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CFD SIMULATION OF MULTIPHASE FLOW: CLOSURE RECOMMENDATIONS FOR FLUID-FLUID SYSTEMS

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Abstract. General closure recommendations for inter-phase interactions were developed using a large number of accurate experimental data sets for dispersed phase holdup profiles in pipeline flows. CFD simulation was used to test a wide range of drag and lift expressions and the most suitable ones were identified. The most suitable dispersion coefficient values in the Viollet and Simonin turbulent dispersion model were also determined. The recommended closure models were found to fairly predict the dispersed phase holdup and its distribution across the pipe diameter and may be used for simulating multi-fluid systems using the Eulerian-Eulerian approach.

Key words: Multiphase systems; CFD simulation; Closure guidelines; Bubbles; Drops; Inter-phase forces.

1. INTRODUCTION

Multi-fluid systems (gas-liquid and liquid-liquid dispersions) are encountered in a wide range of industrial situations such as multiphase reactors, distillation, absorption, solvent extraction, biotechnology, wastewater remediation by oxidation/ozonation, petroleum production and transportation, oil recovery from effluents, direct contact heat transfer, and power generation. They are also encountered in many physical processes such as rain formation, bubble motion in sea water, gas movement in lava flows etc.

It is therefore interesting to note that while CFD is extensively used to simulate and characterize the mixing behaviour of single phase operations, the same does not hold true in the case of multiphase systems. This is mainly attributed to the complex interactions between the phases which result in significant increase in computational demands and the need to make several empirical assumptions. These difficulties are exasperated in the case of multi-fluid systems where, in addition to the aforementioned problems, the individual bubbles/drops can breakup and coalesce throughout the contactor volume, phenomena that still can not be accurately predicted particularly in the case of industrial systems where the presence of contaminants can affect both the breakage and coalescence processes. It is therefore necessary to un-couple the closure problem from that of breakage and coalescence if one is to gain better quantitative understanding of either phenomenon.

The need to limit the amount of information handled by the multidimensional two-fluid models commonly used in CFD simulations, lead to the introduction of averaged equations which are similar to those used for turbulent single-phase flows. Unfortunately, averaging procedures leads to a loss of information which has to be explicitly put back into the equations through modeling of the most important physical phenomena. This is referred to as the closure process which necessitates physical insight in order to identify the phenomena that are of relevance for each particular flow condition [1]. These include items pertaining to mean momentum inter-phase transport (such as the drag and lift forces acting on bubbles and drops) as well as those pertaining to turbulent homogenization of dispersed phase concentration and the coefficient of virtual mass associated with the unsteady motion of dispersed entities. Unfortunately, no generally applicable guidelines for accurately simulating multi-fluid systems have evolved.

The objective of this investigation is to develop general inter-phase closure guidelines that can be used for accurately simulating multi-fluid flow/mixing operations using CFD. However, in order to clearly identify the effect of various closure models on the accuracy of the CFD predictions, it is necessary to use a relatively simple flow field for which there are sufficiently large number of accurate experimental data that can be used for testing and validating the various closure models.

2. SELECTION OF VALIDATION DATA

Most of the previous CFD related studies have focused on mechanically agitated tanks [2,3], Bubble columns [4], or extraction columns [5]. These configurations are characterized by the presence of complex hydrodynamics with very large spatial variations in energy dissipation rates, the presence of a wide range of circulation times, as well as the interference of the complex breakup and coalescence processes. The simulation results obtained using such configurations can therefore not be expected to yield accurate predictions of the fundamental two-phase flow characteristics (such as the local dispersed phase holdup, relative velocity between the phases etc.) without recourse to a fairly large degree of empiricism and know-how.

Two main areas of uncertainties surround the use of E-E approach; namely; the lack of generally acceptable closure recommendations, and the lack of generally acceptable models for describing bubble/drop breakage and coalescence kernels. It is difficult to separate those two issues when addressing the complex hydrodynamics encountered in mechanically agitated tanks, bubble columns etc. and it is therefore necessary to make an assumption concerning the closure issues in order to investigate bubble/drop breakage and coalescence and vice versa. Identification of general closure recommendations requires decoupling of those two issues, a situation which can only be achieved in the case of fully developed two-fluid pipeline flow in which the bubble/drop size is known a priori.

The hydrodynamics of pipe flows are much simpler and the turbulence characteristics of the continuous phase are well known. Attention was consequently focused on the upward pipe flows of gas-liquid and liquid-liquid dispersions in the “bubbly flow” regime; a relatively simple flow configuration which is of significant practical relevance and for which there exists an extensive database of experimental information that can be used to validate the CFD results (radial distribution of the dispersed-phase holdup, phase velocities and turbulence intensities, as well as the bubble /drop size distribution). The experimental data obtained at high L/D ratios were selected in order to eliminate interferences caused by the breakage/coalescence of the dispersed phase entities (bubbles and drops), a situation that is often encountered under the unsteady-state conditions near the inlet. Under those conditions, it is safe to assume that there is very little acceleration/deceleration other than that caused by the response to turbulent eddies.

3. CFD SIMULATION METHODOLOGY

Steady-state CFD simulations were conducted using FLUENT v 6.1.22 and special attention was given to ensure that the CFD simulations are grid-independent and that computational error was minimized. The computational parameters used to assess the various closure approaches are summarized in Table 1,

Table 1 CFD Computation approach

Models and Solution approach	*Gas-liquid and Liquid-liquid dispersions*
Multiphase modeling approach	Eulerian-Eulerian
Continuous phase turbulence	k-ε model
Dispersed phase turbulence	Tchen's theory [18]
Pressure-velocity coupling	Phase coupled SIMPLE

The procedure used for studying grid sensitivity closely follows the recommendations of Ranade [6]. A cell aspect ratio of 1:1 was used wherever possible but in some cases it was necessary to use a non-uniform aspect ratio; however, the aspect ratio never exceeded 5:1 for both gas-liquid and liquid-liquid dispersions in order to avoid numerical errors. A systematic investigation of the number of radial nodes needed to achieve grid independence indicated that whereas 14 nodes were found to be sufficient as the density ratio approaches one a minimum of 60 nodes is required for the low dispersed phase density ratios encountered in gas-liquid systems. The value of y^+ was maintained between 20 to 30 units.

In order to improve the accuracy of the CFD simulation results it was also necessary to adopt a more stringent continuity convergence criteria in which it is reduced from the default value of 10^{-3} to a value of 10^{-6} and 10^{-13} for G-L and L-L systems respectively. The resulting increase in computational demand was reduced without affecting the final results by changing the under-relaxation factor for the dispersed phase holdup from the typical value of 0.2 to 0.8.

The Eulerian-Eulerian approach was chosen for simulating the multiphase systems because its predictions are more accurate than those of the mixture approach under conditions where the dispersed phases are concentrated in certain portions of the domain as opposed to uniformly distributed throughout [6]. It also provides an effective structure to examine and incorporate the various inter-phase forces and is well suited to modeling dispersed flows at high phase fractions. Single phase flow simulations were carried using non-uniform grid cells and excellent agreement with reported velocity and turbulent intensity profiles [7] was achieved.

From the above, it is possible to conclude that the computational requirements for accurately simulating the hydrodynamics of gas-liquid dispersions are significantly more demanding than those required for liquid-liquid dispersions. Consequently, whereas a typical CFD simulation of L-L system converged within 25 minutes using a 2.5 GHz Pentium IV machine, it took approximately 3 hours for G-L cases to converge.

4. INTERPHASE CLOSURE

Several inter-phase forces need to be specified in order to *close* the momentum conservation equation. These include the drag on an assembly of bubbles or drops (under steady and unsteady conditions), the lift forces acting on bubbles/ drops, as well as the diffusive effect turbulent dispersion has on the phase fraction profiles. Due to the strong coupling between these factors, preliminary screening of the various expressions/formulations available in literature was conducted before multi-parameter sensitivity analyses were undertaken.

4.1 Drag forces

The drag forces acting on individual bubbles and drops determine the relative motion between the phases and hence strongly affect the dispersed phase holdup, flooding point, as well as the inter-phase heat and mass transfer coefficients. Numerous expressions were developed to describe the drag forces acting on single bubbles and drops, as well as the effect the presence of neighbouring entities have on such forces. The latter is usually accounted for by semi-empirical expressions that take into account the dispersed phase size and holdup.

Although the presence of neighbouring entities generally results in reducing the slip velocity between the phases, it can also increase the effective slip velocity of clusters. The various expressions tested are summarized in Table 2. The expression for drag on solid spheres was incorporated because many investigators tended to use this simple expression which is strictly applicable to the case of solid particles.

Table 2 Drag coefficient expressions tested

Gas-liquid dispersions	**Liquid-liquid dispersions**
Single bubble Grace et al. [8]; Schiller and Naumann [11]; Tomiyama [17]; Ishii and Zuber [21]	*Single drop* Grace [8]; Hu and Kintner [9]; Klee and Treybal [10]; Schiller and Naumann [11]; Kumar and Hartland [22]
Effect of adjacent bubbles Behzadi et al. [12]; Ishii and Zuber [21]: Dense theory	*Effect of adjacent drops* Behzadi et al. [12]; Ishii and Zuber [21]: Dense theory; Kumar and Hartland [22]

The simulation results suggest that in the case of small bubbles and drops (smaller than 3 mm in diameter), the specific expression used to describe the drag on a single disperse phase entity plays a secondary role in estimating the average dispersed phase holdup. It is however necessary to use expressions that take into account the deformations occurring at larger diameters in order to achieve good correspondence with the experimental values.

On the other hand, the effect of adjacent entities was found to play a significant role in accurately determining the average dispersed phase holdup particularly at higher concentrations ($\varepsilon_{\text{Dispersed}} > 0.05$). The approach proposed by Behzadi [12] yielded the best average fit to the experimental data set for both gas-liquid and liquid-liquid dispersions. Adoption of this approach has the further advantage of eliminating the need to use the empirically-based drift flux models at the local level.

4.2 Virtual mass

Virtual mass is a concept that is commonly used to account for the additional forces acting on dispersed phase entities under accelerating and decelerating conditions. Although virtual mass can play an important role in bubble breakage and coalescence [13], the effect of virtual mass was not included in the present investigation due to the absence of acceleration/deceleration in the continuous flow at the axial point where comparison is made (i.e. high L/D).

4.3 Lift forces:

These forces are somewhat analogous to the Coriolis forces and act in a direction normal to the direction of the relative slip velocity. Their influence is rarely taken into account although they strongly influence the dispersed phase holdup particularly at high shear rates and low concentrations [1].

The magnitude of the lift force acting on a rigid spherical dispersed phase entity depends on the diameter of the entity, the relative velocity between it and the fluid, and the average vorticity at the entity's centroid. Its magnitude can be estimated by Drew and Lahey [14] expression,

$$\vec{F}_{lift} = -C_L\, \rho_q\, \alpha_p \left(\vec{v}_q - \vec{v}_p\right) \times \left(\nabla \times \vec{v}_q\right) \tag{1}$$

where the value of the lift coefficient, C_L, equals 0.5 for inviscid flow and acts in a direction that depends on the relative sip velocity and the degree of deformation (Fig. 1).

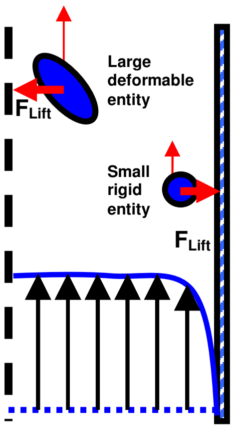

Fig. 1 Lift forces acting on bubbles and drops

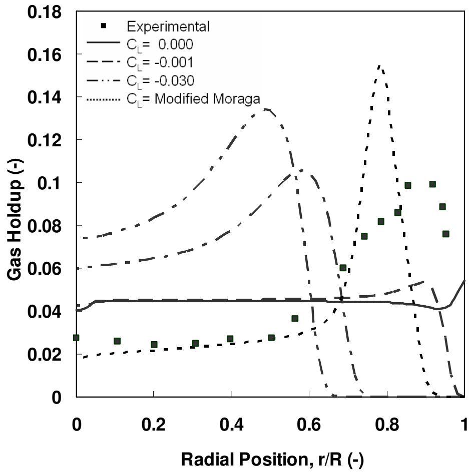

Fig. 2 Effect of incorporating lift forces on bubbles (D_{pipe} =0.0508m, U_l=2.0 m/s, U_g=0.103 m/s, α_g=5.6%)

For a long time, the lift coefficient was treated as a constant, independent of the local relative velocity, equivalent diameter etc., due to the lack of experimental or theoretical work that could quantify it as a function of such variables. Meanwhile, many investigators found it necessary to use lift coefficient values that are significantly less than the inviscid value of 0.5, and in some cases even negative, in order to match their experimental data. Moraga [15] explored the causes for this apparent sign reversal of the lift force and attributed this phenomenon to the mechanism of vortex shedding (wake effects). In the case of bubbles and drops, the situation is further complicated by the observation that shape deformation and/or vortex shedding induced lift forces that act in a direction opposite to that predicted by the inviscid lift theory. The combined effect of these factors resulted in many investigators using *"effective"* lift coefficients that take into account the inviscid and vortex shedding contributions.

Moraga [15] undertook the most comprehensive evaluation of the effective lift coefficient and developed expressions that correlated it with the product of bubble and shear Reynolds numbers (Re_{Bubble} Re_{Shear}). However, the latter had to be slightly modified in order to enhance the stability of the CFD simulation solutions Troshko [16].

As can be seen from Fig. 2, the predicted dispersed phase holdup profiles in pipe flows are strongly influenced by the magnitude of the lift coefficient. This could explain the experimentally observed shift of holdup peaks from the wall region to the core of the pipe as the dispersed phase volume ratio increases.

In order to match the experimental trends it was necessary to use negative lift coefficient with the magnitude being greater the larger the dispersed phase size is. However, identification of the most suitable expression for the lift coefficient could not be properly undertaken without simultaneously incorporating the effect of turbulent dispersion discussed in the following section.

4.4 Turbulent dispersion:

Whereas lift forces are primarily responsible for non-homogeneous radial distribution of the dispersed phase holdup, turbulent dispersion tends to homogenise the dispersed phase holdup by introducing an additional diffusive flux. The formulation developed by Viollet and Simonin [18] was adopted in this investigation because of its ability to accurately predict dispersed phase response in various multiphase systems (S-G, S-L, G-L, L-L), and its ability to account for effect of virtual mass in turbulent dispersion.

5. DEVELOPMENT OF MULTI-FLUID CLOSURE RECOMMENDATIONS

Closure recommendations for multi-fluid systems were developed by comparing CFD simulations with a large database of experimental results published in the open. In total, 16 data sets for liquid-liquid dispersions and 19 data sets for gas-liquid dispersions were used to validate the CFD simulations and identify the most suitable closure models for bubbly flow conditions. The experimental data set (details of which are given in [19] and [20]) covered the following range of experimental conditions:

L-L dispersions: $0.1 < U_L < 1.2$ m/s, $16 < D_{pipe} < 200$ mm, 1 mm $< D_{Drop} < 5$ mm, $25{,}000 < Re_{pipe} < 210{,}000$, $0.678 < \rho_d / \rho_c < 0.781$, and $\varepsilon_{Disp.} < 0.60$,

G-L dispersions; $0.9 < U_L < 2.5$ m/s, $25 < D_{pipe} < 200$ mm, $45{,}720 < Re_{pipe} < 500{,}000$, $\rho_d / \rho_c \approx 0.001$, and $\varepsilon_{Disp.} < 0.20$.

In order to identify the most suitable expressions and parameter values, multi-parameter sensitivity analyses were undertaken. This task was facilitated by the inability of simple drag expressions to match the experimentally obtained average gas holdup over a wide range of bubble/drop sizes. The expressions developed by Ishii and Zuber [21] and Kumar and Hartland [22] for the drag coefficient of single bubbles and drops, were therefore used in subsequent multi-parameter sensitivity analyses.

The radial distribution of dispersed phase holdup was found to be strongly affected by turbulent dispersion and lift forces. So whereas turbulent dispersion tends to homogenize the holdup across the pipe cross-section, lift forces promote non-uniform phase distributions. Attempts were then made to identify the most suitable combination of lift and turbulent dispersion expressions and coefficients that could accurately predict the experimentally obtained holdup profiles under different flow conditions. Wherever possible, the residual sum of squares was used to compare the effectiveness of different simulations; however, the extent and radial location of the peak was used as a secondary criterion when experimental errors reduced the sensitivity of statistical fit.

As exemplified in Figures 3 and 4, the following closure recommendations were found to fairly predict dispersed phase holdup profiles over a wide range of experimental conditions.

Table 3 Recommended Inter-Phase Closure expressions and Parameter Values

Inter-Phase Iteraction	***Gas-Liquid dispersions***	***Liquid-liquid dispersions***
Drag force	Ishii and Zuber expression for single bubbles [21] combined with the expression of Behzadi et al. for the effect of adjacent bubbles [12]	Kumar and Hartland expression for single drops [22] combined with the expression of Behzadi et al. for the effect of adjacent drops [12]
Lift forces	Moraga's expression as modified by Troshko et al. [16]	Moraga's expression as modified by Troshko et al. [16] for Re > 250; and C_L = - 0.05 for Re < 250
Dispersion Numbers in the model of Viollet and Simonin [18]	0.049-0.06 for $0.05<\alpha < 0.20$ 1.33 for $0.20< \alpha< 0.30$	0.01-0.05 for $\alpha < 0.1$ 0.075- 7.5 for $0.1 < \alpha < 0.2$ ≥ 7.5 for $0.2 < \alpha < 0.6$

Although generally applicable recommendations could be made for the drag and lift interactions, the turbulent dispersion numbers were found to be affected by the pipe diameter, D, and the dispersed phase holdup, α. This is very much in accordance with experimental observations where the turbulent dispersion in pipes was found to be reduced in smaller pipe diameters. The dispersion number recommendations given in Table 3 were therefore selected to represent the cases least affected by the presence of walls and are therefore expected to be of generally applicable to multi-fluid dispersions.

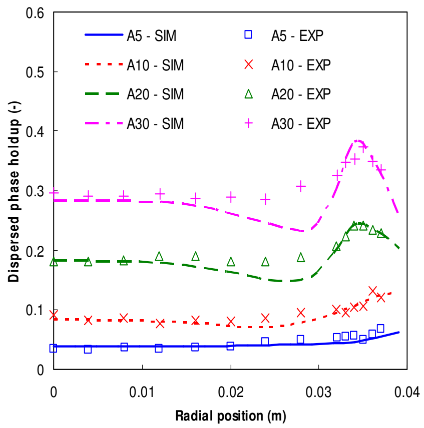

Fig. 3 Radial variation of kerosene holdup (D_{Pipe} =0.078 m; U_l=0.54 m/s, U_d=0.02-,0.2m/s; α_{Disp} =5, 10, 20, 30 %)

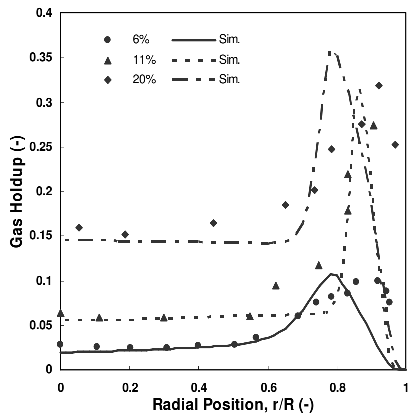

Fig. 4 Radial variation of gas holdup (D_{pipe} =0.0508m; U_l=2.0 m/s, U_g=0.103 m/s, α_g=6%, $D_{Bubb.}$=2.5mm; U_l=0.98 m/s, U_g=0.113, 0.242 m/s, α_g=11, 20%, $D_{Bubb.}$=2.7, 3.0mm)

Similarly, the effect of dispersed phase holdup on turbulent dispersion is inline with the findings of Serizawa [23] and Hibiki [24] who found that the presence of holdups less than 5% reduces turbulence intensity whereas it is enhanced as the holdup increases beyond 5%.

Some of the remaining discrepancy between the predicted and experimental results observed in the case of G-L systems can be attributed to the greater coalescence tendencies in this system and the tendency of the resulting larger bubbles to migrate towards the centre. Efforts are presently underway to incorporate breakage and coalescence processes in the simulation model in order to eliminate the need for knowing the bubble/drop sizes in the flowing systems.

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NOMENCLATURE

U	Superficial velocity
v	Velocity, m/s
ρ	Density, kg/m^3
Subscripts	
Disp.	Dispersed phase
Con.	Continuous phase

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