A multi-dimensional drift flux mixture model for gas-droplet two-phase flow

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Abstract

A multi-dimensional drift flux mixture model was developed to simulate gas-droplet two-phase flows. The drift flux model was modified by considering the centrifugal force on the liquid droplets. Therefore the traditional 1D drift flux model was upgraded to multi-dimension, 2D and 3D. The slip velocities between the continual phase (gas) and the dispersed phase (liquid droplets) were able to calculate through multi-dimensional diffusion flux velocities based on the modified drift flux model. Through the numerical simulations comparing with the experiments and the simulations of other models on the backward-facing step and the water mist spray, the model was validated.

Keywords: drift flux mixture model, slip velocity, two-phase flow, droplet, spray.

Introduction

Liquid spray systems are widely used in many chemical, petrochemical and biochemical industries, such as absorption, oxidation, hydrogenation, coal liquefaction and aerobic fermentation. The operation of these systems is preferred because of the simple construction, ease of maintenance and low operating costs. When the spray is injected from nozzle, it causes a turbulent stream to enable an optimum phase exchange. It is built in numerous forms of construction. The mixing is done by the liquid droplets and it requires less energy than mechanical stirring.

A good understanding of the liquid droplet dynamics of the spray will help the engineers to design the high efficient facilities under optimized operating parameters. Due to the complex two-phase or multi-phase flow and turbulence, normally the flow in spray system is under transient regime. The time average values of the parameters, such as liqud holdup distributions, liquid phase back mixing, gas-liquid interface disturbing, mass and heat transfer between gas and liquid phases, liquid droplet distributions, liquid droplet velocities etc., have to be considering the influence of turbulence. Although the operation of spray system is simple, the actual physical flow phenomena are still lack of complete understanding of the fluid dynamics (Husted, 2007).

Many experimental facilities and methods were introduced to study the multiphase flows in spray systems. Ruck and Makiola (1988) used a laser-Doppler anemometer (LDA) to study the gas-oil droplet passing over a backward facing step. Ferrand et al. (2003) used a phase Doppler and laser induced fluorescence technique to study the gas-droplet turbulent velocity and two-phase interaction through a jet with partly responsive droplets. Esposito et al. (2010) used a monochrome charge-coupled device CCD camera to study the growing of the droplets. The experimental methods can provide very useful information about the liquid droplets at certain measurement points, but they are difficult to show the details of the flow fields and parameters inside the spray.

Following the development of computer technology, it is already allowed to use the numerical method to do the researches in the recent decades (Shang et al., 2008). Therefore, many researchers employ the numerical method, called as computational fluid dynamics (CFD), to study the details of the flows. Griffiths et al. (1996) employed the coupled particle Lagrangian model with Eulerian continual fluid flow model to simulate a cyclone sampler and compared the numerical results with the empirical models. Barton (1999) used the stochastic Monte Carlo scheme coupled with k-ε turbulence model to study the particle trajectories in turbulent flow over a backward facing step. Husted (2007) used the Eulerian-Lagrangian model provided by FDS open source software to simulate a water mist spray system for the fully spray spreading and compared with experiments. Through the former studies of CFD method, it can be seen a good mathematical model will not only help to obtain the agreeable simulation results, but also to be simple, efficient and accurate.

A multi-dimensional drift flux mixture model was developed in this paper. This model was based on the idea of Yang et al. (1999) and Shang (2005). It employed a mixture model to describe the multi-phase flows based on Eulerian model. The slip velocity, which can be developed based on the extended 3D drift flux model. Owing to the the extended 3D drift flux model, the effects of gravity and centrifugal force were considered. Through comparisons with experiments and other model simulations on backward facing step and water mist spray, this model was validated.

Mathematical Modeling

Considering a problem of turbulent multi-component multi-phase flow with one continuous phase and several dispersed phases, the time average conservation equations of mass, momentum and energy for the mixture model as well as the turbulent kinetic energy equation and the turbulent kinetic energy transport equation can be written as the following.

$$\partial \rho_m / \partial t + \nabla \cdot (\rho_m U_m) = 0 \tag{1}$$

$$\partial(\rho_m U_m)/\partial t + \nabla \cdot (\rho_m U_m U_m) = -\nabla p + \rho_m g + \nabla \cdot \left[(\mu_m + \mu_t)(\nabla U_m + \nabla U_m^T)\right] - \nabla \cdot \sum \alpha_k \rho_k U_{km} U_{km} \tag{2}$$

$$\partial(\rho_m h_m)/\partial t + \nabla \cdot (\rho_m U_m h_m) = q + \nabla \cdot \left[\left(\frac{\mu_m}{Pr} + \frac{\mu_t}{Pr_t}\right)\nabla h_m\right] - \nabla \cdot \sum \alpha_k \rho_k h_k U_{km} \tag{3}$$

$$\partial(\rho_m k)/\partial t + \nabla \cdot (\rho_m U_m k) = \nabla \cdot \left[\left(\mu_m + \frac{\mu_t}{\sigma_k}\right)\nabla k\right] + G - \rho_m \varepsilon \tag{4}$$

$$\partial(\rho_m \varepsilon)/\partial t + \nabla \cdot (\rho_m U_m \varepsilon) = \nabla \cdot \left[\left(\mu_m + \frac{\mu_t}{\sigma_\varepsilon}\right)\nabla \varepsilon\right] + \frac{\varepsilon}{k}(C_1 G - C_2 \rho_m \varepsilon) \tag{5}$$

in which

$$\rho_m = \sum \alpha_k \rho_k \tag{6}$$

$$\mu_m = \sum \alpha_k \mu_k \tag{7}$$

$$\rho_m U_m = \sum \alpha_k \rho_k U_k \tag{8}$$

$$U_{km} = U_k - U_m \tag{9}$$

$$G = \frac{1}{2}\mu_t \left[\nabla U_m + (\nabla U_m)^T\right]^2 \tag{10}$$

$$\mu_t = C_\mu \rho_m \frac{k^2}{\varepsilon} \tag{11}$$

where, ρ is the density, U are the velocity vectors, α is the volumetric fraction, p is pressure, g is the gravitational acceleration vector, U_{km} is the diffusion velocity vector of k dispersed phase relative to the averaged mixture flow, h is enthalpy, q is heat input, μ is viscosity, μt is turbulent viscosity, Pr is molecular Prandtl number, Pr_t is turbulent Prandtl number, G is stress production. C_μ, σ_k, σ_ε, C_1, C_2 are constants for standard k-ε turbulence model (Launder & Spalding, 1974), shown in Table 1. The subscript m stands for the averaged mixture flow, and k stands for k dispersed phase.

Table 1 Constants of standard k-ε turbulence model

variable	C_μ	σ_k	σ_ε	C_1	C_2
constant	0.09	1.0	1.3	1.44	1.92

Additional to the above equations, the following conservation equation for each dispersed phase is also necessary.

$$\partial(\alpha_k \rho_k)/\partial t + \nabla \cdot (\alpha_k \rho_k U_m) = \Gamma_k - \nabla \cdot (\alpha_k \rho_k U_{km}) \tag{12}$$

where Γ_k is the generation rate of k-phase.

In order to closure the governing equations (1) ~ (12), it is necessary to determine the diffusion velocities U_{km}. The following equation is employed to covert the diffusion velocities to slip velocities that can be presented as $U_{kl} = U_k - U_l$.

$$U_{km} = U_{kl} - \sum \frac{\alpha_k \rho_k}{\rho_m} U_{kl} \tag{13}$$

Actually the above equation can be developed from the definition of the mixture density equation (6), the definition of mixture mass flux equation (8) and the diffusion velocity equation (9). Once the slip velocities are obtained, the whole governing equations will be closured.

Because the slip velocities present the difference of the movement between the dispersed phase for instance gas and the continuous phase for instance liquid. In gas-liquid two-phase flow, the slip velocity can be modeled through the drift flux model (Yang et al., 1999), shown in equation (14).

$$U_{gl} = \begin{cases} -1.53(1-\alpha_l)^{1.5}\left[\dfrac{\sigma(\rho_l - \rho_g)g'}{\rho_g^2}\right]\dfrac{g'}{|g'|}, & \alpha_l < 0.1 \\ -1.53\left[\dfrac{\sigma(\rho_l - \rho_g)g'}{\rho_g^2}\right]\dfrac{g'}{|g'|}, & \alpha_l \geq 0.1 \end{cases} \tag{14}$$

$$g' = g - \frac{dU_m}{dt} \tag{15}$$

$$U_m = \left(\alpha_g \rho_g U_g + \alpha_l \rho_l U_l\right) / \left(\alpha_g \rho_g + \alpha_l \rho_l\right) \tag{16}$$

where U_{gl} is the slip velocity between gas and liquid, σ is surface tension, g is gravity, Um is mixture velocity.

In equation (14), the drift flux model is different from the traditional 1D drift flux model in Zuber and Findlay (1964) and Hibiki and Ishii (2002). It adopts the form as Yang et al. (1999) and Shang (2005). In Yang et al. (1999), the centrifugal force was induced by the mixture volumetric flux to revise the gravity considering the natural curve movement of gas bubbles. Owing to the concerns, the traditional 1D drift flux model (Zuber and Findlay, 1964; Hibiki and Ishii, 2002) was extended to 3D. Because of the extending, the revised 3D drift flux model is able to describe complex flow conditions and to be adopted by CFD. Further, in this paper, the gradient of mixture velocity, which is used to calculate the centrifugal force, is innovatively induced to revise and update Yang et al.'s (1999) 3D drift flux model. After the updating, the new terminal velocity model, shown in equations (14), (15) and (16), is able to suit the gas-droplet two-phase flows. Since the slip velocity is determined, the whole equations are closured to be solved.

Numerical Procedures

In the simulations, the CFD technique was based on ANSYS FLUENT 13.0. In ANSYS FLUENT, during the numerical computing, all differential governing equations are solved by applying a finite volumes method (FVM). For the fluids, the spatial discretization was performed by upwind scheme of second order for all conservation equations and phase coupled SIMPLE scheme was used for coupling between the pressure and velocity. The overall spatial discretization was of the second order accuracy. The first order implicit scheme was used for the time discretization. During the numerical simulations, the pressure-based solver was employed because all the gas and liquid phases were considered as the incompressible fluids. The fixed time stepping method was employed to run the transient simulations.

The terminal velocity model was accomplished using the concept of user defined functions (UDF). This numerical solution was implemented as a subroutine and linked to the ANSYS FLUENT solver via a set of the original UDFs. The decision whether the UDFs of the coefficients should be used for the interfacial forces at the given calculation step was made automatically by the solver.

Numerical Simulations

For the numerical simulations, two typical cases were chosen as the targets in this paper. They are 2D backward facing step and 3D water mist spray. The backward facing step is a kind of basic facility in many engineering applications, which can be used to investigate the fundamental understanding of important turbulent flow features such as flow separation, flow reattachment and free shear jet phenomena. 3D water mist spray is a very good case to be used to do the validations for the multi-dimensional (3D) drift flux mixture model.

4.1 Backward facing step

Ruck and Makiola (1988) did the experiment on a backward facing step using a laser-Doppler anemometer (LDA) measurement technology, shown in Fig. 1. Hereafter, the experiment data has been cited by other researchers (Tu, 1997; Barton, 1999; Tian, 2006). The backward facing step was with an expansion ratio of 1:2. The step height was 25 mm and the backward channel height after the step was 50 mm. During the experiment, the liquid droplets are kind of oil droplets which were of size of 1 μm generated thought an atomizer. The oil's density was of ρ_l = 810 kg/m^3. The flow Reynolds number (based on the step height h) was of Re = 64000.

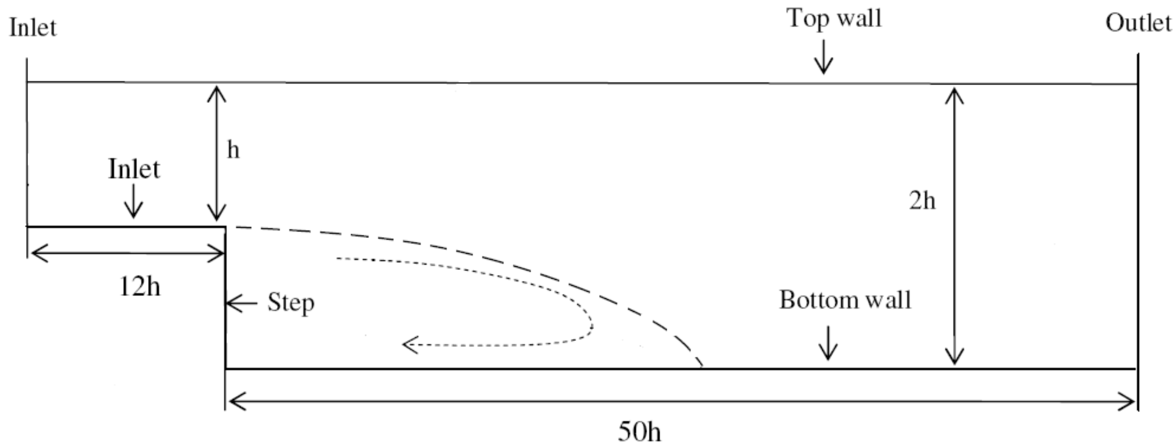


Fig. 1 Diagrammatic sketch of backward facing step

During the simulations, the numerical exercise was performed in a two-dimensional (2D) environment since only 2D representative measurements were available. All the parameters were used same as Ruck and Makiola (1988). The air and oil droplets were under atmospheric pressure. The grid size was employed same as Tian (2006). The computational domain had a size of 12h × 1h before the step and 50h × 2h after the step to ensure the flow was fully developed at the exit. Within the length of 12h before the step, 100 (in the stream-wise direction) × 20 (in the lateral direction) uniform grid points have been allocated. Further downstream, the mesh is with 250 uniform grid points in the stream-wise direction and 40 uniform grid points in the lateral direction. Grid independence was checked by refining the mesh system through doubling the number of grid points along both of the stream-wise and the lateral directions.

Fig. 2 shows the comparisons of the simulation using current drift flux mixture model with the experiment data and the simulation by Tian (2006) using Eulerian-Lagrangian particle tracking model. The computed particle velocity profiles were against measurements for a Reynolds number of 64000, at locations of x/h = 0, 1, 3, 5, 7 and 9 respectively behind the step. The velocity profiles are normalized by the free stream velocity u0 that is with value of 40 m/s.

From Fig. 2, it can be seen that the multi-dimensional drift flux mixture model is able to have the predictions similar with Eulerian-Lagrangian particle tracking model. At the location x/h ≥ 3, the simulation results are even better than Eulerian-Lagrangian particle tracking model comparing with the experiment.

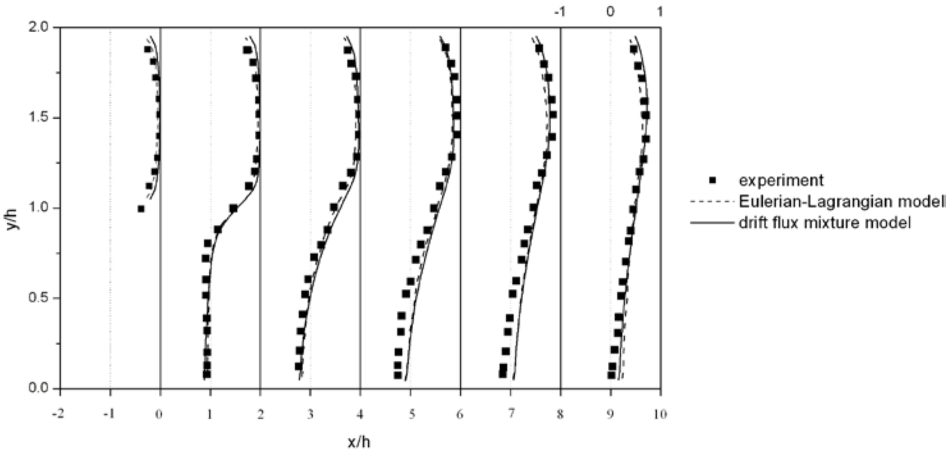


Fig. 2 Comparisons of particle velocities between experiments and simulations

4.2 Water mist spray

Husted (2007) did the experiment on a water mist spray system using a particle image velocimetry (PIV), phase Doppler anemometer (PDA) and a high-speed camera measurement technology, shown in Fig. 3. In Husted's (2007) experiment, the water mist spray is used for fire extinguishing. The purpose of the experiment was to fill the lack of guidelines available for dimensioning water mist systems. The experiment data were good to be used to measure the modeling and numerical simulations. Therefore this experiment was chosen in this paper as the validation tool to validate the drift flux mixture model.

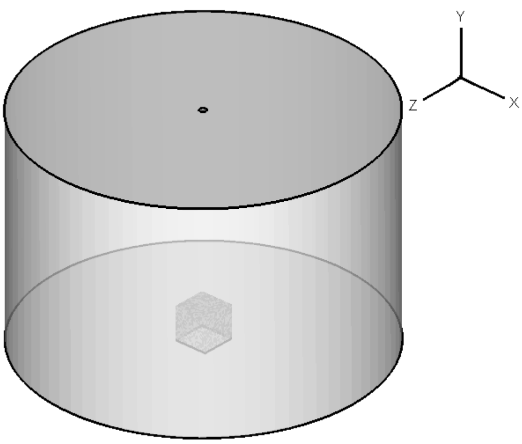


Fig. 3 Diagrammatic sketch of water mist nozzle

During the simulations, the numerical exercise was performed in a three-dimensional (3D) environment. All the parameters were used same as Husted (2007). Fig. 4 shows the mesh distribution. Before the formal simulations, the mesh cell sensitivity studies were carried out among the mesh cells from 154000 to 492000. Fig. 5 shows the comparisons of simulation results of the water mist velocities at different mesh cells. Through the comparisons, it can be seen that among the mesh cells of 154000, 328000 and 492000 the simulation results were not sensitive because there is no evident difference among the results. The averaged errors of the simulation results among the mesh cells were less than ±2.5%. Considering both of the accuracy and the cost of computational time, the formal simulations were carried out by using the mesh cells of 328000. During the simulations, the time step was set as a constant of 0.01 seconds. The simulation time for every case lasted long enough until its steady state.

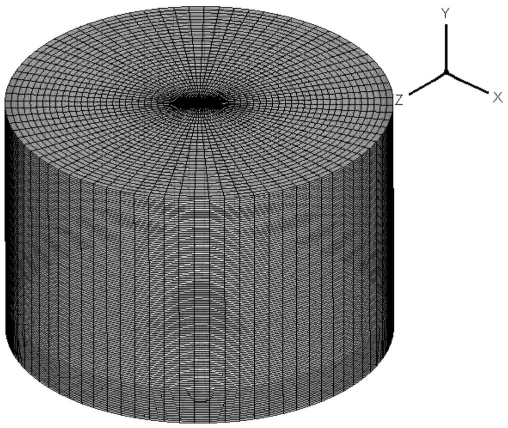


Fig. 4 Mesh distribution

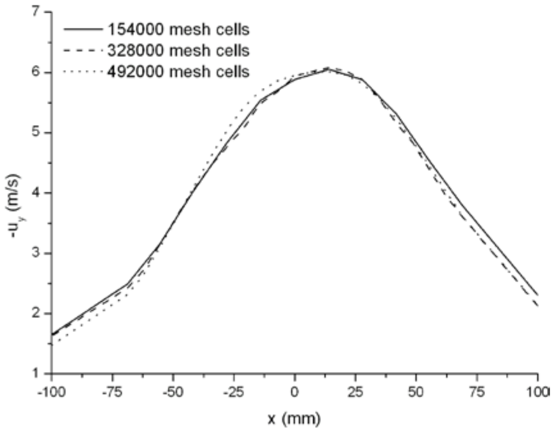
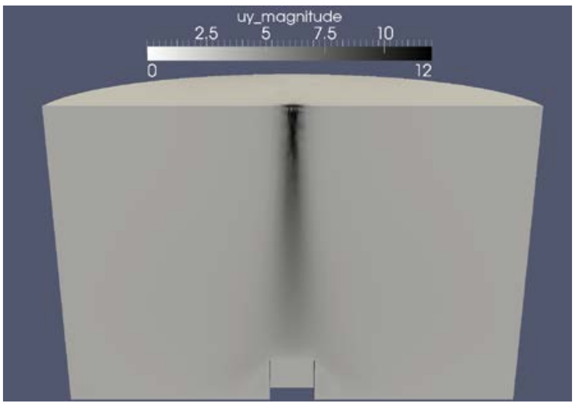
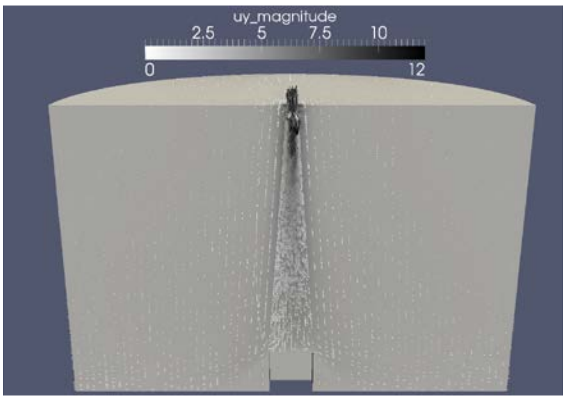


Fig. 5 Mesh sensitivity studies

Fig. 6 shows the distributions of the water mist droplet velocity vector long y coordinate at x-y cross section. From Fig. 6, it can be seen that the droplets flow down in the middle and gradually spreads like a cone shape down from the nozzle. According to the studied of Husted (2007), the stages of the development of the cone spray can be separated as initial conical zone, inflow zone, transition zone, turbulent zone and full cone zone. When the distance is far from 500 mm down from the nozzle, the spray is fully mixed and drop distribution is uniform. The drop velocity becomes flat.



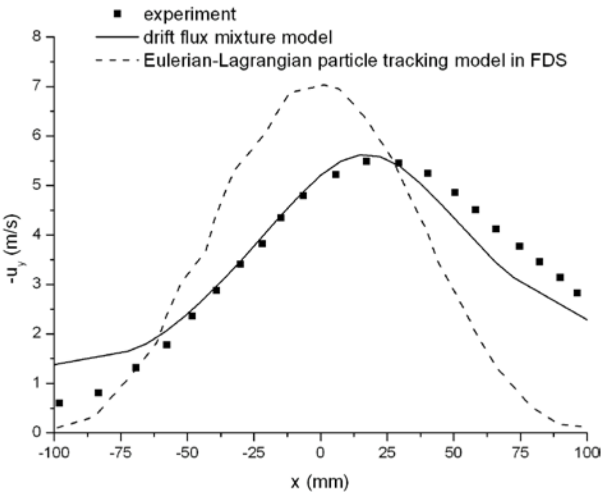
(a) contour of u_y velocity



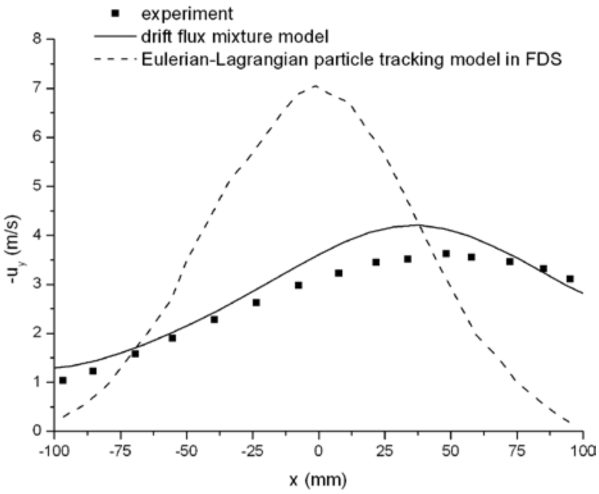
(b) vectors of u_y velocity

Fig. 6 Water mist droplet velocity vector at x-y cross section

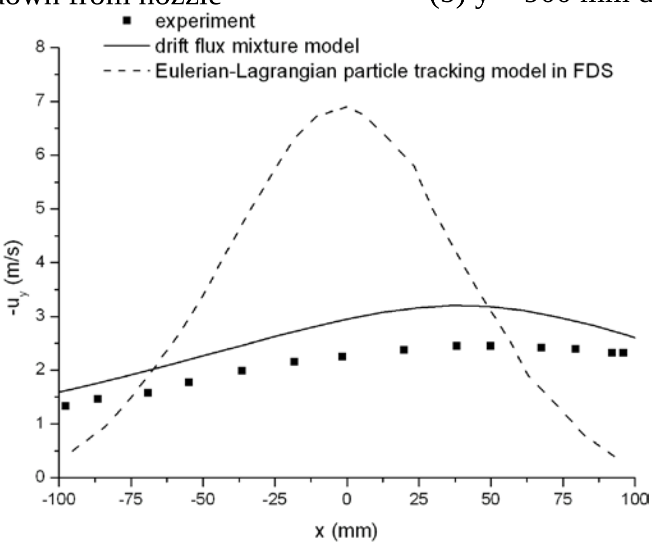
Fig. 7 shows the comparisons of the water mist droplet velocity of the simulations with experiments along different positions down from the nozzle. In Fig. 7, the reference numerical simulations were carried out by Eulerian-Lagrangian particle tracking model in FDS4.0 (FDS, 2013). From the comparisons, it can be seen that the drift flux mixture model is able to capture the velocity profile same as experiments. The numerical predictions have not only the peak value is quite near experiment, but also the position is approaching experiment. The results are much better than the predictions by Eulerian-Lagrangian particle tracking model in FDS4.0.



(a) y = 600 mm down from nozzle



(b) y = 900 mm down from nozzle



(c) y = 1300 mm down from nozzle

Fig. 7 Comparisons of water mist droplet velocity under different positions down from nozzle

Conclusions

The novel multi-dimensional drift flux mixture model is developed based on the mixture multiphase flow model. The diffusion velocity between the dispersed phase and the mixture is closured through the slip velocity. The slip velocity is developed through the drift flux model. Accordingly the multi-dimensional drift flux mixture model is different from the general homogenous model that treats the dispersed phase and the continuous phase flowing under same velocity on multiphase flow. Through the comparisons of the numerical simulations between the multi-dimensional drift flux mixture model and experiments, the model is validated. Through comparisons of the numerical simulations between the multi-dimensional drift flux mixture model and the numerical simulations of Eulerian-Lagrangian particle tracking model, the efficiency and accuracy of the model is confirmed.

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