. An Arbitrary N-Polygon

Our task now is how to efficiently determine the unknown control volumes $\forall_5$ to which the particle has moved after Δt. Consider an arbitrary *N*-polygon, shown in Fig. 2. There are *N* edges and *N* vertices. The positions of *N* vertices can be expressed in terms of the position (Cartesian) coordinates (x_n, y_n) with n = 1, 2, 3, ... *N*. The first question is how to know whether a particle lies inside this polygon. In the present work, the counter-clockwise ordering (Zhou and Leschziner, 1998) is used. As a result, a general linear function can be written for any edge:

$$\Omega_n(x,y) = (x_{n+1-m} - x_n)(y - y_n) - (y_{n+1-m} - y_n)(x - x_n) \qquad (14)$$

where n = 1, 2, 3, ..., *N* for the *N*-polygon. The value of m is given by

$$m = integer\left[\frac{n}{N}\right]N \qquad (15)$$

where *N* stands for the total number of edges of an *N*-polygon, and *integer* denotes the integral operation of n divided by *N*. Under the counter-clockwise ordering, Eq. (14) has the property for a particle in (x_p, y_p):

$$\Omega_n(x_p, y_p) = \begin{cases} <0 & \textit{on the right-hand side of the edge} \\ >0 & \textit{on the left-hand side of the edge} \\ =0 & \textit{on the edge} \end{cases} \qquad (16)$$

where n = 1, 2, 3, ..., *N* for the *N*-polygon. Therefore the particle will be inside a polygon, if and only if $\Omega_n(x_p, y_p) > 0$ is valid for *all* the edges. Generally speaking, it is likely that the particles do not move continuously from one control volume to another. Moreover, the Lagrangian stochastic trajectory model makes it impossible to adequately estimate the moving direction of a particle after each Lagrangian advancing time step. As a consequence, a search path has to be determined for orienting the search direction. To optimize the search path, Chen (1997) developed an efficient numerical algorithm taking advantages of structured grids. The method is outlined as follows. A unit integer variable may be defined in terms of the sign of Ω_n,

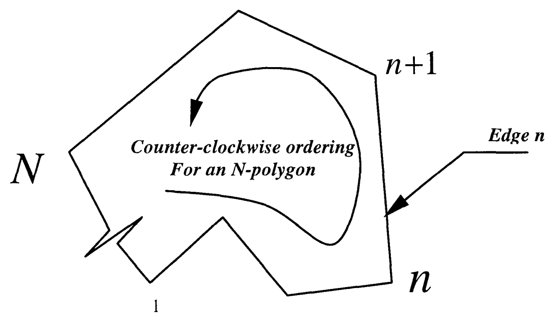

Figure 3. Integral Domain: (a) Right and (b) Arbitrary

$$I_n = sign(1, \Omega_n) = \begin{cases} 1, & \Omega_n \geq 0 \\ -1, & \Omega_n < 0 \end{cases} \quad (17)$$

which is a sign function of Fortran. When I_n = 1, the particle lies on the *left-hand side* of Edge *n* or on the edge. Summing all unit integer variables, we have:

$$I_{sum} = \sum_{n=1}^{N} I_n = \begin{cases} N \\ \text{other values} \end{cases} \quad (18)$$

where *N* is the total number of edges for an *N*-polygon. The particle lies inside the *N*-polygon, if and only if it holds that I_{sum} = *N*. Based on Eq. (17), the index increments for particle location can be calculated, and the search path can thus be determined. For details, the reader is referred to Chen (1997).

PARTICLE SPATIAL DISTRIBUTION

To determine the spatial distribution of physical particles, it is necessary to evaluate the probability distribution of physical particles in irregular Eulerian control volumes. To this end, a robust numerical algorithm is developed for integrating the pdf $f(x, y)$ over irregular Eulerian control volumes $\forall$ (*x, y*). To obtain the integral of a Gaussian probability over an arbitrary Eulerian control volume an auxiliary probability function is defined as follows:

$$P(h, s) = \frac{1}{2\pi} \int_0^h \int_0^{\frac{s}{h}x} g(x) g(y) dx dy \quad (19)$$

where *h* and *s* are defined in Fig. 3(a) for a rectangular triangle, and $g(x)$ and $g(y)$ are the Gaussian probability density functions, having a zero mean and a unity deviation, in the *x*- and *y*-directions, respectively. Based upon the series expansion (Abramowitz and Stegun, 1972), Eq. (19) can be expressed as:

$$P(h, s) = \sum_{n=0}^{\infty} \frac{g^{(n)}(h) g^{(n)}(0)}{(n+1)!} \gamma^{n+1} - \frac{\sin^{-1}\gamma}{2\pi} \quad (20)$$

where $g^{(n)}(x)$ denotes the *n-th* derivative of $g(x)$ with respect to *x*, and γ is defined by

$$\gamma = -\frac{s}{\sqrt{h^2 + s^2}} \quad (21)$$

The *n-th* derivative of $g(x)$ with respect to *x* is given by

$$g^{(n)}(x) = (-1)^n g(x) n! \sum_{m=0}^{M} \frac{(-1)^m x^{n-2m}}{2^m m! (n-2m)!} \quad (22)$$

where *M* is the integer of *n/2* represents the integer of *n/2*. The integral of the probability density function over triangles, see Fig. 3(b), can be written as

$$P(\Delta AOB) = I_A P(h, s_A) + I_B P(h, s_B) \quad (23)$$

where I_A and I_B are taken to be either positive or negative unity, depending on the relative position. The signs of I_A and I_B in Eq. (23) can be determined using Eq. (17). Let P_{ij} be the integral of the pdf over the Eulerian control volume. It follows that

$$P_{ij} = \frac{1}{2\pi\sigma_{px}\sigma_{py}} \iint_{\forall(x,y)} f(x, y) dx dy \quad (24)$$

where $\forall$ (*x, y*) stands for the integral domain, i.e., the control volume *(i, j)*, $f(x, y)$ is given by Eq. (13). Making the following variable transformations,

$$\xi = \frac{x - x_p}{\sigma_{px}}, \quad \eta = \frac{y - y_p}{\sigma_{py}} \quad (25)$$

we have

$$P_{ij} = \frac{1}{2\pi} \iint_{\forall(\xi,\eta)} \exp\left[-\frac{\xi^2 + \eta^2}{2}\right] d\xi d\eta \quad (26)$$

where $\forall(\xi, \eta)$ is the transformed control volume in $\xi - \eta$ coordinates. To obtain the Gaussian pdf over an irregular quadrangle, the quadrangle is decomposed into four triangular domains. As a result, the probability can finally be evaluated over the arbitrary quadrangle.

DEMONSTRATIVE RESULTS

An adequate evaluation of the Lagrangian trajectory model requires providing complete initial conditions from experimental measurements for two phases, since initial conditions were found very important to numerical predictions (Chen and Pereira, 1996b). In the present work, experimental measurements (Sato et al., 1996) were used for the SPEED model validation. Their measurements provided complete initial conditions for both the gas and the particle phases at the inlet.

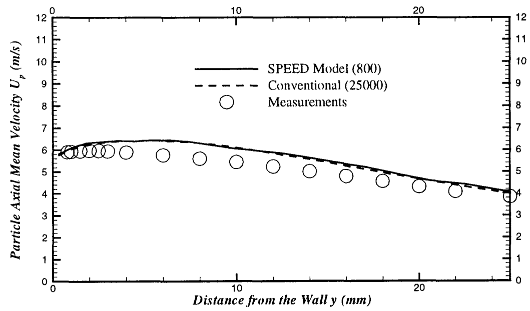

Figure 4. Particle Axial Mean Velocity

In addition, several profiles downstream were provided for the model validation. The turbulent gas flow had a Reynolds number of 3.3 x 10^4, and the glass particles had a mean diameter of 140 μm and a standard deviation of 8.9 μm. The computational domain consisted of 500 *mm* and 100 *mm* in the *x*- and *y*-directions, respectively. The grid-independent solution was obtained using a total of 125 x 80 non-orthogonal grids such the flow domain. The initial conditions for the two phases were obtained by interpolating experimental measurements. The particle diameter at the inlet was obtained by summing over the mean value over a fluctuating value that obeyed a Gaussian distribution having the given standard deviation. The wall-function approach was used to bridge the near-wall layer.

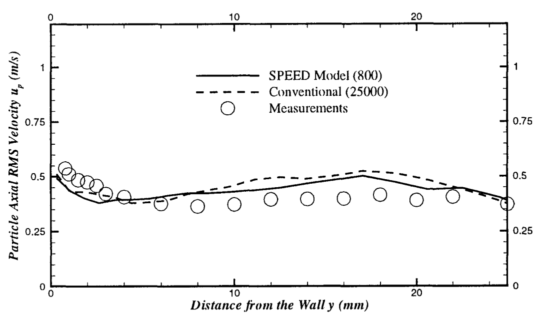

Figure. 5 Particle Axial Fluctuating Velocity

The boundary conditions for the Reynolds stresses were handled using the method of Lien and Leschziner (1994). The solution to the Reynolds-stress equations was based on the apparent-viscosity (Lien and Leschziner, 1996) to enhance the coupling between momentum and Reynolds-stress equations. For the particle phase, a total of 800 particle trajectories were tracked for the SPEED model whereas a total of 25000 particle trajectories were tracked for the conventional particle dispersion model. The conventional Lagrangian stochastic model has been modified (Chen and Pereira, 1996b) to account for the effect of turbulence anisotropy.

In the present work, only demonstrative results are presented. To assess the SPEED model, the numerical results of the conventional Lagrangian stochastic model were also presented for comparison. Figure 4 compares the experimental measurements of Sato et al. (1996) with the numerical predictions of the SPEED model and the conventional Lagrangian stochastic model for the downstream position of x = 250 *mm*. Note that the SPEED model tracked only 800 particle trajectories whereas the modified conventional stochastic model tracked 25000 particle trajectories. It is evident that the two model predictions agree well with each other and with the experimental measurements. It has been found that the particle mean velocity is usually not sensitive to the number of particle trajectories (Chen and Pereira, 1996b).

Compared in Fig. 5 is the profile of the particle axial fluctuating velocity at the downstream station of x = 250 *mm*. Close to the wall region (y < 5 *mm*), where particles were injected at the inlet, particles have large velocity fluctuations. Obviously, this is attributed to both the large turbulence production in this region and the energy transfer from the inlet. As a result, the particles can acquire large turbulence from the gas phase in the region (y < 5 *mm*) close to the wall. In general, the numerical predictions agree satisfactorily with the experimental measurements, even though the velocity fluctuation was underpredicted in the near-wall region and overpredicted in the region away from the wall. Of note is that the SPEED model predictions are slightly better than those of the modified conventional Lagrangian stochastic model.

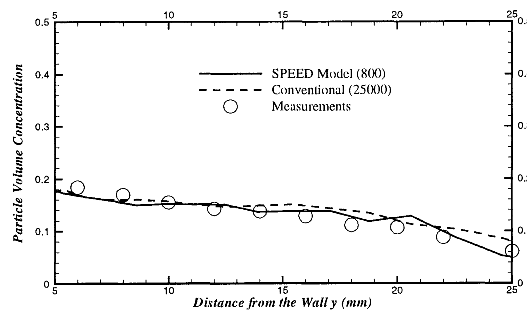

Figure 6. Particle Volume Concentration

Finally, the particle volume concentration is shown in Fig. 6 for the downstream station of x = 250 mm. A similar trend can be observed for the two model predictions. A slightly better agreement with the measurements was achieved with the SPEED model. To evaluate the computational efficiency of the two particle dispersion models, the relative CPU times were monitored since the absolute time depends on many external factors such as the computer itself and the geometry etc. It was found that the SPEED model required about 23.2% the computer CPU time of the conventional Lagrangian stochastic model. Evidently, the computational efficiency was improved as result.

CONCLUDING REMARKS

A general SPEED model was described for an economic prediction of turbulent two-phase flows using non-orthogonal numerical grids. A robust numerical approach was developed to determine the probability distribution of physical particles over irregular Eulerian control volumes. In addition, a simple but efficient numerical approach was developed for rapidly detecting a Eulerian control volume to which the particle has moved after each Lagrangian time step. The present SPEED model has the characteristics that it requires tracking a small number of particle trajectories with reduced statistic noise. Demonstrative numerical results were presented for a particle-laden turbulent gas flow. Compared with the conventional Lagrangian stochastic model, the SPEED model tracked only 3.2 % the number of particle trajectories while yielding agreeable predictions with experimental measurements. It was found that the SPEED model required about 23.2% the computer CPU time of the conventional Lagrangian stochastic model for the present two-phase flow considered, thus offering higher computational efficiency for the Lagrangian solver.

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