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Large Eddy Simulation of Gas-Liquid Flow in a Partially Aerated Bubble Column

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Abstract

In the present work, transient gas-liquid flow dynamics in a partially aerated bubble column (0.15 m wide, 0.15 m deep and 0.5 m high) were studied using large eddy simulation (LES). The Eulerian–Eulerian approach was used to describe the equations of motion of the two-phase flow. The numerical model was validated with the interfacial closures evaluated for drag, lift and virtual mass forces. The column was filled with water up to 0.45 m in the vertical direction. As a result, there exists an air-water interface. A series of superficial gas velocities ranging from 0.005 to 0.025 m/s were used throughout the simulations. The calculated results were compared with numerical predictions using both Reynolds-Averaged Navier–Stokes (RANS) and LES models as well as with experimental data in the literature. The behaviour of the bubble plume observed in the experiments can be captured with the current model, including fluid mean velocity profile, fluid velocity fluctuation and global gas holdup. The current LES results showed better agreement with the experimental data than RANS simulations.

Introduction

Bubble columns are often encountered in the chemical process industries, but also numerous examples can be found in petroleum, pharmaceutical, agricultural, biochemical and power-generation industries. In order to develop design tools for engineering purposes, much research has been carried out in the area of computational fluid dynamics (CFD) modelling of gas-liquid flows.

Numerical simulation of two-phase flows has made significant progress in the past couple decades. Most of the flow models are based on the concept of a domain in the static reference frame for description of the continuous phase, with addition of a reference frame for the description of the dispersed phase. The dispersed phase may be described in a dynamic reference frame, leading to the Eulerian–Lagrangian approach or in the same static reference frame as the continuous phase, leading to the Eulerian–Eulerian approach.

In the Eulerian–Lagrangian approach, the continuous liquid phase is described as a continuum in an Eulerian framework. The dispersed gas phase on the other hand is treated in a Lagrangian manner where the individual bubbles are tracked by solving Newton's Second Law for the forces acting on the individual bubbles. Since each bubble trajectory can be calculated accurately within the control volume, the bubble coalescence and breakup can be incorporated directly and no numerical diffusion is introduced into the dispersed phase computation. However, more equations need to be solved when the system gets larger, making computation of real industrial-scale applications prohibitive.

In the Eulerian–Eulerian approach, also referred as the two-fluid model, both phases are treated as interpenetrating continua occupying the entire domain. The conservation equations are solved for each phase coupled with interphase momentum exchange terms. This approach can suffer from numerical diffusion. Nevertheless, the numerical diffusion can be reduced sufficiently with the help of higher-order discretisation schemes. As a result, the Eulerian approach can offer the same order of accuracy as the Lagrangian approach. The advantage of the Eulerian approach is that the computational demands are much lower compared to the Lagrangian approach when solving systems with higher dispersed void fractions. In the present work, the Eulerian–Eulerian approach was used for the description of both gas and liquid phases.

The turbulence of the continuous phase can be modelled with either Reynolds-Averaged Navier–Stokes (RANS) or large eddy simulation (LES) models. The RANS turbulence model has been a common choice in the literature [2, 18, 21, 17, 25, 3]. The application of LES to multiphase simulations of vertical bubble-driven flows has been identified as a good way to model the turbulence by Jakosen et al. [11]. Deen et al. [4] conducted LES simulations of the gas-liquid flow in a square cross-sectioned bubble column. It was reported that the transient behaviour that was observed in the experiments can be captured when the drag, lift and virtual mass forces acting on the bubbles are modelled. The LES data were found to be in better agreement with the experimental results than the simulations using the k-ε model. Zhang et al. [26] extended the work of [4] to investigate the effect of the Smagorinsky constant and the interfacial closures for drag, lift and virtual mass forces in two columns having aspect ratios of 3 and 6, respectively. Tabib et al. [23] performed LES simulations using the Eulerian approach in a cylindrical column for a series of superficial gas velocities. This work confirmed the importance of a suitable lift coefficient and drag law. The LES was found to successfully predict the average flow behaviour and to be able to simulate the instantaneous vortical-spiral flow regime in the case of a sieve-plate column as well as the bubble plume dynamics in case of a single hole sparger. It was concluded that LES can be effectively used for the study of the flow structures and instantaneous flow profiles. Dhotre et al. [6] studied the influence of the sub-grid scale (SGS) models of Smagorinsky and Germano for a gas-liquid flow in a square cross-sectional bubble column using LES with the Eulerian approach. Both model predictions compared well with the experimental measurements. Dhotre et al. [7] utilised the same model to further studied a gas-liquid flow in a large-scale bubble plume. The LES was shown to be superior in capturing the transient behaviour of the plume and predicting the second-order statistics of the liquid phase accurately. Nicento et al. [16, 15] were the first to apply the one-equation SGS Eulerian–Eulerian LES to a bubble column reactor. Their results revealed that the one-equation model for SGS kinetic energy shows improved predictions over the dynamic model. Sungkorn et al. [22] modelled turbulent gas-liquid bubbly flow in a square cross-sectional bubble column using stochastic Lagrangian model and lattice-Boltzmann scheme. The Smagorinsky model was used to account for the effects of the sub-filter scales. Good agreement with experimental data was found with the presented modelling technique. Bai et al. [1] carried out numerical investigation of gas holdup and phase mixing in bubble column reactors using the same bubble column configuration from the study of [4]. Masood and Delgado [13] investigated the interphase forces and turbulence closure in three-dimensional square bubble columns. This work showed the comparison between different drag force models. The effects of the lift, virtual mass as well as the turbulent dispersion have been examined. All the results showed good quantitative agreement with experiments.

In the present work, transient gas-liquid flow dynamics in a partially aerated bubble column was studied using LES coupled with the Eulerian–Eulerian approach. The numerical model was validated against the studies conducted by [4], in which the interfacial closures were evaluated for drag, lift and virtual mass forces. A series of superficial gas velocities were used throughout the simulations. The calculated results were compared with numerical predictions as well as with experimental data in the literature, including fluid mean velocity profile, fluid velocity fluctuation and global gas holdup.

Numerical Methods

Governing Equations

In the two-fluid approach, a continuity and a momentum equation are solved for each phase present in the system. These governing equations are derived by conditionally averaging the single phase flow equations. The continuity equation for each phase φ has the form

$$\frac{\partial}{\partial t}(\alpha_\varphi \rho_\varphi) + \nabla \cdot (\alpha_\varphi \rho_\varphi \mathbf{U}_\varphi) = 0, \tag{1}$$

where α_φ represents the phase fraction of phase φ, ρ_φ is the density of the material constituting the same phase and $\mathbf{U}_\varphi$ is the phase velocity. The phase momentum equation can be written as

$$\frac{\partial}{\partial t}(\alpha_\varphi \rho_\varphi \mathbf{U}_\varphi) + \nabla \cdot (\alpha_\varphi \rho_\varphi \mathbf{U}_\varphi \mathbf{U}_\varphi) + \nabla \cdot (\alpha_\varphi \mathbf{R}_\varphi^{eff}) = -\alpha_\varphi \nabla p + \alpha_\varphi \rho_\varphi \mathbf{g} + \mathbf{M}_\varphi, \tag{2}$$

in which p is the pressure, $\mathbf{g}$ is the gravitational acceleration vector, $\mathbf{R}_\varphi^{eff}$ is the combination of phase Reynolds (turbulent) and phase viscous stresses and $\mathbf{M}_\varphi$ is the interphase momentum exchange term. The last two terms require further modelling. The stress term of phase φ is described as follows

$$\mathbf{R}_\varphi^{eff} == \rho_\varphi \nu_\varphi^{eff} [\nabla \mathbf{U}_\varphi + (\nabla \mathbf{U}_\varphi)^T - \frac{2}{3}\mathbf{I}(\nabla \cdot \mathbf{U}_\varphi)], \tag{3}$$

where ν_φ^{eff} is the effective viscosity, which is composed of the molecular viscosity, ν_φ and the turbulent viscosity, ν_φ^T. The turbulent viscosity derives from the turbulent effect, which is formulated based on the LES model. In order to deal with the phase inversion in a two-phase syste, the one-equation SGS models of continuousGasKEqn and NicenoKEqn [16] are applied to the gas and liquid phases, respectively. While the equations above allow fully compressible calculations, for the present work, incompressibility is assumed.

Interfacial Momentum Transfer

The total interfacial momentum exchange term between the two phases may arise from several independent physical contributions

$$\mathbf{M}_\varphi = \mathbf{M}_\varphi^D + \mathbf{M}_\varphi^L + \mathbf{M}_\varphi^{VM}, \tag{4}$$

where the terms on the right-hand side of the above equation are the interphase drag, lift and virtual mass forces.

The drag force is modelled from the resolved velocity field, which is given by

$$\mathbf{M}_l^D = -\mathbf{M}_g^D = \frac{3}{4}\alpha_g \rho_l \frac{C_D}{d_b}|\mathbf{U}_g - \mathbf{U}_l|(\mathbf{U}_g - \mathbf{U}_l), \tag{5}$$

where C_D is the drag coefficient and d_b is the bubble diameter. The subscripts l and g stand for liquid and gas phases, respectively. A selection of drag models is considered in the current study, including Schiller and Naumann drag closure (SND) [20], Grace drag closure (GD) [9], Isshi and Zuber drag closure (IZD) [10] and a constant drag closure (CD) [4].

The lift force accounts for the transverse migration of bubbles under the influence of the liquid shear. It can be written as

$$\mathbf{M}_l^L = -\mathbf{M}_g^L = \alpha_g \rho_l C_L (\mathbf{U}_g - \mathbf{U}_l) \times \nabla \times \mathbf{U}_l, \tag{6}$$

where C_L is the lift coefficient. The most straightforward approach is to prescribe a constant lift closure (CL) with $C_L = 0.5$ for a spherical bubble. Bubble size and its shape can also be considered using the Tomiyama lift closure (TL) [24].

The virtual mass force accounts for the extra work performed by the bubbles in accelerating the surround liquid, which is given by

$$\mathbf{M}_l^{VM} = -\mathbf{M}_g^{VM} = \alpha_g \rho_l C_{VM} (\frac{D\mathbf{U}_g}{Dt} - \frac{D\mathbf{U}_l}{Dt}), \tag{7}$$

where C_{VM} is the virtual mass coefficient, which is set to be 0.5.

Grid Requirement

Since the Eulerian–Eulerian approach was coupled with LES in the current study, the resolution requirements of both techniques need to be considered in order to achieve a satisfactory grid. A basic requirement is that the control volume size should be large enough to encompass all the interface details [15]. This is the intrinsic assumption in the derivation of the Eulerian-Eulerian model equations and strictly has to be satisfied at the discrete level as well. The detailed discussion can be found in the studies of [6, 15]. A systematic a-posteriori analysis of the minimum ratio of the cell and bubble sizes (Δ/d_b) for LES modelling of free bubble plume was reported by [14], where Δ is the cell size. The optimum cell size is considered to be $1.2 \leq \Delta/d_b \leq 1.5$, which implies that the interaction of bubbles with the smallest resolved scales is captured without additional approximation.

Simulation Details

An open source CFD package OpenFOAM v5.0 was used to solve the equations of continuity and momentum. Simulations performed were based on the experimental configuration of Deen et al. [4]. The column is 0.15 m wide, 0.15 m deep and 0.5 m high, which was initially filled with water to a height of 0.45 m. As a result, an air-water interface was modelled in the current study. Air was used as the dispersed gas phase and injected in the centre of the bottom plane with an area of 0.03×0.03 m^2 and superficial velocities of 0.005, 0.015 and 0.025 m/s. The bubble diameter was set to 4 mm based on the experimental observation [4]. The gas-liquid flow is assumed to be homogeneous and bubble break-up and coalescence were not considered.

A uniform grid with a cell size of 5 mm was adopted for a Δ/d_b ratio of 1.25. A gas velocity calculated using the superficial gas velocity and gas distributor size was applied at the inlet. At the walls, a no-slip boundary condition is applied for the continuous phase and a free-slip boundary condition for the disperse phase. At the top of the column, a constant pressure of 101.325 kPa is applied. The time step of 0.001 s was selected to satisfy a Courant number less than 0.5. While the equations above allow fully compressible calculations, for the present work, incompressibility is assumed.

Results and Discussion

Interfacial Closures

The first set of simulations performed at a constant superficial velocity of 0.0049 m/s were designed to evaluate the applicability of the aforementioned drag (SND, GD, IZD and CD) and lift (CL and TL) closures. The simulation results averaged from t = 50 s to t = 250 s are quantitatively compared with both numerical predictions and experimental data in the literature as shown in figure 1. The data were taken at the centreline of the horizontal plane at height of 0.25 m. It can be seen that the axial liquid velocity was overpredicted by the TL closure while the the CL closure underpredicted the axial liquid velocity. The SND closure was found to significantly overpredict the axial gas velocity. The TL closure in general overpredicted the axial gas velocity. The turbulent kinetic energy was overpredicted by the TL closure except when it was used with the SND closure. The predictions of the turbulent kinetic energy using the CL closure agreed well with the data in the literature except when it was used with the SND closure. The combination of the GD and the CL closures gave the best overall predictions of the bubble column dynamics for both phases. Hence, this combination of drag and lift closures was used to investigate the global gas holdup.

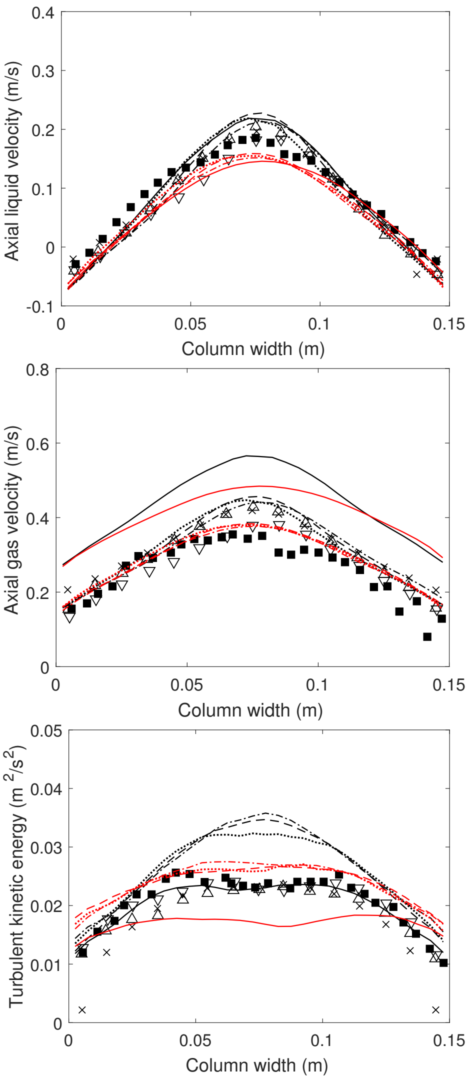

Figure 1: Comparison of the simulated and experimental profiles of the axial liquid velocity (top), axial gas velocity (middle) and turbulent kinetic energy (bottom). The simulated profiles were obtained from different drag (SND, GD, IZD and CD) and lift (CL and TL) closures, (■) Deen et al. 2001 Experiment, (×) Dhotre et al. 2008 RANS, (△) Dhotre et al. 2008 LES Germano model, (▽) Dhotre et al. 2008 LES Smagorinsky model, (—) SND+TL, (−−) GD+TL, (−·− IZD+TL), (···) CD+TL, (—) SND+CL, (−−) GD+CL, (−·−) IZD+CL), (···) CD+CL.

Global Gas Holdup

The global gas holdup in the bubble column for each superficial gas velocity was listed in table 1. Within the adopted range of the superficial gas velocity, the global gas hold up is related to the superficial gas velocity with a multiplication factor of 3 approximately. However, the results from the study of Bai et al. [1] suggested a scaling constant of 4. The bubble column used in the study of Bai et al. [1] was initially filled with water to a heigh of 0.6 m instead of 0.45 m.

Superficial velocity (m/s)	0.005	0.015	0.025
Global gas hold up	0.0171	0.0494	0.0774

Table 1: Global gas holdups at the superficial velocities of 0.005, 0.015 and 0.025 m/s.

In figure 2, the global gas holdups obtained from the simulations are compared with the literature correlations and numerical predictions. It can be seen that the current results agree with the correlations of Fair et al. [8] and Kato and Nishiwaki [12]. The computed global gas holdups from the study of Bai et al. [1] agreed better with the correlation of Ruzicka et al. [19]. These results indicated that the overall gas holdup increases almost linearly with the superficial velocity.

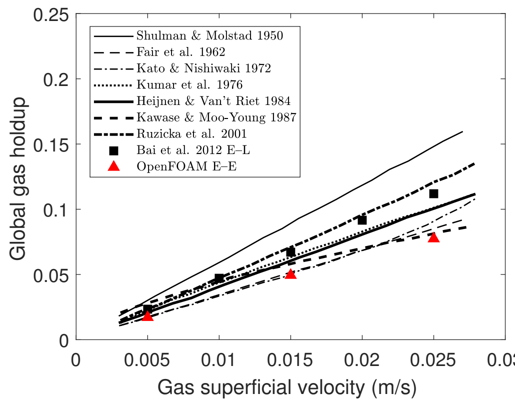

Figure 2: Comparison of the global gas holdup with literature correlations and numerical predictions. The literature correlations are plotted with various types of lines and the numerical predictions are plotted with square and triangle symbols.

Conclusions

The present work utilised LES coupled with the Eulerian–Eulerian approach to investigate the transient gas-liquid flow dynamics in a partially aerated bubble column. The numerical model was validated with the interfacial closures evaluated for drag, lift and virtual mass forces. It was found the combination of the Grace drag closure [9] and the constant lift closure with

$C_L = 0.5$ gave the best predictions of the overall bubble column dynamics, including fluid mean velocity profile, fluid velocity fluctuation and global gas holdup. The LES simulations showed better agreement with the experimental data than RANS simulations. The current results suggested that the global gas holdup increases nearly linearly with the superficial gas velocity with a factor 3 approximately in the adopted range of the superficial gas velocity.

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