

Chinese Society of Aeronautics and Astronautics & Beihang University

Chinese Journal of Aeronautics

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Modeling of finite-size droplets and particles in multiphase flows



JOURNAL

AERONAUTICS

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Received 17 March 2015; revised 1 April 2015; accepted 10 April 2015 Available online 20 June 2015

KEYWORDS

Droplets; Finite-size effects; Large eddy simulation; Multiphase flow; Particle-laden flow

Abstract The conventional point-particle approach for treating the dispersed phase in a continuous flowfield is extended by taking into account the effect of finite particle size, using a Gaussian interpolation from Lagrangian points to the Eulerian field. The inter-phase exchange terms in the conservation equations are distributed over the volume encompassing the particle size, as opposed to the Dirac delta function generally used in the point-particle approach. The proposed approach is benchmarked against three different flow configurations in a numerical framework based on large eddy simulation (LES) turbulence closure. First, the flow over a circular cylinder is simulated for a Reynolds number of 3900 at 1 atm pressure. Results show good agreement with experimental data for the mean streamwise velocity and the vortex shedding frequency in the wake region. The calculated flowfield exhibits correct physics, which the conventional point-particle approach fails to capture. The second case deals with diesel jet injection in quiescent environment over a pressure range of 1.1-5.0 MPa. The calculated jet penetration depth closely matches measurements. It decreases with increasing chamber pressure, due to enhanced drag force in a denser fluid environment. Finally, water and acetone jet injection normal to air crossflow is studied at 1 atm. The calculated jet penetration and Sauter mean diameter of liquid droplets compare very well with measurements.

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1. Introduction

Dispersed droplet (or particulate) flows abound in nature, and they are present in a broad range of applications in atmospheric

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Peer review under responsibility of Editorial Committee of CJA.



fluid dynamics, spray combustion, and two-phase flows in industrial and agricultural processes. In numerical simulations involving liquid–gas flows, the Eulerian–Lagrangian (E–L) method is widely used because of its advantages in predicting turbulent diffusion, droplet breakup, droplet-gas and droplet– droplet interactions.¹ It offers manageable calculations with reasonable turn-round time.^{2,3} The E–L model employs the Eulerian formulation for the carrier (gas) fluid and the Lagrangian formulation for the dispersed phase (particles or droplets). Fig. 1 shows the various inter- and intra-phase couplings between the two phases. One-way coupling refers to models which take into account only the effect of the carrier

http://dx.doi.org/10.1016/j.cja.2015.05.004

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Two-way: mutual coupling between droplets and carrier fluid Four-way: droplet-droplet intractions and interactions (e.g., collision & coalescence)

Fig. 1 Inter-phase couplings between droplets and carrier fluid.

flowfield at the discrete phase. In general, however, the interaction between the two phases is mutual - the carrier phase influences the dispersion and preferential accumulation of the droplets, which in turn modulate the carrier flowfield. This situation is commonly known as two-way coupling.^{1,4–7} The inter-phase exchanges of mass, momentum, and energy are modeled using empirical relations, with the droplets usually treated as point sources. The volumetric displacement of the carrier phase due to the finite-size of droplets is ignored in two-way coupling, as are the ensuing interphase interactions. In a more detailed model, however, in addition to the coupling between the carrier fluid and droplets, the droplet-droplet intractions and interactions (such as collisions and coalescence) should be considered, as the situation prevails in conditions with high loading density of droplets, such as dense sprays. This, combined with two-way coupling, is referred to as the fourway coupling in the modeling of multiphase fluid dynamics.^{5,6} The interactions and intractions, combined with two-way coupling, are referred to as four-way coupling in the modeling of multiphase fluid dynamics.5,6

In typical simulations of particle- (or droplet-) laden flows, the number density of particles is so large that direct resolution of the flow in the vicinity of each particle is not feasible. Particles are usually treated as point sources in an E–L framework.^{8–11} This approach, however, does not necessarily yield accurate results because of its inherent inadequacy in predicting the correct physics, especially when the dispersed phase has finite dimensions. Segura et al.¹² showed that the point-particle approach does not predict turbulence modulation accurately for moderately loaded wall-bounded flows. Similar observations were made by Apte et al.¹³ in simulations of jet fluidization and particle-laden Poiseuille flows.

Typical large eddy simulation (LES) or direct numerical simulation (DNS) studies of dispersed multiphase flows with particles involve grid resolutions that are finer than the particle size. Under such conditions, the assumptions underlying the point-source approach are inadequate to account for the finite size of particles. Furthermore, the drag/lift laws employed in the existing approaches do not capture the key features of particle-induced wakes observed in fully resolved DNS.¹⁴ The effects of the wake and boundary-layer separation behind a particle, as well as particle rotation, become important when

the particle diameter is large. Further, temporal variations of particle size and density distributions in practical applications render the consideration of the finite volume of the dispersed phase imperative in numerical simulations of multiphase flows.

In the present study, the point-source approach is extended by accounting for the finite-size effect of the dispersed phase, and the volume displacement by particles (or droplets) in the carrier flowfield is modeled accurately. The basic idea is that the inter-phase exchange terms in the conservation equations are distributed over mesh volumes spanning the particle size using a Gaussian interpolation function, as opposed to a single cell in the case of the point-particle approach. An empirical model for the drag coefficient C_D , applicable to spheres (or circular cylinders), is adopted and implemented, although any suitable drag coefficient model can be used in conjunction with this approach. The droplets are assumed to remain spherical. Deformation and internal flow motions within droplets are not resolved, thereby substantially reducing the computational time.

This paper is organized in three sections. Section 2 describes the general theoretical formulation based on an E–L framework. The modeling of the finite-size effect of particles on the carrier phase is discussed in detail. Section 3 presents a brief description of the numerical methods. Section 4 discusses the results of three case studies, including the flow over a circular cylinder and liquid jet injection in quiescent and crossflow environments. The calculated fluid physics are benchmarked against experimental measurements. Flow properties of practical interest such as jet penetration depth are systematically compared with published data. Finally, recommendations are made for further improvements.

2. Theoretical formulation

The carrier phase is formulated based on the conservation equations of mass, momentum, and energy in the Cartesian coordinate system.¹⁵ Thermodynamic phase change is neglected in order to focus on the momentum exchange in a particle-laden multiphase flow. The volume fraction of the carrier phase is assumed to be unity since the volume occupied by the discrete phase is exceedingly small in the bulk of the flowfield. The carrier phase is assumed to be a perfect gas.

$$\frac{\partial \rho_{\rm g}}{\partial t} + \boldsymbol{\nabla}(\rho_{\rm g} \boldsymbol{u}) = 0 \tag{1}$$

$$\rho_{g}\left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\boldsymbol{\nabla})\boldsymbol{u}\right) = -\boldsymbol{\nabla}p + \boldsymbol{\nabla}\boldsymbol{\tau} + \boldsymbol{F}^{s}$$
⁽²⁾

$$\rho_{g} \frac{\mathbf{D}e_{t}}{\mathbf{D}t} = \frac{\mathbf{D}p}{\mathbf{D}t} - \nabla \boldsymbol{q} + \boldsymbol{\tau} : \nabla \boldsymbol{u} + \dot{\boldsymbol{Q}}^{s}$$
(3)

where ρ_g is the carrier-gas density, **u** the velocity, **p** the pressure, τ the viscous stress tensor and **q** the heat flux; **F**^s and \dot{Q}^s are the inter-phase momentum and energy coupling terms, respectively. The total specific energy e_t is given by

$$\rho_{g}e_{t} = \rho_{g}e + \frac{1}{2}\rho_{g}\boldsymbol{u} \cdot \boldsymbol{u} = \frac{p}{\gamma - 1} + \frac{1}{2}\rho_{g}\boldsymbol{u} \cdot \boldsymbol{u}$$
(4)

where *e* is the specific internal energy, and γ the ratio of specific heats.

The dispersed-phase dynamics is modeled using a Lagrangian approach, which has been proven to be an efficient way to describe inter-phase interactions. The motion of an individual particle can be determined by Newton's second law of motion as follows:

$$\frac{\mathrm{d}\boldsymbol{x}_{\mathrm{d}}}{\mathrm{d}t} = \boldsymbol{u}_{\mathrm{d}}, \quad m_{\mathrm{d}} \frac{\mathrm{d}\boldsymbol{u}_{\mathrm{d}}}{\mathrm{d}t} = \boldsymbol{F}_{\mathrm{d}}$$
⁽⁵⁾

where x_d is the instantaneous particle location, and m_d the mass. The subscript "d" denotes particles or droplets. Contributions from virtual mass, buoyancy, Basset forces, gravity, and lift are neglected; only the force arising from skin friction and form drag is taken into account.¹¹

$$\boldsymbol{F}_{\rm d} = \frac{1}{8} C_D \rho_{\rm g} \pi d_{\rm p}^2 |\boldsymbol{u}_{\rm R}| \boldsymbol{u}_{\rm R} \tag{6}$$

 $d_{\rm p}$ and $u_{\rm R}$ are the particle diameter and velocity relative to the surrounding carrier fluid, respectively.

The drag coefficient for a sphere C_D is determined based on the empirical correlation by¹⁶

$$C_D = \begin{cases} \frac{24}{Re_d} \left(1 + \frac{Re_d^{2/3}}{6} \right) & Re_d < 1000\\ 0.424 & Re_d \ge 1000 \end{cases}$$
(7)

where Re_d is the particle Reynolds number based on the relative velocity. The source terms F^s and \dot{Q}^s arising from the momentum and energy transfer between the particle and carrier phase are defined, respectively, as¹⁵

$$F^{\rm s} = -\frac{\sum_{k=1}^{N_{\rm p}} (F_{\rm d})_k}{\sum_{k=1}^{N_{\rm p}} V_k}$$
(8)

$$\dot{Q}^s = -\frac{\sum_{k=1}^{N_p} (\boldsymbol{F}_d \cdot \boldsymbol{u}_d)_k}{\sum_{k=1}^{N_p} V_k} \tag{9}$$

where $N_{\rm p}$ is the total number of particles and V_k the volume of the *k*th particle.

To account for the finite-size effect of particles, we consider a computational mesh with a particle centered at x_k in a finite-volume-based numerical framework, as shown schematically in Fig. 2. The domain of influence, $\Delta(x)$, for the point-particle approach is represented by the Dirac delta function, where the force exerted on the carrier phase is treated as a point-source, concentrated in one numerical cell. This methodology works well if the particle size is smaller than the grid encompassing it, but yields erroneous results otherwise. To take into account the volume displaced by a particle and accurately model its effect on the carrier flow, a distribution function, g(x), corresponding to the domain of influence is evaluated for a finite volume containing the particle by means of a Gaussian function.

$$g(\mathbf{x}) = (2\pi\sigma^2)^{-3/2} \exp\left[-\frac{(\mathbf{x} - \mathbf{x}_k)^2}{2\sigma^2}\right]$$
(10)

where

$$\int_{-\infty}^{\infty} g(\mathbf{x}) = 1 \tag{11}$$

and σ is the standard deviation. The Gaussian form provides a smooth interpolation kernel and makes this approach easily adaptable to arbitrarily shaped unstructured grids.¹³ In addition, Gaussian kernels preserve higher-order moments and yield conservative properties in the numerical methodologies



Fig. 2 Particle domain of influence.

used for multiphase flow simulations such as the vortexparticle technique.¹⁷ The inter-phase exchange terms due to the presence of particle k are then distributed over the computational mesh. The distance from the particle center is $(x - x_k)$. The force in the *j*th computational cell is given by

$$\boldsymbol{F}_{i}^{s} = \boldsymbol{g}(\boldsymbol{x})\boldsymbol{F}^{s} \tag{12}$$

The spatial filtering can be adjusted by changing σ relative to the particle size. If the particle diameter d_p is much smaller than σ , the envelop Δ provides a local volume average. Summation of all the particles in the computational domain gives a continuous variation of the local density. On the other hand, if d_p is much larger than σ , the point-source representation can be extended to resolve the motion and the influence of the individual particles.¹⁸ In the present study $\sigma = d_p/\sqrt{2\pi}$ is used. Other forms of forcing envelops and kernel widths can also be used depending on the specific application of interest.¹⁹

The distribution function given by Eq. (10) provides an effective means to treat the finite-size particles in the Eulerian reference frame. The particle wake, vortex shedding and related phenomena are implicitly taken into account without imposing the no-slip boundary condition on the particle surface. Similar distribution functions are used in immersed boundary (IB) methods where the boundary elements are treated as a collection of point sources in the Lagrangian reference frame. The effect of boundary is transmitted to the surrounding fluid either by a localized force (if the IB nodes and computational cells coincide) or a distributed force in the momentum equations.^{20,21} The present work employs a distribution function to simulate the volumetric displacement by a particle and subsequent inter-phase exchanges between the two phases. In theory, our approach approximates the effect of the finite size and rigid boundary of a particle in a manner similar to having finite force monopoles, dipoles and higherorder multipoles.⁴

3. Numerical methods

The numerical scheme for the carrier phase employs a densitybased, finite-volume approach.^{23,24} Temporal integration is carried out using a four-step Runge–Kutta scheme. Spatial discretization is obtained using a fourth-order centraldifferencing scheme in generalized coordinates, and sixthorder numerical dissipation to ensure numerical stability. Further details of the numerical methods used in the present study can be obtained in Wang et al.²³ The finite-size effects are implemented in two steps. The drag force F_d , is first calculated for the particle of concern. The inter-phase momentum exchange in the computed using Eqs. (10) and (12). Once these source terms are evaluated, the governing equations are solved to obtain the resulting flowfield.

4. Sample studies

To verify the numerical treatment and to establish confidence, the approach described in the previous sections for treating finite-size particles is applied to three different sample problems. These include the flow over a circular cylinder and liquid jet injection in both quiescent and crossflow environments. The calculated flowfields are benchmarked against experimental measurements. All the problems are studied in an LES framework, the details of which can be found in Oefelein and Yang²⁵ and Wang et al.²³ The subgrid stress and energy flux are treated by means of a compressible-flow version of the Smagorinsky model proposed by Erlebacher et al.²⁶, because of its reasonable accuracy for turbulent flows in complex geometries. Since all the cases studied here lie in the dilute regime, particle–particle collision and turbulence modulation by particles are not taken into account.

4.1. Flow past a circular cylinder

The flow past a fixed circular cylinder of a diameter $D_0 = 512 \,\mu\text{m}$ is first studied, as shown schematically in



Fig. 3 Flow past a circular cylinder: top and front view of computation domain.

Fig. 3. The computational domain covers a region of $(20 \times 10 \times 10)$ D₀ (length L×width W×height H). Air flows through the channel at a bulk speed, $U_0 = 125$ m/s, at atmospheric conditions $(p_{\infty} = 1.013 \times 10^5 \text{ Pa} \text{ and } T_{\infty} = 298 \text{ K}).$ The Reynolds number based on the cylinder diameter is 3900. The cylinder, represented by a number of finite-size particles, is located at a distance $L_{\rm F} = 5D_0$ downstream of the entrance. The particle density has a large value in the present study because of the fixed geometry of the cylinder. A total of $220 \times 80 \times 200$ (3.52 million) numerical grids are employed in the streamwise, spanwise, and vertical directions, respectively. The grid is clustered downstream of the cylinder to resolve detailed flow structures. Depending on flow configuration, 2-10 grids are used to resolve the cylinder. Fig. 4 shows the drag coefficient C_D for a circular cylinder in a uniform flow.²⁷ It has a value of 0.9 in the present case.

Fig. 5 shows a snapshot of the calculated vorticity magnitude $|\omega|$ in the *x*-*z* plane at $y/D_0 = 5$. Vortex shedding is clearly observed downstream of the cylinder in the form of a Kármán vortex street. Fig. 6 uses vortex filaments to detail



Fig. 4 Drag coefficient of flow over a cylinder for $10^{-1} < Re_d < 10^4$.



Fig. 5 Instantaneous vorticity magnitude for flow over a cylinder at $y/D_0 = 5$, $Re_d = 3900$.



Fig. 6 Vortex filament lines downstream of a bluff body.

the mechanism underlying vortex shedding phenomena behind bluff bodies.²⁸ The shear layer on the top surface of the cylinder folds into a vortex and becomes progressively stronger through the continuous feeding of vorticity from the boundary layer. Fluid from the lower shear layer crosses the wake axis and is entrained into the upper vortex. The source of vorticity to the top vortex is eventually cut off due to reverse flow 1, and entrainment 2, and it detaches.²⁸⁻³⁰ This process continues alternately from the top and bottom of the cylinder, forming a shedding pattern as evidenced in the present study. Beaudan and Moin³¹ reported similar vortex shedding phenomena using an LES-based approach (see Fig. 5(b)) for the same Reynolds number. Their simulation employs no-slip boundary condition on the cylinder surface, and thus resolves the boundary layer and its separation explicitly. A detailed discussion about flow past circular cylinders for a wide range of Reynolds numbers can be found elsewhere.^{29,32}

For comparison, another numerical simulation is conducted with exactly the same flow conditions and grid resolution as the above case (Fig. 5(a)), but with the point-particle assumption. The vorticity contours shown in Fig. 5(c) do not demonstrate any sort of vortex shedding phenomenon. Instead, symmetric shear layers are observed in the wake; these are manifestations of the momentum exchanged between the carrier phase and the point source. The vorticity values are almost an order of magnitude less than those obtained for the finite-size approach.

The vorticity in the wake of a bluff body is caused by the no-slip boundary. Vorticity penetrates the wake via viscous diffusion and is distributed by advection, stretching and bending.³³ The local disturbance created by the cylinder due to force coupling is a strong source of small scale vorticity and interacts with the gas-phase flow. The distributed momentum exchange between the two phases thus mimics the vorticity-generation mechanism in the shear layer at the top and bottom surfaces of the cylinder. Asymmetric disturbances which initiate the shedding phenomena are not possible if the inter-phase coupling source terms are concentrated in one (or a few) computational cell. This explains why the point-particle assumption is incapable of predicting vortex shedding.

To explore the limitations and capabilities of the present approach, the mean streamwise velocity \overline{U}/U_0 at downstream locations of $x/D_0 = 3$, 4 and 6 are compared with experimental measurements.³⁴ The LES result of Beaudan and Moin³¹ at $x/D_0 = 4$ is also included, as shown in Fig. 7. The wake deficit decreases and the spreading angle of the streamwise velocity profile increases with distance downstream of the cylinder. Excellent agreement with experimental data is observed in the near field. Farther downstream, the momentum deficit is slightly under-predicted in the central region. Higher-order statistics are not compared with measurements due to the lack of information about turbulence intensity at the inlet. The calculated Strouhal number of 0.21 for the dominant shedding frequency matches closely with the experimentally measured values.^{27,35}

To further explain why the point-particle approach does not yield the correct flowfield, a parametric study is conducted by varying the filter width. Table 1 lists the Strouhal number



Fig. 7 Mean streamwise velocity at $x/D_0 = 3$, 4 and 6 for flow past a cylinder, $Re_d = 3900$.

Table 1 Strouhal number as a function of $\sigma/\Delta x$.		
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Case	$\sigma/\Delta x$	Strouhal number
1	0.79	0.16
2	1.59	0.20
3	2.39	0.21

obtained for flow over cylinder for various values of $\sigma/\Delta x$, the ratio of the filter size to the computational grid. For Case 1, regular vorter shedding is damped very quickly, and the evolution of large eddies cannot be maintained. The kernel width, even though larger than the Dirac delta function, is not sufficient to ensure proper numerical resolution.¹⁸ For Cases 2 and 3, the calculated Strouhal numbers match closely with measurements.³⁵

4.2. Diesel injection in quiescent environment

The experiments conducted by Hiroyasu and Kodata³⁶ on diesel injection into a quiescent nitrogen environment are studied next. Table 2 lists the fuel properties and operating conditions.³⁶ The chamber pressure covers a range from 1.1 to 5.0 MPa. The corresponding jet velocities at the injector exit are 86.4–102 m/s. A total of 10⁶ droplet parcels are discharged into the chamber to accurately describe the spray dynamics.

The hydrodynamic stability analysis of Reitz³⁷ is implemented to model liquid injection and primary atomization. The fuel jet is modeled as a series of blobs having a characteristic size equal to the injector exit diameter, D_0 , i.e.,

$$d_{\rm int} = D_0 \tag{13}$$

The number of blobs injected per unit time is determined by the injector mass flow rate. Each blob is assigned an initial radial velocity component $V_0 = U_0 \tan(\theta/2)$, where U_0 is the injection velocity, and the spray angle θ is assumed to be uniformly distributed between 0 and Θ , with

$$\tan\frac{\Theta}{2} = A_1 \Lambda \Omega / U_0 \tag{14}$$

In the present study, $A_1 = 0.188$, corresponding to a sharpentrance nozzle with a length-to-diameter ratio of 5. The frequency of the fastest growing Kelvin–Helmholtz wave Ω , and the corresponding wavelength Λ , are determined using a curve-fit solution of the linearized hydrodynamic equations, as follows:

$$\frac{\Lambda}{a} = 9.02 \frac{(1+0.45Z^{0.5})(1+0.4Ta^{0.7})}{(1+0.87We_{\rm g}^{1.67})^{0.6}}$$
(15)

$$\Omega\left(\frac{\rho_{\rm d}a^3}{\sigma}\right)^{0.5} = \frac{0.34 + 0.38We_{\rm g}^{1.5}}{(1+Z)(1+1.4Ta^{0.6})} \tag{16}$$

where $Z = W e_d^{0.5} / R e_d$ is the Ohnesorge number, $W e_d = \rho_d U_R^2 a / \sigma$ the liquid Weber number; $W e_g = \rho_g U^2 r_d / \sigma$ the gas Weber number, and $Ta = Z W e_g^{0.5}$ the Taylor number. The variable *a* is the parent droplet radius. It is assumed that the sizes of the child droplets are proportional to the

Table 2 Fuel properties and operating conditions. ³⁶	
Parameter	Value
Density (kg/m ³)	840
Viscosity (mm ² /s)	2.5
Surface tension (kN/m)	29.5
Operating pressure p (MPa)	1.1-5.0
Operating temperature $T(\mathbf{K})$	298
Orifice diameter D_{jet} (µm)	300
Nozzle opening pressure P_{inj} (MPa)	9.9
Coefficient of discharge C_{dis}	0.705

wavelength of the most unstable surface wave and are modeled as follows:

$$r = B_0 \Lambda \quad (B_0 \Lambda \leqslant a) \tag{17}$$

$$r = \min((3\pi a^2 W/2\Omega)^{0.33}, (3a^2 \Lambda/4)^{0.34})$$

$$B_0 \Lambda > a, \text{ one time only}$$
(18)

where $B_0 = 0.61$. Breakup is determined by tracking the change in the radius of the parent droplet, collecting the mass that would have been shed due to wave stripping, and assigning it to the child droplets. The rate of change of the parent droplet radius is assumed to obey the following equation

$$\frac{\mathrm{d}a}{\mathrm{d}t} = -\frac{a-r}{\tau} \tag{19}$$

where $\tau = 3.726$. $B_1 a / \Lambda \Omega$ is the breakup time constant with $B_1 = 1.73$.³⁸ The Taylor analogy breakup (TAB) model³⁹ is implemented to model secondary breakup.

Fig. 8 shows the instantaneous spray field and the details of the jet tip for diesel injection at 1.1 MPa. Primary atomization proceeds immediately after fuel injection because of the large Weber number. As the spray penetrates and breaks up further, the smaller droplets lag behind, because of the wake created downstream of the larger drops.

Fig. 9 shows the root-mean square of the jet penetration depth for three different chamber pressures of 1.1, 3.0 and 5.0 MPa. Also shown is the result obtained from the point-particle approach.⁴⁰ Excellent agreement is observed with experimental data. Jet penetration decreases with increasing chamber pressure because of the enhanced aerodynamic drag force experienced by the liquid spray in a denser environment.



(a) Instantaneous spray field for diesel injection at p = 1.1 Mpa, T = 298 K, $D_0 = 300 \mu$ m



(b) Close up view of diesel spray tip

Fig. 8 Instantaneous spray field and details of jet tip for diesel injection at 1.1 MPa.



Fig. 9 Diesel jet penetration depth at p = 1.1, 3.0 and 5.0 MPa.

The slight deviation from measurements in the downstream region can be attributed to particle–particle collision and coalescence, and turbulence modulation by particles and its ensuing effect on the particle trajectory, which are not considered in the present study. These effects may become prominent as the particle-loading density increases.

4.3. Water and acetone injection in air crossflow

Water injection into an air crossflow is also investigated. Fig. 10 shows the computational domain with dimensions of 38.1 mm × 25.4 mm × 25.4 mm ($L \times W \times H$). Air enters the duct at a velocity of 125 m/s. The temperature and pressure of the gas phase are 297 K and 1 atm, respectively. The Reynolds number of the gas phase based on the flow velocity and duct width is 2.1×10^5 . The injector with a diameter of 0.254 mm is located 12.7 mm downstream of the entrance. Water is injected into the duct with a momentum flux ratio, $q = \rho_d u_d^2 / \rho_g u_g^2 = 18$. A total of 1.5 million numerical grids are used.

Fig. 11 shows a snapshot of the flowfield. Water is injected into the crossflow in the form of discrete blobs, which break up to form droplets. They are rapidly convected downstream by the air flow because of their small Stokes number. The large-size parent droplets penetrate farther into the central region of the duct. Fig. 11(b) shows a wake that starts immediately downstream of the liquid injection location and extends to the end of the computational domain. This is consistent with the flow structure typically observed behind a liquid column in a crossflow. Since intensive momentum exchange takes place between the air and the normally injected water stream through drag force, the axial velocity in the downstream region of the liquid column is significantly lower than that of the free stream.



Fig. 10 Water injection in high-speed air crossflow.



(b) y-z cross sections

Fig. 11 Snapshot of air/water flowfields (gas phase: contours of *x*-velocity; spray phase: distribution of droplets).



Fig. 12 Temporal evolution of vorticity magnitude and spray field at cross section y = 0 mm.

Fig. 12 shows the temporal evolution of the vorticity and spray fields. High vorticity is observed immediately behind the liquid jet and convects downstream with the local flow velocity. The maximum vorticity magnitude decreases as the



Fig. 13 Spatial distribution of Sauter mean diameter of water droplets, D_{32} at $x/D_0 = 100$.

blobs in the injected column undergo fragmentation and penetrate farther into the duct. The whole process is similar to the flow over a blunt-body at high Reynolds number. A symmetric recirculating-flow topology is first observed. It becomes laterally unstable due to the disturbance arising from the downstream region and develops into a periodic vortex shedding pattern. Detailed examination of two-phase interactions in the flowfield at $x/D_0 = 20$ indicates an oscillation frequency of 70 kHz. This agrees reasonably with the intrinsic frequency of vortex shedding behind a circular cylinder under the same flow conditions (i.e., 88 kHz for $Re = 2.1 \times 10^5$).³⁵

Fig. 13 shows the time-average Sauter mean diameter D_{32} of the droplet size distribution. The calculated $D_{32} = 60 \,\mu\text{m}$ agrees reasonably well with measurements. Experimental data indicate an accumulation of droplets near the bottom surface in the downstream region of the injector, which is not observed in the present results. The predicted height of the liquid jet is higher than the measured value. These differences may be attributed to the particular primary breakup model employed in the present analysis.

Simulations are further conducted to study acetone injection into an air crossflow, simulating the experiments conducted by Stenzler et al.⁴¹ The computational domain includes a duct with dimensions of 28.9 mm \times 25.8 mm ($W \times H$). High velocity air



Fig. 14 Penetration of acetone jet in air crossflow.

enters the duct at a velocity of 90 m/s. The temperature and pressure of the gas phase are 291 K and 1 atm, respectively. The injector diameter is 0.254 mm. Acetone is injected with a velocity of 21.16 m/s, giving a momentum flux ratio of 36 and a Weber number of 106.2. The spray field shown in Fig. 14 shows excellent agreement with experimental measurements. The other flow features are similar to those observed with the case of water injection in air crossflow.

5. Conclusions

- (1) A general approach was developed to take into account the effect of finite-size of particles in multiphase flows. The conventional point-particle approximation is extended by distributing the inter-phase exchange terms in the conservation equations over the volume encompassing the particle size using a Gaussian interpolation function.
- (2) The spray-field dynamics is treated in an Eulerian– Lagrangian framework in which the carrier phase is discretized using a density-based, finite-volume approach, and the discrete phase trajectory is calculated using Newton's second law of motion. Large-eddy simulation is employed to achieve turbulence closure. The disintegration of the liquid column and secondary atomization are treated by means of the wave breakup and Taylor analogy breakup models respectively.
- (3) The overall approach was benchmarked against three different flow configurations. In a study of flow past a circular cylinder at $Re_d = 3900$, the near wake profiles and the vortex shedding frequency downstream of the cylinder were found to agree very well with measurements. Diesel jet injection in a range of pressures from 1.1 to 5.0 MPa was also considered; jet penetration depth matched very well with experimental data. The third case dealt with water and acetone injection in an air crossflow. The calculated Sauter mean diameter of droplet size distribution for water injection compared closely with measured values. The approach developed in the current paper to treat the finite-size effect of particles and droplets can be used effectively in large-scale numerical simulations to obtain accurate physics while maintaining computational efficiency.

Acknowledgement

This work was sponsored by the William R. T. Oakes Endowment of the Georgia Institute of Technology.

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