Prediction of Turbulent Diffusion Coefficient of Liquid Droplet Using Lagrangian Simulation

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Droplet behavior in turbulent flow field was analyzed based on Lagrangian simulation of droplet and droplet diffusion coefficient was predicted. In Lagrangian simulation of droplet, turbulent field of gas flow was calculated by low Reynolds number type k-ε model and the equation of motion of droplet in turbulent gas field was solved for each droplet considering the stochastic interaction between droplet and turbulent eddy of gas flow. An improved eddy interaction model was used where stochastic models of eddy life time and eddy size considered in details. As for the forces on acting on droplet, drag force and lift force were considered. Various models for lift force were evaluated and anisotropy of turbulence field is also considered. Based on these models, trajectory of droplet in the turbulent gas field was calculated for each droplet. Statistical treatment of trajectories of sufficiently large number of droplets, dispersion of droplets was calculated and turbulent diffusion coefficient was derived. It is revealed that the fluctuation of the droplet velocity at inlet has a large effect on the turbulent diffusion coefficient when the relaxation time of droplet was larger than time scale of velocity fluctuation of droplet. This indicated that turbulent diffusion of droplet shows different value for different inlet velocity fluctuation although other operational conditions of annular droplet flow are same. The effect of lift force on the turbulent diffusion coefficient was shown to be small. The predicted turbulent diffusion coefficients well reproduced those obtained in experiment.

KEYWORDS : droplet flow, turbulent diffusion, Lagrangian simulation, lift force

I. Introduction

Annular droplet flow is one of the most important flow regimes in gas-liquid two-phase flow. In many industrial equipments such as boiler, nuclear reactor, chemical plant, this flow regime is often encountered both in normal and anomaly conditions. Therefore, considerable researches have been carried out on this flow regime both experimentally and analytically1,2) and a lot of knowledge has been accumulated. However, due to the complexity of the phenomena, there are still some subjects to be studied further. In annular droplet flow, gas velocity is usually very high and gas flow is in turbulent condition. In this turbulent gas flow field, droplet moves in quite complicated way due to the interaction with turbulent eddy of gas phase (turbulent diffusion). Some droplets finally reach to the pipe wall or liquid film on it (deposition). When there is liquid film in the pipe wall, droplets entrained from the liquid film due to the strong shear of gas flow (entrainment). In order to predict the thermohydrodynamic characteristics of annular droplet flow, accurate knowledge of such droplet behavior is indispensable. Of course, there have been considerable experimental and analytical works on droplet behavior in annular droplet flow1-14). However, experimental data and constitutive equations still show considerable scatters15) due to the difficulties of experimental techniques.

II. Basic Equation of Droplet Behavior Simulation

In order to analyze the droplet behaviors in more accurate ways, numerical analyses of annular droplet flow and droplet behavior by Lagrangian method, in which the trajectory of each droplet is calculated, becomes more and more important along with remarkable progresses of computer and numerical technologies. This method has prevailed especially in the area of solid-gas flow analysis6). Using such method, detailed analyses of annular droplet flow and droplet behavior under high pressure and high temperature, under complicated flow geometries become possible17).

Based on this Lagrangian method, analytical research was carried out on the droplet behavior particularly focused on the droplet diffusion phenomenon. Effects of various model and boundary conditions on droplet diffusion were evaluated and the predicted results were compared with experimental results with reasonable agreements.
various methods to obtain turbulent velocity field of gas phase such as direct numerical simulation, large eddy simulation and simulation by appropriate turbulence models. Among these, simulation by $k$-$\varepsilon$ turbulence model is most commonly used in practical calculation of turbulence flow field. However, in this model, the local instantaneous velocity of gas phase is not given. Instead, averaged velocity, turbulence kinetic energy and turbulent dissipation are calculated. Therefore, in this model, one needs some stochastic method to evaluate local instantaneous velocity from averaged velocity and turbulent kinetic energy. Furthermore, in this model, the time of interaction between droplet and gas turbulent eddy should be evaluated based on appropriate model. The result of Lagrangian simulation of droplet is strongly dependent on these models. In what follows, the basic equations and models for Lagrangian simulation of droplet will be described.

1. Calculation of Turbulent Flow Filed of Gas Phase

In calculating the turbulent flow filed of gas phase, low Reynolds number type $k$-$\varepsilon$ model proposed by Myong-Kasagi \cite{18,19} was used. Here, droplet flow in axisymmetric pipe flow is analyzed. Therefore, following basic conservation equations of mass, averaged momentum, turbulence kinetic energy and turbulence dissipation were solved in cylindrical coordinate assuming axisymmetry under steady state. Here, $x$ is coordinate in flow direction and $r$ is coordinate of radial direction.

(Mass)

$$\frac{\partial (\rho U)}{\partial x} + \frac{\partial (\rho V)}{\partial r} = 0$$  \hspace{1cm} (1)

where $\rho$, $U$ and $V$ are density, averaged velocity in $x$ direction and averaged velocity in $r$ direction.

(Averaged momentum in flow direction)

$$\frac{1}{r} \left[ \frac{\partial}{\partial x} (\rho U U) + \frac{\partial}{\partial r} (\rho V U) \right]$$

$$= -\frac{\partial \rho}{\partial x} + \frac{1}{r} \left[ \frac{\partial}{\partial x} \left( \mu_{\text{eff}} \frac{\partial U}{\partial x} \right) + \frac{\partial}{\partial r} \left( \mu_{\text{eff}} \frac{\partial U}{\partial r} \right) \right]$$

$$+ \frac{\partial \mu_{\text{eff}}}{\partial x} \frac{\partial U}{\partial x} + \frac{1}{r} \frac{\partial \mu_{\text{eff}}}{\partial r} \frac{\partial V}{\partial x} - F_d$$  \hspace{1cm} (2)

(Turbulence kinetic energy, $k$)

$$\frac{1}{r} \left[ \frac{\partial}{\partial x} (\rho U k) + \frac{\partial}{\partial r} (\rho V k) \right]$$

$$= \frac{1}{r} \left[ \frac{\partial}{\partial x} \left( r \left( \frac{\mu_{\text{eff}}}{\sigma_k} \right) \frac{\partial k}{\partial x} \right) + \frac{\partial}{\partial r} \left( r \left( \frac{\mu_{\text{eff}}}{\sigma_k} \right) \frac{\partial k}{\partial r} \right) \right]$$

$$+ G - \rho C_D \varepsilon$$  \hspace{1cm} (3)

Here, $G$ is given by

$$G = \mu_{\text{t}} \left[ 2 \left( \frac{\partial U}{\partial x} \right)^2 + \left( \frac{\partial V}{\partial r} \right)^2 + \left( \frac{V}{r} \right)^2 \right] + \left( \frac{\partial U}{\partial r} + \frac{\partial V}{\partial x} \right)^2$$

$\frac{2}{3} \mu_{\text{t}} \left[ \frac{1}{r} \frac{\partial}{\partial r} \left( r V \right) + \left( \frac{\partial U}{\partial x} \right)^2 \right]$

(Turbulent dissipation, $\varepsilon$)

$$\frac{1}{r} \left[ \frac{\partial}{\partial x} \left( \rho (u \sigma) \right) + \frac{\partial}{\partial r} \left( \rho (v \sigma) \right) \right]$$

$$= \frac{1}{r} \left[ \frac{\partial}{\partial x} \left( \left( \mu + \frac{\mu_{\text{eff}}}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial x} \right) + \frac{\partial}{\partial r} \left( \left( \mu + \frac{\mu_{\text{eff}}}{\sigma_k} \right) \frac{\partial \varepsilon}{\partial r} \right) \right]$$

$$+ \frac{\varepsilon}{k} \left( C_{\varepsilon_1} f_1 G - \rho C_{\varepsilon_2} f_2 \varepsilon \right)$$

The parameters in above equations are given by

$$\mu_{\text{t}} = \rho C_{\mu} f_{\mu} \frac{k^2}{\varepsilon}$$  \hspace{1cm} (6)

$$C_{\mu} = 0.09$$  \hspace{1cm} (7)

$$f_{\mu} = \left( 1 + \frac{3.45}{\sqrt{R_t}} \right) \left[ 1 - \exp \left( - \frac{y^*}{70} \right) \right]$$  \hspace{1cm} (8)

$$R_t = \frac{k^2}{\nu \varepsilon}$$  \hspace{1cm} (9)

$$\sigma_k = 1.4, \quad \sigma_{\varepsilon} = 1.3, \quad C_{\varepsilon_1} = 1.4, \quad C_{\varepsilon_2} = 1.8$$  \hspace{1cm} (10)

$$f_1 = 1.0$$  \hspace{1cm} (11)

$$f_2 = \left[ 1 - \frac{2}{9} \exp \left( - \left( \frac{R_t}{6} \right)^2 \right) \right] \left[ 1 - \exp \left( - \frac{y^*}{5} \right) \right]^2$$  \hspace{1cm} (12)

Equations (1) through (5) are discretized by finite volume method and solved by SIMPLE method using Eqs.(6) through (12).

2. Calculation of Droplet Trajectory

Each trajectory of droplet is calculated by solving the equation of motion considering, gravity, buoyancy, drag and lift force acting on droplet. The equation of motion is given by

$$\frac{d^2 x}{dt^2} = \frac{F_{\text{drag}}}{m}$$

where $x$ is the position of droplet, $m$ is the mass of droplet, and $F_{\text{drag}}$ is the drag force acting on droplet.
\[ m_d \frac{d^2 \mathbf{X}_d}{dt^2} = -\frac{1}{2} C_d \rho_d \left| \mathbf{v}_d - \mathbf{v}_g \right| \left| \mathbf{v}_d - \mathbf{v}_g \right| \frac{\pi D_d^2}{4} \]

\[ + K_{Mei} \frac{K \mu D_d^2}{v^2} \text{sgn} \left( \frac{dU}{dy} \right) \left| \frac{dU}{dy} \right| \left( \mathbf{U}_g - \mathbf{U}_d \right) \]

\[ + m_d g \left( 1 - \frac{\rho_g}{\rho_d} \right) \]

Here, \( m_d \), \( \mathbf{X}_d \) and \( D_d \) are mass, position vector and diameter of droplet. Suffix \( d \) denotes droplet and \( g \) denotes gas phase.

The last term of the right hand side of Eq.(13) is gravitational force (considering buoyancy) acting on droplet where \( g \) is gravity vector.

### 3. Interaction between Droplet and Turbulence Eddy

Integrating Eq.(13) using Eqs.(14) through (20) under appropriate initial and boundary conditions, the trajectory of each droplet can be calculated. For this purpose, the local instantaneous gas velocity in Eq.(13) should be given. However, as described in Sec.1, in the calculation of turbulent flow field of gas phase by k-\( \varepsilon \) model, only averaged velocity and turbulent kinetic energy are predicted. Therefore, based on some models, local instantaneous gas velocity is estimated. The typical method is stochastic method considering the behavior of turbulence eddy. In the present study, this method is used.

In this method, turbulence eddy has uniform velocity and certain size and lifetime. Droplet interacts with this turbulence eddy. First, at certain time and droplet location, droplet starts to interact with one eddy. The velocity in the eddy is estimated stochastically by Eqs.(21) and (22)

\[ u_g = U_g + u'_g \]

\[ v_g = V_g + v'_g \]

Here, \( u_g \) and \( v_g \) are local instantaneous velocity of gas phase in \( x \) and \( r \) direction. \( u'_g \) and \( v'_g \) are fluctuating velocity of gas phase in \( x \) and \( r \) direction and they are assumed to obey Gaussian distribution with standard deviation of \( (2k/3)^{1/2} \) and given stochastically.

Droplet is assumed in this uniform velocity field given by Eqs.(21) and (22) for droplet eddy interaction time \( T_i \). Here, droplet contact time is given by

\[ T_i = \min(T_L, T_c) \]

In Eq.(23), \( T_L \) is lifetime of eddy and \( T_c \) is contact time in which droplet pass through the eddy due to the relative velocity of droplet and eddy.

For lifetime of eddy, the following equations proposed by Corrsin \(^{23}\) were used. These equations were confirmed experimentally by Snyder and Lumley \(^{24}\)

\[ T_L = \frac{\Lambda}{\left( \frac{2}{3} k \right)^{3/2}} \]

\[ \Lambda = \frac{\varepsilon \alpha k^{3/2}}{3} \]

\[ \alpha = 0.165 \]

Here, \( \Lambda \) is the size of eddy.
On the other hand, contact time $T_C$, is given by the time when the distance from the eddy and droplet become $\Lambda$ after they start to interact with the droplet velocity $u_{po}$ and gas velocity $u_{go}$. It is finally given by

$$T_C = -\tau \ln \left( 1 - \frac{\Lambda}{u_{po} - u_{go} \tau} \right)$$

(27)

where $\tau$ is the relaxation time of droplet.

Above mentioned equations are most commonly used in Lagrangian simulation of particle including droplet. However, base on more detailed analysis of droplet eddy interaction $^{25,26}$, it is recommended that the values of $T_L$ given by Eq.(24) and $\Lambda$ in Eq.(27) are doubled.

For the calculated droplet eddy interaction time $T_I$, gas phase velocity is assumed to be constant value as obtained by Eqs.(22) and (23). During this droplet eddy interaction time, Eq.(13) is solved by 4th order Runge-Kutta method for appropriate time mesh. At the end of the calculation, a new droplet position is determined. Then for this new droplet position, a new gas velocity is calculated by above mentioned method. The trajectory of droplet will be calculated such calculation procedure is iterated.

4. Anisotropy of Gas Phase Turbulence

Turbulence in the central portion of pipe is considered to be equilateral. However, in the region near pipe wall, turbulence becomes nonequilateral. Since the droplet behavior depends strongly upon gas phase turbulence, it is necessary to consider anisotropy of turbulence near wall. Here, correlation proposed by Matida$^{27}$ is used which is given by

$$\frac{u'_{rms}}{u^*} = \frac{0.5241 \cdot y^+}{1 + 0.0407 \cdot y^{+1.444}}$$

(28)

$$\frac{v'_{rms}}{u^*} = \frac{0.00313 \cdot y^{+2}}{1 + 0.00101 \cdot y^{+2.253}}$$

(29)

$$\frac{w'_{rms}}{u^*} = \frac{0.160 \cdot y^+}{1 + 0.0248 \cdot y^{+1.361}}$$

(30)

where $u^*$ is friction velocity and $y^+$ is dimensionless distance from the pipe wall. The nonequilateral turbulence velocity calculated by Eqs.(28) through (30) is shown in Fig.1.

III. Result and Discussion

Using the basing equations and constitutive relations described above, one can carry out Lagrangian simulation of droplet in turbulent gas flow. Here, in order to confirm the validity of the present model, Lagrangian simulation was carried out and compared with reference experiments by Ginsberg$^{28}$ and Vames$^{29}$ where droplet diffusion phenomena were measured.

1. Comparison with Ginsberg’s Experiment

Ginsberg$^{28}$ carried out the experiment on the droplet diffusion coefficient in downward flow in 11.58 m long straight tube with 190.5mm diameter. Experimental apparatus is shown in Fig.2. Droplets with uniform diameter are introduced at the center of the pipe and the radial distribution of droplet concentration was measured at the positions of 1.22m, 3.66 m and 6.9 m downstream of droplet injector. From the radial distributions of droplet concentration and diffusion theory, droplet diffusion coefficients were calculated. Experiments were carried out for droplet diameters of 80, 150, and 200 $\mu$m and gas phase Reynolds number of 2.5 $\times$ 10$^4$, 5.0 $\times$ 10$^4$, 1.0 $\times$ 10$^5$.

For the same conditions as experiments, Lagrangian simulation was carried out. Trajectories of many droplets were calculated and the results are treated statistically and radial droplet concentration distributions by Lagrangian simulation were obtained. From these radial concentration distributions, diffusion coefficients were predicted. In Lagrangian simulation, the effects of various parameters and constitutive correlations were evaluated.

As for the effect of the droplet number, the result of simulation showed that when the droplet number is more than 10000, the results of simulation were almost same. Therefore, in this study, number of droplet in the simulation was fixed to 10000.

The effect of models of transverse lift force and anisotropy were also evaluated. However, in this case, droplet diffusion phenomena occur at the central portion of pipe where turbulence considered to be equilateral and radial.
gradient of averaged gas velocity is small. Therefore, no appreciable effects of transverse lift force and anisotropy were observed from the simulation result.

Lagrangean simulation to Eq.(30), the initial velocity and its fluctuation of droplet and turbulent field of gas at the position of introduction of droplet have quite important effects on the droplet trajectories as shown in the following section. In the Ginsberg’s experiment, droplet is introduced in the developing region of gas phase turbulent field. Therefore, calculation was carried out estimating the turbulent velocity of developing region so as to obtain the best fit between experiment and calculation.

\[ \frac{C(r,x)}{C_{\text{MAX}}} = \exp\left( -\frac{\nu_r r^2}{4\varepsilon_d x} \right) \]

where \( C(r,x) \) droplet concentration and \( C_{\text{MAX}} \) is the maximum value. \( \varepsilon_d \) is the droplet diffusion coefficient.

From the fitting of experimental result and Lagrangian simulation to Eq.(30), \( \varepsilon_d \) is obtained Figure 6 shows the comparison of droplet diffusion coefficient between experiment and Lagrangian simulation. As shown in this figure, Lagrangian simulation in the present study well predicted the droplet diffusion coefficient.

In the Lagrangian simulation of droplet, the initial velocity and its fluctuation of droplet and turbulent field of gas at the position of introduction of droplet have quite important effects on the droplet trajectories as shown in the following section. In the Ginsberg’s experiment, droplet is introduced in the developing region of gas phase turbulent field. Therefore, calculation was carried out estimating the turbulent velocity of developing region so as to obtain the best fit between experiment and calculation.

\[ C_{r,z}/C_{\text{max}} = \exp\left(-1027r^2/1.31 \times 10^8\right) \]

\[ C_{r,z}/C_{\text{max}} = \exp\left(-31800r^2/1.77 \times 10^7\right) \]

\[ C_{r,z}/C_{\text{max}} = \exp\left(-3021r^2/1.77 \times 10^7\right) \]

\[ C_{r,z}/C_{\text{max}} = \exp\left(-31800r^2/5.96 \times 10^7\right) \]

\[ C_{r,z}/C_{\text{max}} = \exp\left(-31800r^2/5.96 \times 10^7\right) \]
2. Comparison with Vames’ s Experiment

Vames 29) carried out experiment on droplet diffusion in downward flow in pipe with a diameter of 5.08 mm. In the well developed region of gas turbulence (107 diameter length from the inlet of test section), droplets are introduced into gas flow through injected nozzle located in the center of the pipe. Experiment was carried out for droplet diameters of 50 µ, 90 µ and 150 µ. Droplet concentration distributions were measure using optical method. Gas Reynolds number ranged from $10^4$ to $10^5$. Experimental apparatus is shown in Fig.7.

![Experimental apparatus of Vames' Experiment](image)

At various positions from the injector, the distribution of droplet number passing per unit time $N(r,x)$ was measured. Measured distribution of droplet number is approximated by Gaussian distribution curve which is given by

$$\frac{N(r,x)}{N_{\text{MAX}}} = \exp\left( -\frac{r^2}{2X_P^2} \right)$$

(32)

From the Eq.(32), averaged square displacement $X_P^2$ is obtained as a function of the distance from injector, $x$. In Vames’ experiment, the distance, $x$ is converted to the time during which droplet moves from injector to the location $x$, which is given by

$$t = \frac{x}{V_p}$$

(33)

The relation between $X_P^2$ and $t$ expresses the droplet diffusion.

Prediction of distribution of droplet number per unit time is carried out based on Lagrangian simulation for the same condition as experiment. The effects of various constitutive relations and boundary conditions were evaluated. The comparison was made between prediction and experiment.

Figures 8 through 10 show that the comparison of $X_P^2 - t$ relation between experiment and prediction. In these figures, the predicted values are shown considering the effects of constitutive relation of lift force, turbulence anisotropy and initial velocity condition of droplet.

In order to evaluate the effect of the constitutive relation of transverse lift force, Lagrangian simulation was carried out using Saffman’s original correlation 21) for transverse lift force and Mei’s modified correlation 22) (Eq.(17) through (20)). As shown in Figs.8 through 10, in the present condition, the effect of transverse lift force correlation is not appreciable because droplet diffusion phenomenon occurs at the central part of pipe where the velocity gradient of averaged gas velocity is small.

In respect to anisotropy, the effect is negligible in the present analyses as shown in Figs.8 through 10 because droplet diffusion phenomenon occurs at the central part of pipe where turbulence is considered to be equilateral.

On the other hand, the effect of initial velocity condition of droplet is remarkable for large droplet diameter (90 and 150µ) whereas the effect is negligible for smaller droplet diameter (50 µ). When the droplets are introduced into the turbulent gas field through nozzle, initial velocity of droplet may change due to the turbulence fluctuation of gas phase velocity. Therefore, in the Lagrangian simulation, two cases of calculations were carried out with and without including turbulence fluctuation velocity into the droplet initial velocity. As shown in Figs.9 and 10, the prediction well agreed with the experiment when one considers the turbulence fluctuation velocity. The importance of the turbulence fluctuation velocity on Lagrangian simulation of droplet depends upon the relaxation time of droplet which is given by
\[ \tau = \frac{D_d^2}{18 \mu_g} \]

(34)

For smaller droplet diameter (50 µ), relaxation time is small which means the droplet soon become momentum equilibrium. Therefore, the effect of initial fluctuation velocity is not appreciable. On the other hand, for larger droplet diameter, effect of initial fluctuation velocity droplet last relatively longer time due to the larger relaxation time of droplet.

Fig.8 Comparison of \( X_p^2 - t \) relation between experiment and prediction \((D_d=50\mu, Re=2.1 \times 10^4)\)

Fig.9 Comparison of \( X_p^2 - t \) relation between experiment and prediction \((D_d=90\mu, Re=5.6 \times 10^4)\)

IV. Conclusions

Lagrangian simulation of droplet in turbulent velocity field of gas phase was carried out and diffusion phenomenon of droplet is predicted. The effects of various constitutive correlations and models are evaluated and appropriate basic equations of gas phase turbulence and equation of motion of droplet were presented. Mei’s modified correlation was used for transverse lift force and detailed model for droplet eddy interaction time was considered. The anisotropy of gas phase turbulence is also considered near the pipe wall. The experimental results of droplet diffusion by Ginsberg and Vames were compared with the prediction by Lagrangian simulation based on the present basic equations and constitutive models. The predicted result well agreed with the experimental data. Among various parameters and constitutive models, the initial fluctuation velocity of droplet is found to be most important particularly for the larger droplet diameter where relaxation time is large.

The present study showed that using appropriate basic equations and models, the droplet behaviors in turbulent velocity field can be successfully predicted by Lagrangian simulation of droplet.

References
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