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CFD Simulation of Air-Water in a Spouted Bed

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Computational fluid dynamics (CFD) is employed to simulate the air-water system in a spouted column with a draft tube. Numerical results of Reynolds-averaged Navier-Stokes (RANS) equations using the k-ε and k-ω two-equation turbulence models are compared with Pironti at al. (1995) experimental data. CFD predictions of the k-ε and k-ω turbulence models are in good agreement with the reported experimental data. The interfacial momentum transfer in modeling air-water system in the spouted bed indicated the importance of using turbulent dispersion force besides the most often used drag and lift forces to better predict flow behavior and air hold-up. Ishii-Zuber liquid-gas drag model with the lift and turbulent dispersion forces yields very good results; it correctly determines a hold up within 1% when used along with the k-ε turbulence model, while it under-predicts the hold-up by 4.08% when used with the k-ω model.

Introduction

Bubble columns are the reactor of choice for processes with mass and heat transfer limitations, thus providing a competitive alternative to achieve gas–liquid and gas–liquid–solid reactions. They are used in chemical engineering processes, such as hydrogenation, oxidation, chlorination, and alkylation processes among others.
Knowledge of the prevalent hydrodynamics effects is fundamental, because local flow, turbulence and gas hold-up distribution have an impact on the mass, heat and momentum transfer between the phases and are coupled to the operating and design variables. Computational fluid dynamics (CFD) is employed to describe the observed physical phenomena in bubble columns. The interaction between the dispersed gas phase and the continuous liquid phase is characterized by bubble–liquid interphase forces (e.g. drag force, lift force and added mass forces, i.e., virtual mass and close-to-wall lift and lubrication forces) and turbulence in the column. Therefore, the correct modeling of interphase forces and turbulence is fundamental to correctly describe the observed physical phenomena of the bubble column (Jakobsen et al., 2005). The drag, lift and virtual mass forces are considered as the predominant interphase forces and the most implemented closure for turbulence is the k-ε because it is computationally and numerically inexpensive, and yet satisfactorily accurate (Zhang et al,. 2006; Tabid et al. 2008). The Computational fluid dynamics

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(CFD)simulation between the disperse gas phase and the continuous liquid phase in a two phase bubble columns can be achieved with the Euler–Lagrange (E–L) and/or the Euler–Euler (E–E) modeling framework. With the (E–L) approach, the gas–liquid system is treated as a pseudo–continuous phase with variable density, while the discrete nature of the disperse phase is depicted by tracking a large number of individual bubbles through the flow. E–L is the method that better characterize the physics of the fluid–particle interaction; however, the highly disperse phase volume fraction of this system makes it computationally prohibitive. The (E–E) approach models the disperse phase as another continuum phase. Regarding the geometry (cylindrical or rectangular), and dimensions (Zhang et al,. 2006; Emkambara et al. 2005) indicated that the 3D simulation provides a better insight of the physics of the two-phase bubble column, since 1D and 2D simulations lack of accuracy when describing this type of flow.
To gain a better understanding of the dominant interphase forces between the air-water system of a spouted column with a concentric draft tube and a conical base, computational fluid dynamics (CFD) techniques are here employed to simulate the air-water system in a 3D, cylindrical geometry. The Euler–Euler modeling framework and a two–fluid model are adopted to simulate the dispersed gas–liquid flows within the reactor. The interaction between the disperse gas phase and the continuous liquid phase is characterized by bubble–liquid interphase forces (e.g. drag force, lift force and turbulent dispersion force) and turbulence in the column is characterized by k-ε and k-ω turbulence closures to compare the prediction capability of both methods for this phenomenon. The Ishii-Zuber drag model (1975) is used to determine the draft coefficient of the liquid phase. The numerical results are compared with Pironti at al. (1995) holdup experimental data.

Theory

In the E-E approach the bubble is treated as a continuous medium with properties analogous to those of a fluid. The time-averaged continuity without mass transfer and momentum transfer equations for phase q can be written as:

$$\frac{\partial}{\partial t}(\upsilon_q \rho_q) + \nabla \cdot (\upsilon_q \rho_q \vec{u}_q) = \sum_{p=1}^{n} R_{pq} \tag{1}$$

$$\frac{\partial}{\partial t}(\upsilon_q \rho_q \vec{u}_q) + \nabla \cdot (\upsilon_q \rho_q \vec{u}_q \vec{u}_q) = -\upsilon_q \nabla \cdot P + \nabla \bar{\bar{\tau}}_q + F_{interfacial} + F_{external} \tag{2}$$

This system of equations is constrained by the fractional sum of the hold up: $\sum_{i=1}^{n} \upsilon_q = 1$. Here, ρ_q, ν_q, u_q, represent, respectively, density, volume fraction, time–averaged velocity, P is pressure, $F_{interfacial}$ is the averaged interfacial momentum transfer between the phases, $F_{external}$ is the gravitational acceleration, and $\nabla \bar{\bar{\tau}}_q$ the shear stress tensor.

$$\bar{\bar{\tau}}_q = \mu_{eff} \left(\nabla U_k + (\nabla U_k)^T - \frac{2}{3} I \nabla \cdot U_k \right) \tag{3}$$

Where the liquid phase effective viscosity, $\mu_{L,eff}$, is composed of two contributions: the molecular viscosity $\mu_{L,L}$, and the shear induced turbulent viscosity $\mu_{L,Turb}$, $\mu_{L,eff} = \mu_{L,L} + \mu_{L,Tur}$, The gas phase effective viscosity is calculated from the effective liquid viscosity $\mu_{G,eff} = \mu_{L,eff}\frac{\rho_G}{\rho_L}$. The shear-induced turbulent viscosity in the liquid phase is calculated using the chosen turbulence model. When the k-ε model is used, the shear-induced turbulent viscosity in the liquid phase is formulated as follows: $\mu_{L,Tur} = C_\mu \rho_L \frac{k_L^2}{\varepsilon_L}$ with C_μ=0.09. The conservation equations for k and ε are, respectively, given by:

$$\frac{\partial(\upsilon_L \rho_L k_L)}{\partial t} + \nabla \cdot \left(\upsilon_L \rho_L k_L \vec{u}_L - \upsilon_L \left(\mu_{L,L} + \frac{\mu_{L,L}}{\sigma_k} \right) \nabla k_L \right) = \varepsilon_L (G_L - \varepsilon \rho_L) \tag{4}$$

$$\frac{\partial(\upsilon_L \rho_L \varepsilon_L)}{\partial t} + \nabla \cdot \left(\upsilon_L \rho_L \varepsilon_L \vec{u}_L - \upsilon_L \left(\mu_{L,L} + \frac{\mu_{L,Turb}}{\sigma_\varepsilon} \right) \nabla \varepsilon_L \right) = -\nabla \left(\upsilon_L \frac{\mu_{L,eff}}{\sigma_\varepsilon} \nabla \varepsilon_L \right) + \upsilon_L \frac{\varepsilon_L}{k} (C_{\varepsilon 1} G_L - C_{\varepsilon 2} \varepsilon_L \rho_L) \tag{5}$$

With the production of turbulent kinetic energy, $G_L = \upsilon_L (\nabla U_L + (\nabla U_L)^T) : \nabla U$, and experimentally defined constant, $C_{\varepsilon 1}$=1.44, $C_{\varepsilon 2}$=1.92, σ_k=1.00, σ_ε =1.217. The interfacial momentum transfer, $F_{interfacial,}$ can be attributed to the sum of interfacial forces such as the Magnus effect, Basset effect, drag force, lift force, lubrication, virtual mass force, and turbulent dispersion forces.

$$F_{interfacial} = f_{drag} + f_{lift} + f_{lubrication} + f_{VM} + f_{TD} \tag{6}$$

Table 1: Interphase forces models and parameter

Interphase force	Model	Parameter
Drag	$f_D = -\frac{3}{4}\upsilon_g \rho_L \frac{C_D}{d_P} \lvert \vec{u}_g - \vec{u}_L \rvert (\vec{u}_g - \vec{u}_L)$	Ishii-Zuber (1975) $C_{D,Sphere} = \frac{2}{3} Eo^{1/2}$, $C_{D,Ellipse} = \frac{24}{\mathrm{Re}_P}(1 + 0.1\mathrm{Re}_P^{0.75})$
Lift	$f_L = C_L \upsilon_g \rho_L (\vec{u}_g - \vec{u}_L) \nabla \cdot u_L$	C_{Lift}=[0.1,0.5]
Turbulent dispersion	$f_{TD} = -C_{TD} \rho_L k_{TD} \nabla \upsilon_L$	C_{TD}=[0.1,0.5]

In this work it is taken into account only the drag force, drag, lift and turbulence dispersion forces since most authors report that the momentum transfer is mostly attributed due to the drag, lift forces (Tabid at al., 2008; Zhang et al., 2006). The drag force is originated by the differences in velocities between the phases and is expected to have the largest influence in the momentum transfer between the gas and liquid phases. The lift force (f_L) is caused by the effect of the pressure and stress over the bubble surface and is the principal mechanism that determines the phase distribution in bubble flow. The lift coefficient CL is between 0.1 and 0.5 for viscous liquid. The dispersion force characterizes the disperse phases eddies in the continuum. Lopes de Bertodano´s model (1991) is the most often used in bubble column, with turbulent dispersion coefficient C_{TD} between 0.1 and 0.5. The virtual mass force is caused by the relative acceleration between phases, Tabid et al. (2008) and Zhang et al. (2006) observed that the virtual mass force has an insignificant effect over the interfacial moment transfer in a bubble column.

Physical Problem

Pironti et al. (1995) experimental set-up, converts pressure drop into air holdup. The bubble column was employed in semi-batch mode, the column was filled with tap water and then air was introduced in the column at the bottom of the conical section through a nozzle with internal diameter of 0.63cm. The column has a draft tube. All the measures were taken a 25° Celsius and atmospheric pressure. The bubble column has two regions: (a) a conical base; and (b) a cylindrical region. The height of the cylindrical region is 3 m long, with an internal diameter of 15 cm. The draft tube is 2 m long, with a diameter of 7 cm and 0,5 cm of thickness. The conic section has a height of 43 cm and an angle of 34°. The draft tube was located 20 cm above the column entry. The superficial gas velocity is 5 cm/s. For the numerical analysis, the domain was discretized with a mesh chosen to guarantee a difference in pressure drop of less than 5 % for a sequential 50% of refinement. The simulation of a spouted bed air-water reactor is presented. Simulation is carried out by using a finite element-based finite volume numerical scheme together with a coupled solution algorithm (ANSYS-CFX). A typical run simulation took about 2 hours in a 1.6 GHz Intel core 2 duo processor and 1 GB RAM PC.

Results

Numerical results from RANS two-equation turbulence models are used to compare with Pironti at al. (1995) experimental data. The spouted column simulation provides a qualitative agreement with the observed experimental behavior and the expected hydrodynamic flow characteristics in the conical and exit sections of the draft tube, for both k-ε and k-ω turbulence models. Based on results with k-ε, the flow reflects the high mixing and turbulence in the entry of the cone (Fig 1a), and represents the spouted flow or fountain region in the exit section of the draft tube (Fig. 1b).

As it can be shown in Table 1, first the k-ε (Launder and Spalding,1974) is used with: (A) the Ishii-Zuber (1975) liquid-gas correlation for drag force; (B) adding the lift force; and (C) adding simultaneously the lift and Lopes de Bertodano´s turbulent dispersion force (1991). Secondly, the k-ω (Wilcox 1988) is used with: (D) the Ishii-Zuber correlation for drag force, adding the lift and turbulent dispersion forces simultaneously.

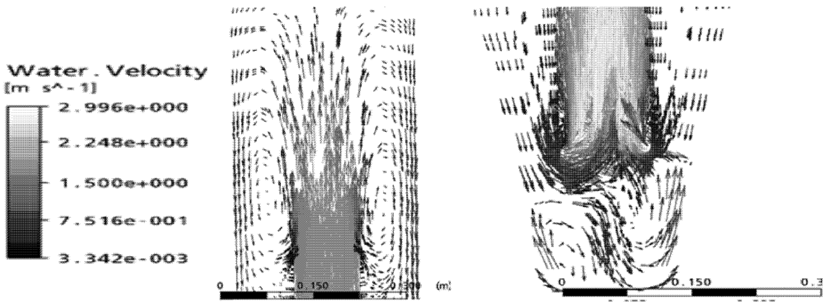

Figure 1: Conical section mixing: 1a conical section (right), 1b draft tube outlet (left)

Table 2: Error (%) in air hold up Momentum transfer modeling, *Ishii-Zuber(1975)*

Case	Turbulence model	C_{lift}	C_{TD}	Re_p	ε_g error (%)
A	k-ε			1159	18.69
B	k-ε	0.2		1114	0.18
C	k-ε	0.2	0.1	1086	0.14
D	k-ω	0.2	0.1	1248	4.08

The added effect of the interphase forces (e.g. drag force, lift force and turbulent dispersion forces), and the k-ε turbulence model, in the CFD modeling of the air-water system in the spouted bed improved the prediction of the air hold up. The k-ε and k-ω turbulence models predicted the air hold up within experimental error. Moreover, the k-ε with Ishii-Zuber liquid-gas drag model and lift force yielded very good results; in fact, the absolute error decreased from 18.69 to 0.18%. Adding the Lopes de Bertodano´s turbulent dispersion force model, the absolute error decreased further from 0.18% to 0.14% for the turbulence model, while the k-ω turbulence model predicted the air hold up within 4.08% when accompanied by the lift force and Lopes de Bertodano´s dispersion force.

The physical properties of the system, turns the interfacial force closures into a complex function of the bubble Reynolds number (Re), the Eötvös number (Eo), and the Morton number (M). For all cases, the Eötvös and Morton numbers were defined a priori supposing constant transport properties and uniform equivalent bubble diameter of 6mm. For the low experimental air hold-up of 14.70, the phenomena of coalescence and break–up are less probable and the assumption of uniform equivalent bubble diameter of 6mm is valid. The operating Eötvös and Morton numbers are 4.82 and 1.58e-11, respectively. The observed particle Reynolds number in the draft tube ranged between 1159 and 1086, indicating a Newton regime for the drag force using the k-ε turbulence model. The combination of the observed Re and defined Eo and M numbers are indicative of no spherical bubbles. The combination of the observed Re and defined Eo of 4.82, identified the same bubbles flow regime, which at these conditions is called wobbling flow regime (Grace et al., 1978). The almost uniform Re, of equal–sized bubbles is characteristic of decreasing rise velocity.

Conclusion

Numerical results explored the capabilities of two-equation turbulence models, as well as the inclusion of lift and turbulence dispersion forces in the correct prediction of the air hold-up. The results proved that: The momentum exchange is qualitatively characterized by equally balanced free-wall turbulence as the k-ε/ k-ω turbulence models both captured equally well the main features of the mixing region. However, the turbulence models by themselves do not suffice in the modeling of the quantitative features of the mixing flow. In fact, when no lift and turbulence dispersion forces were considered, very large errors were found in the quantitative prediction. Whereas, the inclusion of these extra interphase forces may reduce dramatically the error to less than 1% in the prediction of the air hold-up.

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