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Numerical Simulation of Hold-Up And Velocity Profiles for Two-Phase Developed Flows in a Column

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The purpose of this article is to simulate and analyse two-phase fluid dynamics in a bubble column, through two different numerical approaches, in a fast and effective way, to minimize project costs and increase productivity. Bubble column reactors are commonly employed in chemical processes because of their wide application area, such as simple construction and operation, high heat and mass transfer coefficients. Despite the model chosen in this article does not consider the reaction rate, bubble columns usually feature complex hydrodynamic interactions that requires a high computational effort for modelling. In this study, to simulate a bubble column reactor with continuous flow (e.g., air-water), two approaches were compared to predict axial and radial profiles for the two-phase, the finite volume and the variational method. The values of holdups and the axial velocity are in agreement with the experimental results in the literature.
Key Words: fluid dynamic, hold-up, finite volume method, variational method, modelling.

1. Introduction

Bubble columns are a multiphase reactors or contactors which performs interaction between gas and liquid phases with the purpose of promoting heat and mass transfer. This equipment is widely used in chemical, biochemical and petrochemical industries for having excellent heat and mass transfer coefficient, low maintenance and operating costs, simple design and operation such as the absence of moving parts. Despite its simple structure the column provides a good environment for the complex fluid dynamics interactions, which is the focus of this work.

The mixing behaviour and complex flow found in bubble columns are linked to the geometry column and the operation conditions, and often can be described as the global gas holdup and liquid circulation velocity (Wu and Al-Dahhan, 2001). The gas holdup (ε_g) is a dimensionless parameter that expresses the volumetric gas fraction over the total volume inside the column. This parameter is of great importance in the design of bubble columns for being directly attached to the phenomena of mass transport between the gas and liquid phases.

The characterization of fluid dynamics has a significant effect on the operation and performance of a bubble column. According to Hyndam et al. (1997) and Deckwer et al. (1980), the experimental results obtained by parameters investigations, strictly depend on the prevailing column regime. The flow regime is classified and maintained according to the superficial gas velocity and the column diameter.

In multiphase flows, the interaction between the phases is determined by solving the momentum equation which includes interfacial forces, e.g., drag force, lift force, turbulent dispersion and virtual mass. Eulerian-Eulerian approach often uses the drag force as the predominant interfacial force to predict flow pattern and hydrodynamics properties in the bubble column. Moreover, literature has shown that although the effect of drag force is significantly higher than the others interfacial forces, it is necessary to consider the lift force to solve the equation bring more accuracy to the bubble column simulation, improving predictions of the axial liquid velocity, turbulent kinetic energy and radial gas holdup (Gupta and Roy, 2013) and (Tabib and Roy, 2008).

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2. Mathematic model

The equations regarding the fluid dynamics in a bubble column are based on the continuity equations and momentum balance, using a Eulerian approach enabling the write for cylindrical or squared column systems with axis symmetry.
The general mass and momentum equation for two-phase flow can be found in Torvik and Svendsen (1990), and Grienberger and Hofmann (1992). For this paper the fluid dynamic model considers a general heterogeneous system with two-phases in a fully developed flow with all quantities e.g., holdups (ε_i), radial velocity (v_{ir}), axial velocity (v_{iz}) varying only in the radial direction. The two-phase are designated here by *i,j.*
The equations for the steady state isothermal two-phase flow in cylindrical coordinates with axisymmetric (r, z) are given by:

- Mass balance:

$$\frac{1}{r}\cdot\frac{\partial}{\partial r}[r\cdot\rho_i\cdot\varepsilon_i\cdot v_{ir}-r\cdot D_{ij}\cdot\frac{\partial}{\partial r}\cdot(\rho_i\cdot\varepsilon_i)]=\xi_i \tag{01}$$

For this paper the mass transfer was not considered, ξ_i= 0.

- Momentum balance:

Momentum equation in radial and axial direction, respectively, are given by:

$$\frac{1}{r}\cdot\frac{\partial}{\partial r}(r\cdot\rho_i\cdot\varepsilon_i\cdot v_{ir}\cdot v_{ir})=\rho_i\cdot\varepsilon_i\cdot g+\xi_i\cdot v_{ir}+F_{ijr}+L_{ijr}-\varepsilon_i\cdot\frac{\partial p}{\partial r}+\frac{1}{r}\cdot\frac{\partial}{\partial r}\cdot\left[r\cdot\mu_i\cdot\varepsilon_i\cdot 2\cdot\frac{\partial v_{ir}}{\partial r}\right]-\mu_i\cdot\varepsilon_i\cdot 2\cdot\frac{v_{ir}}{r^2} \tag{02}$$

$$\frac{1}{r}\cdot\frac{\partial}{\partial r}\cdot(r\cdot\varepsilon_i\cdot\rho_i\cdot v_{iz}\cdot v_{iz})=\rho_i\cdot\varepsilon_i\cdot g\cdot F_{ijz}+L_{ijz}-\varepsilon_i\cdot\frac{\partial p}{\partial z}+\frac{1}{r}\cdot\frac{\partial}{\partial r}\cdot\left[r\cdot\mu_i\cdot\varepsilon_i\cdot\frac{\partial v_{iz}}{\partial r}\right] \tag{03}$$

The turbulent viscosity ($\mu^{(t)}$) was calculated using a zero order turbulence model proposed by Chen et al. (1995) and Menzel et al. (1990):

$$\mu^{eff}=\mu+\mu^{(t)} \tag{04}$$

The diffusivity of one phase into another (D_{ij}) affects the distribution of the phases volume fraction (ε_i) inside the column. The eq. (05) shows that the diffusivity coefficient can be equal to turbulent viscosity divided by the density of a given phase (*i,j*).

$$D_{ij}=\frac{\mu_i^{(t)}}{\rho_i}=\frac{\mu_j^{(t)}}{\rho_j}=f(r)=k\cdot\frac{R}{6}\cdot\frac{\sqrt{P_w}}{\rho_m}\cdot\left[1+2\left(\frac{r}{R}\right)^2\right]\cdot\left[1-\left(\frac{r}{R}\right)^2\right] \tag{05}$$

The momentum balances account for two interfacial forces. The Magnus force, commonly known as the transversal lift is a phenomenon in which the rotation of a body modifies the trajectory of the fluid. It is generated by velocity gradients at relative speed across the bubble diameter, forcing it to move against the liquid phase velocity gradient.

$$L_{ijr}=0{,}5\cdot C_L\cdot\varepsilon_i\cdot\varepsilon_j\cdot(v_{iz}-v_{jz})\cdot\left[\rho_i\cdot\left(-\frac{\partial v_{iz}}{\partial r}\right)+\rho_j\cdot\left(-\frac{\partial v_{jz}}{\partial r}\right)\right] \tag{06}$$

The other interfacial force used is the drag force. It is a resistance force offered by the system, slowing down the bubbles' movement due to the flow of liquid phase near at the bubble's boundary layer.

$$F_{ijr}=C_D\cdot\varepsilon_i\cdot\varepsilon_j\cdot(v_{jr}-v_{ir}) \tag{07}$$

- Boundary conditions:

$$\frac{\partial v_{iz}}{\partial r}=0\quad r=0 \tag{08}$$

$$v_{ir}=0\quad r=0 \tag{09}$$

$$v_{ir} = 0 \quad r = R \tag{10}$$

$$v_{iz} = 0 \quad r = R \tag{11}$$

3. Numerical Methods

3.1 Finite Volume Method

The finite volume method is a class of finite difference method where the domain is subdivided into a finite number of smaller control volumes. The main characteristics of this method is the simple and easy derivation where the equations can be interpreted in physical terms as the tendency to solve partial different equations to iterative calculations through its non-linear equations. This method was widely used by Patankar and Spalding (1972), that contributed to fill the gap in the calculation procedures for three-dimensional flow at that time. Currently is one of the most used methods to calculate fluid dynamics. In this study, Excel was chosen to run this simulation because of its simple calculation platform and easy access.

3.2 Variational Method

The variational method is a numerical method that allows to obtain an accurate or estimated solution for an objective function, with unknown parameters and functions. The unknown terms are determined by the operating conditions and restrictions that are applied to the system. The principle of this method is to transform a differential equation into an integral equation, mathematically equivalent, by using the Euler-Lagrange equation (Gal-Or et al., 1972). The variational model used in this work was described in Guirardello (2019). This method is solved by GAMS software and usually is defined to maximize or minimize the objective function. The software solves the designated problem in order to deliver the optimum value.

4. Simulation

To investigate the fluid dynamics inside of a column, two main components of phases distributions were predicted, axial liquid velocity and gas hold-up, one-dimensional in the radial direction. The simulation was conducted for a bubble column with 29 cm inner diameter, operating in a fully developed flow, with a co-current upward flow of liquid and gas phases (air-water).

In this study no chemical reaction was considered. A zero order turbulence model was assumed to express the liquid dispersion and the fluid is considered Newtonian (Menzel et al., 1990; Chen et al., 1995). The simulation was conducted in GAMS software and Excel to calculate the turbulent flow of two-phase bubble column through variational and finite volume methods. The cases were solved using 20 intervals in the radial direction and a lift coefficient (C_L) of -1. In GAMS code program was used CONOPT3 to solve nonlinear equations.

The values of drag coefficient (C_D) and root mean square of pressure at the wall divided by apparent mixture density $\left(\frac{\sqrt{P_w}}{\rho_m}\right)$ were estimated to find an agreement between experimental and predicted results.

5. Results and discussion

Two main local parameters were evaluated in the simulations of the fluid dynamics, the gas holdup and axial velocity. Two cases simulation were conducted in order to analyse the profiles predicted for different flow regimes by distinct superficial gas velocity.

In the model used local gas holdup was calculated by using the volumetric fraction balance equation (12) and the liquid holdup (13).

$$\varepsilon_g + \varepsilon_l = 1 \tag{12}$$

$$\varepsilon_l \cdot v_{lr} = f(r) \cdot \frac{\partial \varepsilon_l}{dr} \tag{13}$$

The axial liquid velocity was calculated by sum of the eq. (03) for gas and liquid phases, canceling the drag and lift force ($F_{ijr} = -F_{jir}$, $L_{ijz} = -L_{jiz}$). It was also considered that physical properties of the liquid phase e.g., the density and viscosity, are extremely higher than the gas phase ($\rho_g \ll \rho_l, \mu_g \ll \mu_l$) and that radial liquid velocity is significantly lower than the axial liquid velocity ($v_{lr} \ll v_{lz}$).

$$-\left(\rho_l \cdot \varepsilon_l + \rho_g \cdot \varepsilon_g\right) \cdot g \cdot \frac{\partial p}{\partial z} + \frac{1}{r} \cdot \frac{d}{dr} \cdot \left[r \cdot \mu_l \cdot \varepsilon_l \cdot \frac{\partial v_{lz}}{\partial r}\right] = 0 \tag{14}$$

The axial gas velocity was calculated considering the sum of momentum balance eq. (03) for the gas and liquid phases. It was also considering that radial liquid velocity is significantly lower than the axial liquid velocity, ($v_{lr} \ll v_{lz}$).

$$C_D \cdot \varepsilon_l \cdot (v_{gz} - v_{lz}) - \frac{1}{\varepsilon_g} \cdot \frac{1}{r} \cdot \frac{d}{dr} \cdot \left[r \cdot \mu_g \cdot \varepsilon_g \cdot \frac{\partial v_{gz}}{\partial r} \right] + (\rho_g \cdot g - k) = 0 \quad (15)$$

The radial liquid velocity was calculated from the eq. (4) divided by ε_i, then subtracting the liquid equation from the gas equation. Also was considered that the gas phase density and viscosity are extremely lower the liquid phase.

$$\frac{1}{r} \cdot \frac{\partial}{\partial r} \cdot \left[r \cdot \mu_l \cdot \varepsilon_l \cdot 2 \cdot \frac{\partial v_l}{\partial r} \right] - \mu_l \cdot \varepsilon_l \cdot 2 \cdot \frac{v_{lr}}{r^2} - C_D \cdot \frac{\varepsilon_l}{\varepsilon_g} \cdot v_{lr} = 0.5 \cdot C_L \cdot (v_{gz} - v_{lz}) \cdot \rho_l \cdot \left(- \frac{\partial v_{lz}}{\partial r} \right) \quad (16)$$

For case 1, it was considered a superficial gas velocity (U_g) of 0,04 m/s and superficial liquid velocity (U_l) of 0,01 m/s, with a $\frac{P_w}{\rho_m}$= 7650 cm²/s², the drag force was calculated using C_D = 40 g.cm^{-3}.s^{-1}. The predictions for the main local parameters from the numerical methods used were compared with the experimental results from Yao et al. (1991) presented in Figure1. Others parameters that were calculated are presented in table 1, indicating the values distributed along the 20 intervals evidenced by the ratio distribution in the first column. The 2nd to 5th column refer to the simulation via GAMS and the 6th and 7th through Excel. The effective viscosity (μ^{eff}) was equal to both methods while the radial liquid velocity had a difference less than 0,5%. The Axial and radial gas velocity had a slightly difference between the finite volume and variational method.

Table 1: Comparison calculated parameters in case 1 (all units in CGS).

r	μ^{eff}	v_{lz}	v_{gz}	v_{gr}	v_{gz}	v_{gr}
0.00	21.0748	0.0000	59.3642	0.0000	59.4746	0.0000
0.73	21.1272	0.0803	58.8547	-0.2943	58.9996	-0.2945
1.45	21.2813	0.1551	57.3265	-0.5791	57.5790	-0.5719
2.18	21.5276	0.2148	55.0991	-0.8262	55.3304	-0.8112
2.90	21.8503	0.2553	52.3066	-1.0196	52.4170	-1.0005
3.63	22.2273	0.2767	49.0869	-1.1542	49.0256	-1.1344
4.35	22.6300	0.2817	45.5843	-1.2312	45.3422	-1.2134
5.08	23.0239	0.2741	41.9381	-1.2566	41.5346	-1.2425
5.80	23.3676	0.2579	38.2725	-1.2390	37.7433	-1.2292
6.53	23.6139	0.2364	34.6919	-1.1877	34.0789	-1.1819
7.25	23.7090	0.2121	31.2789	-1.1109	30.6242	-1.1084
7.98	23.5928	0.1865	28.0971	-1.0154	27.4398	-1.0151
8.70	23.1990	0.1606	25.1951	-0.9055	24.5700	-0.9063
9.43	22.4549	0.1346	22.6113	-0.7832	22.0493	-0.7841
10.15	21.2813	0.1083	20.3802	-0.6478	19.9109	-0.6477
10.88	19.5930	0.0808	18.5395	-0.4944	18.1955	-0.4917
11.60	17.2984	0.0499	17.1385	-0.3111	16.9679	-0.3026
12.33	14.2993	0.0111	16.2478	-0.0696	16.3502	-0.0471
13.05	10.4915	-0.0488	15.9597	0.3030	16.6171	0.3654
13.78	5.7644	-0.1728	16.3184	0.9673	18.6248	1.1542
14.50	0.0010	0.0000	0.0000	0.0000	0.0000	0.0000

In the case 2, it was considered a U_g of 0,08 m/s and U_l of 0,01 m/s, $\frac{P_w}{\rho_m}$ = 14400 cm²/s², the drag force between phases was calculated using C_D= 40 g.cm^{-3}.s^{-1} The local values for axial liquid velocity and gas holdup calculated were compared with the experimental results from Torvik and Svendsen (1990) presented in Figure2. The axial and radial velocities and the effective viscosity was calculated for these conditions are showed in Table 2. However, it only displays the results from GAMS because the values obtained are quite similar and among them the variational method was the one that showed a lightly better axial liquid velocity profile.

Table 2: Calculated parameters in case 2 (all units in CGS).

r	μ^{eff}	v_{gz}	v_{gr}	v_{lr}
0.00	28.9140	76.5568	0.0000	0.0000
0.73	28.9859	75.7951	-0.3488	0.2279
1.45	29.1973	73.5100	-0.6863	0.4391
2.18	29.5353	70.1974	-0.9807	0.6071
2.90	29.9780	66.0510	-1.2132	0.7202
3.63	30.4952	61.2730	-1.3768	0.7790
4.35	31.0478	56.0747	-1.4718	0.7913
5.08	31.5881	50.6605	-1.5045	0.7682
5.80	32.0597	45.2135	-1.4849	0.7209
6.53	32.3977	39.8871	-1.4239	0.6590
7.25	32.5281	34.8032	-1.3317	0.5896
7.98	32.3687	30.0553	-1.2163	0.5170
8.70	31.8284	25.7138	-1.0831	0.4438
9.43	30.8074	21.8341	-0.9348	0.3707
10.15	29.1973	18.4652	-0.7701	0.2968
10.88	26.8811	15.6600	-0.5831	0.2194
11.60	23.7328	13.4893	-0.3588	0.1326
12.33	19.6181	12.0600	-0.0651	0.0239
13.05	14.3939	11.5390	0.3674	-0.1366
13.78	7.9083	12.1610	1.0264	-0,4195
14.50	0.0010	0.0000	0.0000	0.0000

The values presented in Table 3 refer to the mean squared error of the main parameters calculated in the cases 1 and 2. These values are referred to experimental dada used in each case. The 2nd. and 3rd. columns refer to finite volume method, and the 3rd. and 4th. columns refer to variational method.

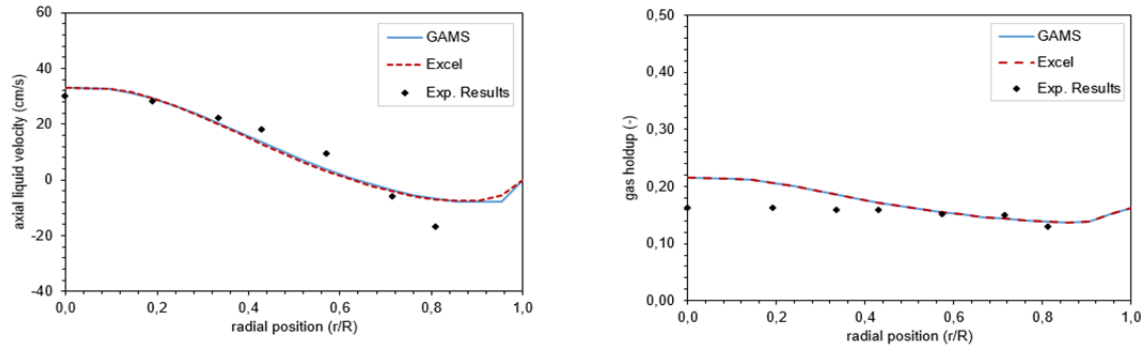

Figure1- Results for (a) axial liquid velocity and (b) local gas holdup, comparing with experimental results from Yao et al. (1991).

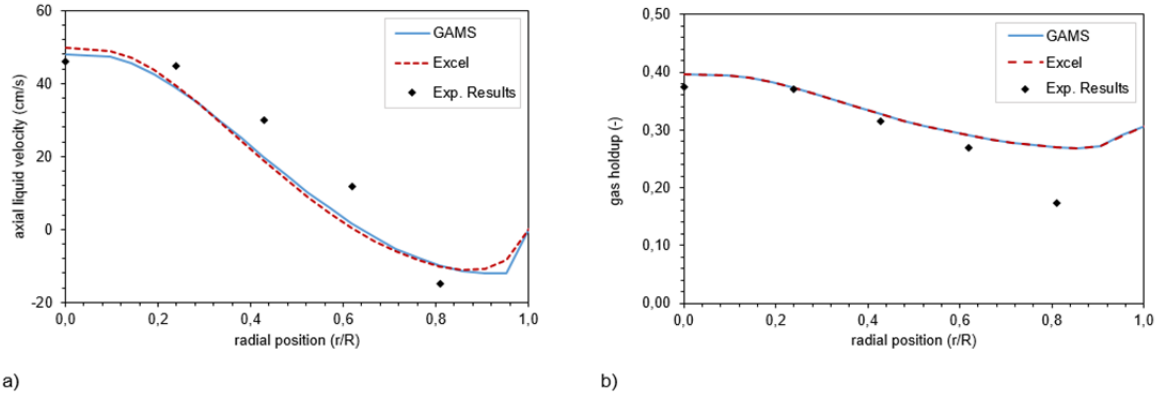

Figure 2- Results for (a) axial liquid velocity and (b) local gas holdup, comparing with experimental results from Torvik and Svendsen (1990).

Table 3: Mean squared error obtained (all units in CGS).

	ε_g	v_{lz}	ε_g	v_{lz}
Case 1	0.0008	26.0817	0.0008	24.5105
Case 2	0.0021	63.0019	0.0021	52.8591

According information presented in Kantarci et al. (2005), the operation condition and column geometry presented in the 1st case is considered a homogeneous bubble regime while in the 2nd case it is a churn turbulent regime. Despite of its different flow regimes seen in Figure 1(b) and 2 (b) it has shown a good similarity on the axial liquid velocity curves between experimental dada and calculations results. Although the case 2 has a higher quadratic error. Probably it was caused by the increase in the superficial gas velocity in the column forming larger bubbles destabilizing the bubble flow due to the coalescence effect. As a result, it increases the recirculation patterns inside the column.

6. Conclusions

The numerical methods proposed for a two-phase bubble column showed good results, being able to give reliable results for the two cases studied. Proving that for one-dimensional system both methods have precise results. A nonlinear problem is usually sensitive to initial estimates, therefore variational method program used the values of liquid hold-ups from finite volume method to run calculations. That may be the reason why some of the calculated values are similar in both methods. For future studies some improvement on the programing code will be necessary. This study also proves that Excel, can be used to calculate fluid dynamics problems without an expensive optimization software with a proper mathematical method, minimizing project cost.
For this study all physical properties were considered constant, calculation should be revised in future problems for chemical reaction or if the physical properties change with pressure.

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