Development of New Coalescence and Breakup Closures for the Inhomogeneous MUSIG Model

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ABSTRACT

In the present study we propose new coalescence and breakup closures for the inhomogeneous multiple bubble size group (MUSIG) model. The major purpose is to consider bubble coalescence and breakup due to different mechanisms and to develop a general applicable constitutive model for CFD applications. For bubble coalescence the new model includes coalescence due to turbulence, laminar shear, wake entrainment and eddy capture. Bubble breakup mechanisms encompass turbulent fluctuation, laminar shear and interfacial slip velocity. The new models were implemented in ANSYS-CFX and applied to the case of turbulent air-water mixtures in a large vertical pipe (DN 200). Simulation results for the evolution of radial gas volume fraction, bubble size distribution were compared to as default used closure models of Luo & Svendsen and Prince & Blanch [1, 2] as well as TOPFLOW experimental data. Better prediction of bubble size distribution is accomplished.

1 INTRODUCTION

Flow fields in the safety research of nuclear reactors are usually complex and often involve two-phase flows, where one of the phases is continuous and the other phase consists of disperse bubbles. Interfacial heat and mass transfer within such flows is directly related to the interfacial area density, and to the residence time of the disperse phase. Conventional methods used in 1D system codes are inadequate to resolve the local distribution and redistribution of disperse phase. Computational fluid dynamics (CFD) has been identified as a viable tool for the analysis of such cases. In polydisperse bubbly flows, where the volume fraction of disperse phase is not small, collision, coalescence and breakup of bubbles becomes of paramount importance. It determines not only the local bubble size distribution, but the main hydrodynamical features of both continuous and disperse phases.

In many CFD simulations of two-phase flows, the disperse phases, i.e. bubbles in the gas-liquid flow, are assumed to have an equal size and shape which might be correct for low gas fractions. In the reality of polydisperse flows, due to bubble coalescence and breakup a wide spectrum of sizes and shapes may exist throughout the flow. The inhomogeneous Multiple Size Group (MUSIG) model has led to notable success in the prediction of polydisperse flows by taking the bubble size distribution into account. This model was developed by the cooperation of ANSYS-CFX and Forschungszentrum Dresden-Rossendorf and implemented into the CFD code CFX. During the validation process, the default constitutive models of Luo & Svendsen [1], Prince & Blanch [2] for bubble coalescence and breakup were diagnosed as the weakest point, which needs further investigation. Details can be found in our previous work [3, 4, 5, 6].
Thus, a series of work was done for the purpose of more fundamental models to model bubble coalescence and breakup, which would apply to a large range of flow conditions, e.g. gas and liquid superficial velocity. Based on an extensive literature study on breakup and coalescence models available for fluid particles [7, 8], a basic model has been proposed, which considers coalescence and breakup due to different mechanisms, including coalescence due to turbulence, laminar shear, wake entrainment and eddy capture. Breakup mechanisms encompass turbulent fluctuation, laminar shear and interfacial slip velocity. In the previous work [9, 10], the basic model was implemented in a 1D Test Solver and compared with the experimental data of TOPFLOW test facility. The new model was shown to be capable of tracing the evolution of bubble size distribution due to coalescence and breakup, even for large gas volume fractions.

In this work, the basic model is implemented into the CFD code CFX through user FORTRAN routines, and it serves to the inhomogeneous MUSIG approach as the new constitutive model. Simulations for the evolution of radial gas volume fraction, bubble size distribution along a vertical pipe are presented. For the TOPFLOW experimental data, the new constitutive model shows better prediction of bubble size distribution than the default one.

2 THE BASIC MODEL

The model is formulated on the basis of existing findings with the attempt to combine advantages and overcome limitations of other models [7, 8]. It includes a model for bubble coalescence frequency and a model for bubble breakup frequency, which are required to compute the birth and death rates in the inhomogeneous MUSIG model.

2.1 Coalescence Frequency \( \Gamma(d_i, d_j) \)

The coalescence frequency \( \Gamma(d_i, d_j) \) between two bubbles of diameter \( d_i \) and \( d_j \) is usually calculated as a product of collision frequency and coalescence efficiency [2]. By considering various mechanisms, we rewrite the basic correlation as follows:

\[
\Gamma(d_i, d_j) = C_{coal} \sum_k S_k(d_i, d_j) \cdot \lambda_{rel,k}(d_i, d_j) \cdot \lambda(d_i, d_j)
\]

where the subscript, \( k \), represents different collision mechanisms, \( turb \) (turbulence fluctuation), \( slip \) (slip resulted from laminar shear and buoyancy), \( eddy \) (eddy-capture) and \( wake \) (wake entrainment).

\( S_k(d_i, d_j) \) in Eq. (1) is the collision cross-sectional area of the “collision tube” swept by a bubble of diameter \( d_i \):

\[
S_{turb}(d_i, d_j) = S_{slip}(d_i, d_j) = S_{eddy}(d_i, d_j) = \frac{\pi}{4}[d_i + d_j]^2
\]

\[
S_{wake} = \frac{\pi}{4}[d_i]^2
\]

For the mechanism of wake-entrainment, it is assumed that the bubble with size \( d_i \) is the leading one, who generates a wake region.
In Eq. (1), $w_{rel,k}(d_i, d_j)$ is the relative velocity between the two colliding bubbles, which depends on collision mechanisms.

\[
w_{rel,turb} = \sqrt{2\varepsilon \left[d_i^{2/3} + d_j^{2/3}\right]^{1/2}}, \quad \left[d_i + d_j > \eta\right]
\]

\[
w_{rel,eddy} = C_0 \left[d_i + d_j\right] \left[\frac{\varepsilon}{\nu}\right], \quad \left[d_i + d_j \leq \eta\right]
\]

\[
w_{rel,slip} = \pm \left[u_T(d_i) - u_T(d_j)\right] \pm C_0 \left[d_i + d_j\right] \frac{du_i}{dr}, \quad \left(d_i \geq d_c\right)
\]

\[
w_{rel,wake} = C_1 u_T(d_i) C_D^{1/3}, \quad \left(d_i \geq d_c\right)
\]

where $C_0$ is a constant with a value $0 \sim 0.5$. Its value is dependent on the horizontal distance perpendicular to the velocity gradient between two bubbles. The constant $C_1$ is related to the geometry and size of the wake region. $C_D$ is the drag coefficient and $\eta$ Kolmogorov length scale.

In his theory, Kolmogorov [11] introduced in 1941 the idea that the smallest scales (time, velocity and length) of turbulence are universal and that they depend only on the energy dissipation rate $\varepsilon$ and the kinematic viscosity $\nu$. With these two parameters, the unique length, which is called Kolmogorov length scale, can be obtained by dimensional analysis is:

\[
\eta = \left(\frac{\nu^3}{\varepsilon}\right)^{1/4}
\]

For the calculation of $d_c$ in Eq. (4), the correlation of Ishii and Zuber is used [12]:

\[
d_c = 4 \sqrt{\frac{\sigma}{g\Delta\rho}}
\]

For the calculation of coalescence efficiency $\lambda(V_i, V_j)$, we use the popular film drainage model, which argues that coalescence can occur only if two colliding bubbles keep in contact till the liquid film captured between them drains out to a critical thickness.

\[
\lambda(d_i, d_j) = \exp\left(-\frac{t_{drainage}}{t_{contact}}\right)
\]

The contact time of the two colliding bubbles, $t_{contact}$ is defined as a length scale, dependent on the sizes of bubbles, divided by the maximum of resultant relative velocities arising from different mechanisms.

\[
t_{contact} \propto \frac{d_i + d_j}{\text{max}(w_{rel,k})}
\]
For the determination of film drainage time $t_{\text{drainage}}$, the expression of Prince and Blanch [2] was used,

$$
t_{\text{drainage}} = \left( \frac{r_{\text{eq}}^2 \rho_1}{16 \sigma} \right)^{1/2} \ln \left( \frac{h_0}{h_c} \right)
$$

(9)

where $h_0$ and $h_c$ is the initial and critical film thickness, respectively, and $r_{\text{eq}}$ is the equivalent radius, given by Chesters and Hofman [13],

$$
r_{\text{eq}} = \frac{d_i d_j}{d_i + d_j}
$$

(10)

2.2 Breakup Frequency $\Omega(d_i, d_j)$

The velocity $u_b$ at which the breakup process takes place can be assumed proportional to the difference between the disruptive stress $\tau$ and the minimum required stress $\tau_c$ for the breakage to occur [14]

$$
\nu_b \propto (\tau - \tau_c)^n
$$

(11)

The disruptive stress $\tau$ is dependent on breakup mechanisms,

$$
\tau_{\text{turb}} = \frac{1}{2} \rho_i (\varepsilon d_i)^{2/3}
$$

$$
\tau_{\text{shear}} = \mu_i \dot{\gamma}
$$

$$
\tau_{\text{fric}} = \frac{1}{2} C_2 \rho_i [u_r (d_i)]^2
$$

(12)

The subscripts of $\tau$ in Eq. (12) represent different breakup mechanisms, $\text{turb}$: turbulence fluctuation; $\text{shear}$: velocity shear; $\text{fric}$: interfacial friction force, respectively.

When a relative motion exists between air bubbles and water, small bubbles can be sheared off from the “skirt” at the rim of a large bubble due to the interfacial friction force. $C_2$ is an adjustable constant determined by the interfacial frictional coefficient and the proportional factor between the size of the small bubble and the “skirt” length.

The critical stress $\tau_c$ might be determined by the surface tension of the smallest daughter bubble and the increase of surface energy required for such a breakage [15]:

$$
\tau_c \propto \max \left( \frac{c_{fvv} \sigma}{d_i}, \frac{\sigma}{d_j} \right)
$$

(13)

where $d_j$ is the diameter of the smallest daughter bubble and $c_{fvv}$ is defined as:
The breakup frequency of a bubble with size $d_i$ breaking into a daughter bubble with size $d_j$, $\Omega(d_i,d_j)$, is given by:

$$\Omega(d_i,d_j) = C_{br} \sum_k \frac{n_{b,k}}{d_i}$$  \hfill (15)$$

where the subscript $k$ represents different breakup mechanisms in Eq.(12).

3 INHOMOGENEOUS MUSIG MODEL

The multiple size group model (MUSIG) was first proposed by Lo [16], where the whole diameter range of the disperse phase is divided into $M$ size groups and only one common momentum equation is solved for all size groups (homogeneous MUSIG, see Figure 1a). This model approach has found a number of successful applications because it allows sufficient size groups for the calculation of coalescence and breakup to be accurate. Unfortunately, the restriction of the original model was revealed quickly due to its assumption that the slip velocities of bubbles are independent of bubble size.

Alternatively, the inhomogeneous MUSIG model was developed owing to the cooperation of the Forschungszentrum Dresden-Rossendorf and ANSYS-CFX. In the inhomogeneous MUSIG model the disperse phase is divided firstly into $N$ velocity groups (or phases), where each group is characterized by its own velocity field. Furthermore, each velocity group $j$ is divided into a number of sub-size groups $M_j$, $j=1, 2, \ldots, N$. The population balance model considering coalescence and breakup is applied to the sub-size groups (see Figure 1b).

![Figure 1: Schema of the Homogeneous and Inhomogeneous MUSIG model](image)

Detailed information about the inhomogeneous MUSIG model can be found in the reference [4].

4 RESULTS AND DISCUSSIONS

The basic model depicted in the section §2 was implemented in the inhomogeneous MUSIG model of CFX 12.0 via user subroutine and applied to the case of upwards air-water mixture inside a large pipe (DN 200). Simulation results using the new closure model and the standard one were compared with the experimental data of TOPFLOW test facility where the
interested parameters are determined in the corresponding cross sectional plane by wire mesh sensors [17]. As an example, the validation results for the test point 118 ($J_L=1.017\text{m/s}$, $J_G=0.219\text{m/s}$) are shown here.

4.1 Radial Gas Volume Fraction

By considering that the lift force changes its sign for $d_b$ values of around 6mm [18], the gaseous phase was divided into 2 velocity groups, i.e. $N=2$, the first velocity group (small bubbles, $0<d_b<6\text{mm}$) is subdivided into 3 sub-size groups ($M_1=3$) and the second velocity group (large bubbles, $6<d_b<50\text{mm}$) having 22 sub-size groups ($M_2=22$). The evolution of radial gas volume fraction from the inlet (Level A, $z=0.221\text{m}$) to Level R ($z=7.802\text{m}$) is shown in Figure 2.

![Figure 2: Evolution of Radial Gas Volume Fraction at Different Distance Levels: (a)(b) Small Bubbles ($0<d_b<6\text{mm}$); (c)(d) Large Bubbles ($6<d_b<50\text{mm}$); (e)(f) Total](image)

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Figures 2a ~ 2d show that at the beginning both small and large bubbles swarm towards the pipe center due to the effect of turbulent dispersion. And then under the action of the lift force, small bubbles concentrate near the pipe wall (R=0.098m), while large bubbles migrate further to the pipe centre (R=0.0m). Figures 2e and 2f indicate that the gas migration velocity is overpredicted for both closure models, especially at the early stage (from Level A to Level F). This might be caused by the fact of a too large turbulent dispersion force, which considers the smoothing of radial gas volume profiles by turbulence. In our case, the force disperses the bubbles from the injection position near the wall to the pipe center. The influence of the inlet conditions for turbulent parameters needs further investigation.

Figure 3 is the level-averaged and local bubble size distribution at different distance levels.

Figure 5: Evolution of Bubble Size Distribution: (a) (b) Average Distribution at Different Distance Levels; (c) (d) Local Distribution at the Pipe Bottom (Level A: Inlet); (e) (f) Local Distribution at the Pipe Top (Level R)
Figures 3a and 3b show that in comparison to experimental data, the new closure model predicts a lower number of small bubbles (0<d<6mm) while the standard closure provides an overprediction. Both models can not reproduce the formation of very large bubbles (d>30mm), i.e. the transition from bubbly to churn-turbulent flow. Figures 3e and 3f indicate that according to the new model at the Level R there are more large bubbles concentrated at the pipe center.

Finally, it is noted that the total gas volume fraction from calculation is obviously less than that from the experiment (see Figures 2e, 2f) which might be caused by the assumption of incompressible flows.

5 CONCLUSIONS AND OUTLOOK

The inhomogeneous multiple bubble size group (MUSIG) model is a promising supplement to commercial CFD-codes, e.g. ANSYS-CFX, for their application in polydisperse flows. Its closure models for coalescence and breakup were shown to be the weakest point, which restricts the application range of the MUSIG model. In the present work, effort was made to develop a more general closure model. For the first step, a basic model was proposed to overcome limitations in models available in the literature.

The new model was implemented into the inhomogeneous MUSIG model of CFX 12.0. Simulations were performed for the case of upwards air-water two-phase flows in a vertical pipe. The results were compared with experimental data from TOPFLOW test facility and the standard closure model. Results for one example test point (J_L=1.017m/s, J_G=0.219m/s), a transition between bubbly and churn-turbulent flow, are presented. Generally speaking, both closure models can reproduce the evolution of bubble size distribution and radial gas volume fraction at different distance levels. However, they are unable to predict the regime transition from bubbly flow to churn-turbulent flow, which indicates that the coalescence of very large bubbles is not correctly modelled. Furthermore, there is a substantial deviation between simulated radial gas migration velocity and the measured one. That might be caused by the accuracy of interfacial force modelling. Finally, it is worth to mention that the new model has a notable improvement for the size limit of smallest daughter bubbles during breakage.

Development work for the new closure model is still in progress by considering the effect of models for bubble-induced turbulence and interfacial forces as well as gas compressibility. Further the validation will be done for other test points of TOPFLOW test matrix as well as other flow configurations, e.g. bubble column. A generally applicable set of model parameters, C_0, C_1, C_2, C_coal and C_br should be accomplished.

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