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AN ASSESSMENT OF MECHANISTIC BREAKAGE AND COALESCENCE KERNELS IN POLY-DISPERSED MULTIPHASE FLOW

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ABSTRACT

Gas-liquid bubbly flows (i.e. swarm of discrete gas bubbles suspended in continuous liquid) have a wide range of applications; including mining, pharmaceutical and petroleum industries. Many researches have been carried out to develop an effective design tool for these industries and enhance the efficiency of their systems. Population balance (PB) approach in conjunction with Computational Fluid Dynamics (CFD) technique has been widely recognized as a robust methodology in solving such complex bubbly flows and providing a better understanding of the local flow behaviour. Nonetheless, to model the microscopic bubble interactions, an accurate coalescence and breakup kernel is crucial. Several models have been proposed within literatures for modelling breakup frequency and the daughter size distribution in the breakup mechanism; as well as coalescence frequency and efficiency in coalescence (Liao and Lucas 2009; Liao and Lucas 2010). A thorough assessment of the performance of a number of gas-liquid coalescence and breakage kernels has been carried out to find its effect in modelling the evolution of bubble size distribution in large scale vertical bubble column. A total of four different models were considered (one for breakage and three for coalescence) (Coulaloglou and Tavlarides 1977; Prince and Blanch 1990; Luo and Svendsen 1996; Lehr et al. 2002). To assess the performances under complex flow conditions, validation has been carried out against experimental data of Prasser et al. (2007) measured in the Helmholtz-Zentrum Dresden-Rossendorf (HZRD) facility.

NOMENCLATURE

a	growth rate
p	pressure, Pa
u	velocity, m/s
g	gravity acceleration factor, m/s^2
F	force, N
f	size fraction
S	source or sink term
d	Bubble diameter, mm
h_i, h_f	Initial and critical film thickness, m
$h(d_i, d_j)$	collision frequency of bubbles d_i and d_j.
Pc	coalescence efficiency
P^C, P^B	production due to coalescence and breakage
D^C, D^B	death due to coalescence and breakage
C_{1-4}	Adjustable parameter
ρ	density, kg/m^3
α	void fraction
ε	Turbulent eddy dissipation rate, m^2s^{-3}
μ	dynamic viscosity, Pa.s
σ	surface tension, Nm^{-1}

INTRODUCTION

The study of fluid flow behaviour is believed to be one of the prime requisite in many industrial applications involving multiphase flow because of the fact that significant environmental and safety benefits can be achieved by improved ability to accurately predict the hydrodynamic conditions in multiphase reactors. Therefore computational fluid dynamics (CFD) has been arisen as promising tool which permits the combination of population balance equations (PBE) with the continuity equations in order to gain insight into the factors affecting interfacial transfer processes and flow pattern distribution. To predict the nature of interaction between fluid particles conservation equation will require fluid particle coalescence and breakage rates.

A variety of models have been published in the literature for breakup and coalescence model. Interesting reviews and analysis on breakup and coalescence kernels are given by Liao and Lucas (2010). The coalescence kernel is given by the product of collision frequency and coalescence efficiency for the physical model. The collision frequency can be induced by viscous shear, buoyancy, turbulence, wake entrainment or capture in turbulent eddies. Various coalescence efficiency models have also been proposed in the literature such as critical velocity model, film drainage model and energy model. In this study, coalescence kernel proposed by Lehr et al. (2002) based on critical velocity approach has been compared with kernels proposed by Coulaloglou and Tavlarides (1977) and Prince and Blanch (1990). Based on film drainage model, Coulaloglou and Tavlarides (1977) developed their coalescence model which has become one of the widely adopted models. Later Prince and Blanch (1990) simplified the model of Oolman and Blanch (1986) and proposed the coalescence model for deformable particles with fully mobile interfaces. In case of breakup kernel, model proposed by Luo and Svendsen (1996) has been combined in conjunction with coalescence model. Luo and Svendsen (1996) developed their model concerning the criteria that the turbulent kinetic energy of hitting eddy is greater than a critical value. There have been lot more breakup models published in the literature based on determining the breakup frequency in terms of turbulent fluctuation and

collision, viscous shear stress, shearing off and surface instability (Liao and Lucas 2009).
Different bubble breakup and coalescence models developed by various researchers are implemented into commercial CFD package (Ansys 12.1) through user Fortran subroutine. Breakup and coalescence rates estimated by various researchers are qualitatively compared by implementing different kernel combinations. Bubble size distribution, radial void fraction and interfacial area concentration resulting from CFD analysis are compared with experimental data by Prasser et al. (2007) measured in the HZRD facility.

MATHEMATICAL MODEL DESCRIPTION

Governing Equations

The two-fluid model treating both the gas and liquid phases as continua solves two sets of conservation equations governing mass and momentum. Denoting the liquid as the continuum phase (α_l) and the gas (i.e. bubbles) as disperse phase (α_g), these equations can be written as

$$\frac{\partial}{\partial t}(\rho_i \alpha_i) + \nabla.(\rho_i \alpha_i \bar{u}_i) = 0 \qquad (1)$$

$$\frac{\partial}{\partial t}(\rho_i \alpha_i \bar{u}_i) + \nabla.(\rho_i \alpha_i \bar{u}_i \bar{u}_i) = -\alpha_i \nabla P + \alpha_i \rho_i \bar{g} + \nabla.\left[\alpha_i \mu_i^e \left(\nabla \bar{u}_i + (\nabla \bar{u}_i)^T\right)\right] + F_i \qquad (2)$$

where $\bar{g}$ the gravity acceleration vector and P is the pressure. The closure law is required to determine the momentum transfer of the total interfacial force. This force strongly governs the distribution of the liquid and gas phases within the flow volume. On the right hand side of equation (2), F_i represents the total interfacial force which is composed of the drag force, lift force, wall lubrication force and the turbulent dispersion force respectively. Numerical details on handling these interfacial forces can be found in Cheung et al. (2007) and references therein. For handling the turbulence effects, the Shear Stress Transport (SST) model is adopted for the liquid phase (Menter 1994), while the Sato's bubble-induced turbulent viscosity model (Sato et al. 1981) was employed for the gas phase.

In accordance with the work by Fleischer et al. (1996), the bubble size distribution is calculated with population balance equation (PBE) that is generally expressed in an integro-differential form describing the local Bubble Size Distribution (BSD) written as

$$\frac{\partial f(x,\xi,t)}{\partial t} + \nabla.(V(x,\xi,t) f(x,\xi,t)) = S(x,\xi,t) \qquad (3)$$

where $f(x,\xi,t)$ is the bubble number density distribution per unit mixture and bubble volume, $V(x,\xi,t)$ is velocity vector. On the right hand side, the term $S(x,\xi,t)$ contains the bubble source/sink rates per unit mixture volume due to the bubble interactions such as coalescence, break-up and phase change.

A sophisticated model and most commonly used technique, namely MUltiple SIze Group (MUSIG) was first introduced by Lo (1996) has been considered for solving PBE. The technique proposed by Kumar and Ramkrishna (1996) that allows the usage of variable M bubble size groups to reduce the numerical effort is adopted, such as:

$$\frac{\partial n_i}{\partial t} + \nabla.(u_i^g n_i) = S_i \qquad (4)$$

The interaction term $S_i = (P^C + P^B - D^C - D^B)$ contains the source rates of P^C , P^B, D^C and D^B, which are the production rates due to coalescence and break-up and the death rate to coalescence and break-up of bubbles respectively. The birth and death rates can be formulated in terms of size fraction.

$$P^C = (\rho_j^g \alpha_j^g)^2 \frac{1}{2} \sum_k \sum_l f_k f_l \frac{M_k + M_l}{M_k M_l} a(M_k, M_l) \qquad (5)$$

$$D^C = (\rho_j^g \alpha_j^g)^2 \sum_k f_i f_k \frac{1}{M_k} a(M_i, M_k) \qquad (6)$$

$$P^B = \rho_j^g \alpha_j^g \sum_k r(M_k, M_i) f_k \qquad (7)$$

$$D^B = \rho_j^g \alpha_j^g f_i \sum_k r(M_i, M_k) \qquad (8)$$

All breakup kernels comprise three important sub-processes: (i) breakage frequency, (ii) number of daughter bubbles and (iii) size distribution of the bubbles formation. In this present study breakage kernel by Luo and Svendsen (1996) was tested. Luo and Svendsen (1996) developed based on surface energy criterion and isotropic turbulence to formulate the theoretical binary bubble breakup model was tested.

Coalescence Kernels

Prince and Blanch (1990)

$$h(d_i, d_j) = C_1 (d_i + d_j)^2 ({d_i}^{2/3} + {d_j}^{2/3})^{1/2} \varepsilon^{1/3}$$

$$P_c = \exp\left(-\frac{{\rho_c}^{1/2} {r_{eq}}^{5/6} \varepsilon^{1/3} \ln(h_i / h_f)}{4\sigma^{1/2} {r_{ij}}^{2/3}}\right),$$

$$r_{eq} = \frac{1}{2}\left(\frac{1}{r_i} + \frac{1}{r_j}\right)^{-1}$$

Coulaloglou and Tavlarides (1977)

$$h(d_i, d_j) = C_2 (d_i + d_j)^2 ({d_i}^{2/3} + {d_j}^{2/3})^{1/2} \varepsilon^{1/3}$$

$$P_c = \exp\left[-C_3 \frac{\rho_c \mu_c \varepsilon}{\sigma^2}\left(\frac{d_i d_j}{d_i + d_j}\right)^4\right]$$

Lehr et al. (2002)

$$h(d_i, d_j) = C_4 (d_i + d_j)^2 ({d_i}^{2/3} + {d_j}^{2/3})^{1/2} \varepsilon^{1/3}$$

$$P_c = \max\left(\frac{u_{crit}}{u_{rel}}, 1\right), u_{crit} = 0.08$$

$$u_{rel} = \max\left(1.414\varepsilon^{1/3}\left(d_i^{\,2/3} + d_j^{\,2/3}\right)^{1/2}, \left|u_i - u_j\right|\right)$$

Breakage kernel

Luo and Svendsen (1996)

$$S(d_i, d_j) = 0.923(1-\alpha)\left(\frac{\varepsilon}{d_i^{\,2}}\right)^{1/3} \int_{\xi_{\min}}^{1} \frac{(1+\xi)^2}{\xi^{11/3}} \exp\left(-\frac{\Delta E_i(d_i)}{E(d_e)}\right) d\xi$$

$$\xi_{\min} = d_{e,\min} / d_i$$

$$d_{e,\min} = (11.4 \sim 31.4)(\mu_f / \rho_f)^{0.75} / \varepsilon^{0.25}$$

Table 1: Coalescence and breakage models

On the other hand coalescence process can be divided mainly into three steps: (i) the approach of one bubble colliding with another, (ii) the formation and thinning of a thin film between the interfaces and (iii) finally the rupture of the thin film. To model above three steps coalescence kernels are thus normally expressed as a function of the collision frequency and the coalescence efficiency. Three different binary bubble coalescence kernels were tested in the current study. Mathematical formulations have been summarised in Table 1. Coulaloglou and Tavlarides (1977) believe coalescence to occur if the contact time between two intervening bubbles exceeds the time required for the complete film drainage and rupture. Afterward Prince and Blanch (1990) superimposed the effects of turbulence, buoyancy and laminar shear to derive the expression for collision frequency. They postulated that the fluctuating turbulent velocity is the primary cause of bubble collision. Recently, Lehr et al. (2002) considered collision contribution arising from two sources (i.e. namely turbulence and buoyancy)- in order to reflect the conditions in bubble columns. In this case a characteristic velocity has been multiplied with the collision cross sectional area to obtain the collision frequency. The characteristic velocity assumed to be the turbulent eddy velocity having the length scale of bubbles. But for larger bubbles it is assumed to be the difference between rise velocities of bubbles.

	Kernel combination	Model
Case 1	Luo and Svendsen (1996) Coulaloglou and Tavlarides(1977)	Breakup Coalescence
Case 2	Luo and Svendsen (1996) Prince and Blanch (1990)	Breakup Coalescence
Case 3	Luo and Svendsen (1996) Lehr, Millies et al. (2002)	Breakup Coalescence

Table 2: Simulation cases

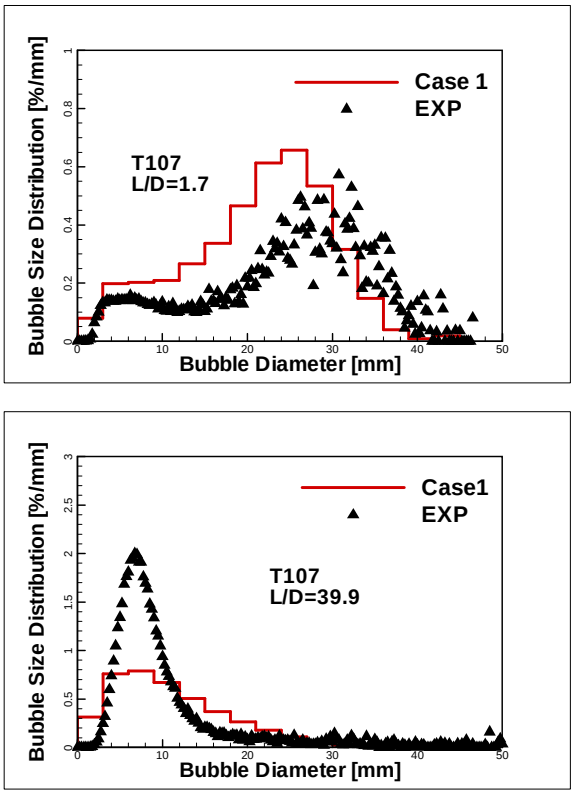

Figure 1: Predicted Bubble Size Distribution for Case 1.

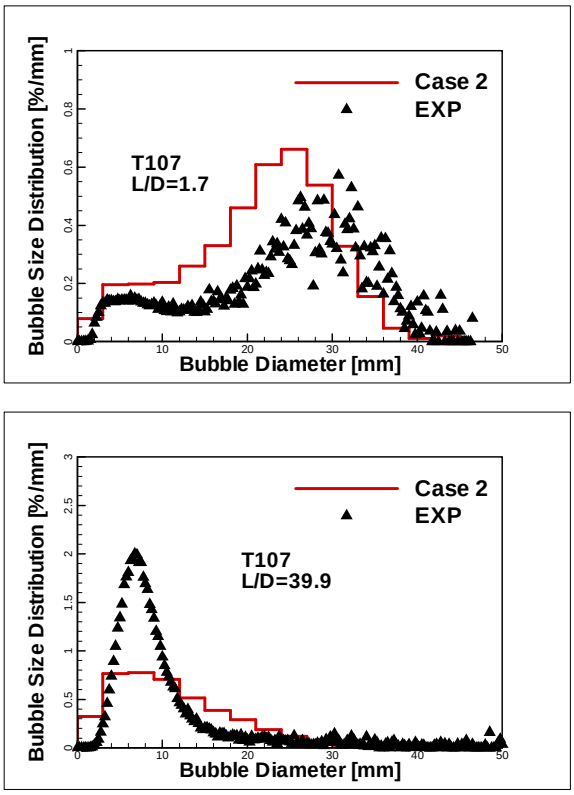

Figure 2: Predicted Bubble Size Distribution for Case 2.

EXPERIMENTAL AND COMPUTATIONAL DETAILS

Numerical predictions from all simulation cases were validated and assessed against the TOPFLOW experimental data measured in the HZRD facility. In TOPFLOW experimental facility, a large size vertical cylindrical pipe with height 9000 mm and inner diameter of 195.3 mm inner diameter was adopted. Water was circulated from the bottom to the top with a constant temperature of 30ºC, maintained by a heat exchanged installed in the water reservoir. A variable gas injection system was constructed by equipping with gas injection units at 18 different axial positions from Z/D = 1.1-39.9. Details of experimental setup can be found out from literature (Prasser et al. 2007).

Numerical calculations were achieved through the use of the generic computational fluid dynamics code ANSYS-CFX12.1. Transport equation with appropriate source and sink terms describing the coalescence and break-up rate of bubble was implemented through the CFX Command Language (CCL). Computational geometry was simplified through consideration of a 60^{o} radial sector of the pipe with symmetry boundary conditions being imposed at both vertical sides of the computational domain.

TOPFLOW Experiment (T107)	
$\langle j_g \rangle\|_{Z/D=0}$	1.017 m/s
$\langle j_l \rangle\|_{Z/D=0}$	0.140 m/s
$\alpha_g\|_{Z/D=0}$	12.1 %
$D_s\|_{z/D=0.0}$	20.18 mm

Table 3: Flow condition

RESULTS AND DISCUSSION

In order to identify the combination of kernels that can be used to accurately predict the flow, PBE was solved at a particular operating condition of the experiments to obtain the bubble size distribution at the bottom and top of the column. Details of the operating condition are summarized in Table 3.

Figure 1-3 shows the bubble size distribution for different kernel combinations at the bottom of the column as well as at the top of the column. It can be seen that the fraction of larger bubble sizes at the bottom of the column is greater than the top of the column. Moreover it indicates that the breakage is acting predominantly in this case study. For breakup mechanism the popular Luo and Svendsen(1996) kernel model has been applied for all the three case study. So it is not surprising that the change of bubble size distribution predicted by different combinations of breakup and coalescence model is quite similar from case to case.

Moreover, these kernels have been developed on the assumption that the bubbles are finely dispersed and in spherical shape. Bubbles would start to distort from spherical shape if they exceeds a critical value of 10.9 mm for 25^{0}C air-water flow under atmospheric pressure. As can be found from the figures, close to the inlet majority of the bubbles were above that size limits. So appropriate consideration of cap bubble coalescence and breakage could be place into calculations to reduce the discrepancies between measurement and predicted results.

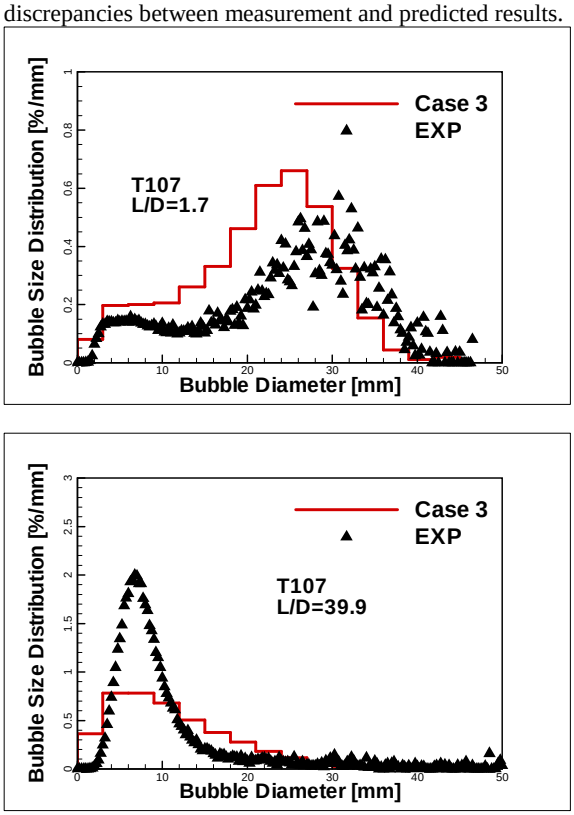

Figure 3: Predicted Bubble Size Distribution for Case 3.

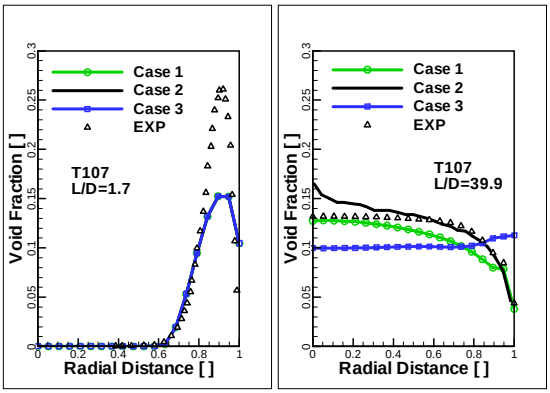

Figure 4: Comparison of Void fraction profile.

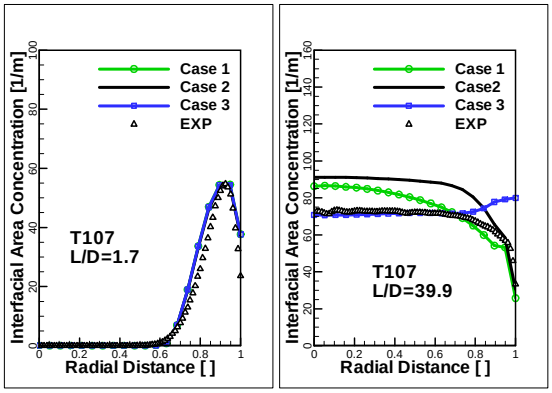

Figure 5: Comparison of Interfacial area concentration.

As shown in Figure 4, Lehr et al. (2002) kernel was found to be unable to capture the near wall void fraction profile and over-predicted the gas holdup near the wall when combined with Luo and Svendsen break up kernel model. Based on the critical approach velocity model, Lehr et al. (2002) considered that collision would result in coalescence only if the characteristic velocity is lower than a certain critical value. The experimental observation of Doubliez (1991) and Duineveld (1994) also supports this theory of having an impact of approach velocity on coalescence efficiency. Thus this over-prediction near the wall indicating to producing higher rate of small bubbles might caused by high approach velocity that could lead to a low coalescence efficiency. Sauter mean diameter obtained numerically by solving population balance equation is an important parameter that has direct impact on non-drag force. Thus it is essential to get the bubble size distribution correctly to determine the magnitude of non drag forces that affects the radial void fraction profile. Nevertheless, as seen in Table 4, Cases 1, 2 and 3 for the predominant bubble breakup flow, The sauter mean bubble diameter predicted by Lehr et al. (2002) is smaller in comparison to the other two kernels. Therefore it suggests that coalescence rate estimated by Lehr et al. (2002) is lower than the one by Prince and Blanch (1990) and Coulaloglou and Tavlarides (1977).

	Sauter Mean Diameter at L/D=39.9
Case 1	8.86 mm
Case 2	8.68 mm
Case 3	8.46 mm

Table 4: Predicted bubble diameter for different cases

Figure 5 shows the comparison between predicted and measured IAC. Predicted interfacial area concentration (IAC) also roughly followed the same trend as void fraction profile.

CONCLUSION

A preliminary numerical study of bubble breakup and coalescence models has been investigated in this paper. Performance of coalescence kernels by Prince and Blanch (1996), Coulaloglou and Tavlarides (1977) and Lehr et al. (2002) were considered and assessed for coalescence mechanism. For breakup mechanism, the widely adopted model proposed by Luo and Svendsen (1996) was applied. In general, satisfactory agreement was observed in comparing model prediction of Coulaloglou and Tavlarides (1977) and Prince and Blanch (1990) with experimental data. Nonetheless, for the Lehr et al. (2002) model the void fraction profile was over predicted at near wall locations. Incompatible kernels of coalescence and breakup might produce this poor result. Chen et al. (2005) also studied different coalescence and breakage closures and reported about compatibility of kernels. Thus it is important to have compatible kernels for coalescence and breakage that could lead this two competing mechanism to reach a certain equilibrium. Further study is currently being carried out to investigate different breakage kernel as well as coalescence to explore the effect of different closures and their compatibility with each other.

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