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COMPARISON BETWEEN 2D AND 3D TRANSIENT FLOW SIMULATION OF GAS – LIQUID DYNAMICS IN TWO-PHASE CYLINDRICAL BUBBLE COLUMN REACTORS BY CFD

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ABSTRACT

In this research paper, we evaluated the applicability of using computational fluid dynamics (CFD) to simulate a transient, two-dimensional axisymetric and three-dimensional dynamic Eulerian-Eulerian two-phase model and for the modeling of bubble column hydrodynamics in the homogeneous flow regime. A two fluid model along with the standard k-ε model for turbulence in liquid phase is considered. Further numerical studies investigate the influence of additional turbulence production through the dispersed gas phase. The experimental data, with reference to the works literature experimental data of Dudukovic et al. (1999) that was obtained via Computer Automated Radioactive Particle Tracking System (CARPT) and Pleger et al. (2001) works literature that was obtained via particle image velocimetry, allow for the validation of the model simulation. The comparison between experimental data and CFD modeling focus on the local axial liquid velocity. The simulations are done using Fluent CFD software. Reasonably good quantitative agreement is obtained between the experimental data and simulations profiles defined points. Also these results will expect for the turbulent kinetic energy and the other variables profiles. Employing finer grids improves the description of the flow structure in the bubble column and the agreement with the experimental data. However, the computation power increases significantly and a compromise between efficiency and quality of results has to be found.

Key words: CFD, Bubble column, Hydrodynamics, Two-phase model, Axial liquid velocity, Liquid recirculation

INTRODUCTION

Bubble column reactors are widely used as gas liquid contactors in industrial fermentation, hydrogenation and other chemical operations because of their simple

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construction and case of maintenance. Bubble column combine efficient gas transfer and mixing with low shear forces. The behavior of these reactors is determined by their hydrodynamic properties. The complex flow and mixing behavior found in bubble column are often described by means of local parameter such as gas holdup and axial liquid velocity. There are currently strong efforts in academic institutions and industry to enable the use of computational fluid dynamics (CFD) for the design, scale-up, and optimum operation of bubble column reactors. The simulation of bubbly flows is still not fully mastered mainly due to its complexity and the manifold interacting phenomena. The bubble column hydrodynamics are dominated by the movement of the bubble plume and the three-dimensional (3D) vertical flow structures in the liquid phase that continuously change sizes and positions[1].

It is generally accepted that only dynamic 3D flow models are able to simulate theessential features encountered in bubble columns to a reasonable extent[1-3]. Most of the transient CFD studies of the last decade focused on flat bubble columns with a rectangular cross section because they have a less complex flow structure. They proved to be a useful tool for numerical model development and validation. Characteristic flow structures of gas and liquid phases are formed in cylindrical bubble columns depending on operating parameters such as gas flow rate, aspect ratio, and sparger location. For certain configurations the bubble plume moves periodically in lateral direction[3-5]. This unsteady flow behaviour can be measured and described quantitatively[6]. Its simulation is sensitive to the applied physical model and the chosen model parameters[1,3,7]. The correct prediction of shape and movement of the bubble hose in a flat bubble column is therefore considered as a criterion of quality for dynamic flow models. This investigation transfers the knowledge and experiences obtained from dynamic modeling of bubbly flows in flat bubble columns[3] to a bubble column with cylindrical geometry. This important step away from academic test cases brings the two-phase flow modeling closer to industrial-scale apparatus.

Most of the publications on cylindrical bubble columns focused up to now on time-averaged hydrodynamics. The dynamic flow behaviour that dominates the liquid-phase mixing and interacts with mass transfer and reaction processes is usually not considered. Only a few time dependent experimental data are available. It is well known that the transient flow is very important in many processes (i.e. stirred tank and plug reactors) for achieving to residual time (RTD) and having initial condition for arriving to steady state time. Also difference of results accuracy, CPU time and the other computational effort are depending on the computational setup. Therefore, we attempted to make two models with deference types of computational setup. In the present work, the transient flow dynamics behavior in full 3D and 2D axisymetric bubble column is

simulated using Fluent 6.0 CFD commercial package and prediction of results is compared against the experimental data and its computational setup differences compared through the error bar chart.

THEORY

Numerical simulation

In the present work the flow in the bubble column reactor is modeled using the Eulerian multiphase model and the k-ε model with fluent simulation. We observed that for simulation with better results, the Eulerian multiphase model and the k-ε model would both be applied. Although both models are used to predict multiphase flows, there are fundamental differences in their respective approaches, which are outlined here.

The Eulerian multiphase model

In the Eulerian two-fluid approach, the different phases are treated mathematically as interpenetration continua. The derivation of the conservation equations for mass, momentum and energy for each of the individual phases is done by ensemble averaging the local instantaneous balances for each of the phases[8]. The basic assumptions of this formulation used in the present computations are as follows:

(i) All phases are treated as interpenetrating continua and the probability of occurrence of every phase in multiple realizations of the flow is given by instantaneous volume fraction of that phase at that point. Total sum of all volume fractions at a point is identically unit.

(ii) Both fluids are treated as incompressible, and a single pressure field is shared by all phases.

(iii) Continuity and momentum equations are solved for each phase.

(iv) Momentum transfer between the phases is modeled through a drag term, which is a function of the local slip velocity between the phases. A characteristics diameter is assigned for the dispersed phase gas bubbles, and a drag formulation based on a single sphere settling in an infinite medium is used. The turbulence in either phase is modeled separately. The conservation equations can be written as follows:

$$\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla.(\alpha_k \rho_k \mathbf{u}_k) = \sum_{\rho = 1}^{n} \dot{m}_{pk.} \quad \ldots (1)$$

$$\frac{\partial}{\partial t}(\alpha_k \rho_k \mathbf{u}_k) + \nabla.(\alpha_k \rho_k \mathbf{u}_k \otimes \mathbf{u}_k) = -\alpha_k \nabla_p + \nabla.\bar{\bar{\tau}} + \mathbf{F}_k + \sum_{\rho=1}^{n} (K_{pk}(\mathbf{u}_p - \mathbf{u}_k) + \dot{m}_{pk}\mathbf{u}_{pk}) \quad \ldots(2)$$

The fourth term on the right hand side of Eq. (2) represents the interphase drag term, with K_{pk} being the momentum exchange coefficient between the pth and the kth phases. The evaluation of the needed drag coefficient requires the bubbles Reynolds number, which are based on the local slip velocity for a single sphere with constant diameter sediment in stagnant fluid. In the present computations, the drag coefficient, K_{pk} is based on the generalized correlations[9]. The turbulence in the continuous phase is modeled through a set of modified k-ε equations with extra terms that include inter phase turbulent momentum transfer[10]. This term can be derived exactly from the instantaneous equation of the continuous phase and it involves the continuous-dispersed velocity covariance. The turbulent quantities for the dispersed phase in Fluent are based on characteristic particle relaxation time and Lagrangian time scale[11].

For the dispersed gas phase, the turbulence closure is affected by the correlation of the dispersion theory, which becomes discrete by homogeneous turbulence[12]. The equations discussed above are solved using an extension of the SIMPLE algorithm[13]. The momentum equations are decoupled using the full elimination algorithm (FEA). By using SIMPLE-FEA[14], the variables for each phase are eliminated from the momentum equations for all other phases. The pressure correction equation is obtained by summing the continuity equations for each of the phases. The equations are then solved in a segregated, iterative fashion and are advanced during the time. At each time step, with an initial guess for the pressure field, the primary- and secondary-phase velocities are computed. These are used in the pressure correction equation (continuity), and based on the discrepancy between the guessed pressure field and the computed field, the velocities, holdups and fluxes are suitably modified to obtain convergence in aniterative manner –

The k-ε model

In the k-ε model, the basic equation set consists of the continuity and momentum equations for N_p phases. The first one is expressed by.

$$\frac{\partial}{\partial t}(\rho_a r_a) + \frac{\partial}{\partial x_i}(\rho_a r_a u_{a,i}) = \sum_{\beta=1}^{N_p} (\dot{m}_{\alpha\beta} - \dot{m}_{\alpha\beta}) + r_\alpha S_\alpha \quad \ldots(3)$$

The right-hand side of the continuity equation describes mass transfer from phase α

to β as well as vice versa and includes additional source terms. In this work, mass transfer and source terms were neglected. Therefore, Eq. (3) simplifies to –

$$\frac{\partial}{\partial t}(\rho_a r_a) + \frac{\partial}{\partial x_i}(\rho_a r_a u_{a,i}) = 0 \qquad \ldots(4)$$

Where r_a represents the volume fraction of phase α . The sum over all N_p phases satisfies below relation –

$$\sum_{i=1}^{N_p} r_i = 1 \qquad \ldots (5)$$

In analogy with the mass conservation, the momentum conservation for multiphase flows is described by the Navier– Stokes equations expanded by the phase volume fraction r_α and the interphase transfer term $M_{\alpha, i}$

$$\frac{\partial}{\partial t}(\rho_\alpha r_\alpha u_{\alpha,i}) + \frac{\partial}{\partial x_i}(\rho_\alpha r_\alpha u_{\alpha,i} u_{\alpha,j}) = - r_\alpha \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i} r_\alpha \mu_\alpha \left(\frac{\partial u_{\alpha,i}}{\partial x_j} + \frac{\partial u_{\alpha,i}}{\partial x_i} \right) + \rho_\alpha r_\alpha g_i + M_{\alpha,i} \ldots(6)$$

The terms on the right–hand side describe all forces acting on a fluid element of phase α in the control volume. These are the overall pressure gradient, the viscous stresses, and the gravitational force and interphase momentum forces combined in $M_{\alpha i}$. Only the drag force is included up to now in our model, which is based on Weber et al.

$$M_{\alpha,i} = \frac{3}{4} (C_d r_\beta \rho_\alpha \frac{1}{d_b} \left| u_\beta - u_\alpha \right| (u_\beta - u_\alpha) \qquad \ldots(7)$$

The drag coefficient (C_d = 0.44) and bubble diameter (d_b = 4 mm) is set constant in the simulations to define a fixed slip velocity between bubbles and surrounding liquid of around 20 cm/s. The use of a more complex drag model did not result in better agreements. Due to the fact that simulation results are not sensitive with respect to a fixed slip velocity in our regime, it is reasonable to use this model assumption. Coalescence and bubble breakup are not considered in this model. The impact of these phenomena is negligible for our test case configuration and conditions. Turbulence is taken into consideration for the continuous phase. The dispersed gas phase is modeled laminar but influences the turbulence in the continuous phase by a bubble-induced turbulence model. The well-known single-phase standard *k*- ε turbulence model[15] is used to model the turbulence phenomena in the continuous phase of the gas–liquid flow. Its transport equations for the turbulent

kinetic energy, k and turbulent dissipation rate, ε is –

$$\frac{\partial}{\partial t}(\rho_\alpha r_\alpha k_\alpha) + \frac{\partial}{\partial x_i}(r_\alpha \rho_\alpha u_{\alpha,i} k_\alpha) - \frac{\partial}{\partial x_i}\left(r_\alpha \left(\mu_{\alpha,lam} + \frac{\mu_{\alpha,tur}}{\sigma_k} \right) \frac{\partial k_\alpha}{\partial x_i} \right) \quad \ldots(8)$$
$$= - r_\alpha \left(G_\alpha - \rho_a \varepsilon_a \right) + S_{\alpha,k}$$

$$\frac{\partial}{\partial t}(r_a \rho_a \varepsilon_a) + \frac{\partial}{\partial x_i}(r_a \rho_a u_{a,i} \varepsilon_a) - \frac{\partial}{\partial x_i}\left(r_\alpha \left(\mu_{\alpha,lam} + \frac{\mu_{\alpha,tur}}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon_\alpha}{\partial x_i} \right) \quad \ldots(9)$$
$$= r_\alpha \frac{\varepsilon_a}{k_a} \left(C_{\varepsilon 1} G_a - C_{\varepsilon 2} \rho_a \varepsilon_a \right) + S_{a,\varepsilon}$$

The standard model is taken without any further modifications. The source terms $S_{\alpha,\varepsilon}$ and $S_{\alpha,k}$ on the right-hand side of the equations are not considered in the mean of interphase turbulence exchange. The effective viscosity of phase α in Eq. (4) is combined by –

$$\mu_{a,eff} = \mu_{a,lam} + \frac{\mu_{a,tur}}{\sigma_k} \quad \ldots(10)$$

Using the standard k- ε model, the turbulent viscosity of the continuous phase is calculated by –

$$\mu_{c,\,tur} = C_\mu \rho_c \frac{k_c^2}{\varepsilon_c} \quad \ldots(11)$$

One of the main objectives of our investigations is the evaluation of bubble-induced turbulence in gas-liquid flows, which seems to have an important impact on the correctness of simulation results[16]. A direct coupling of turbulence equations via an interphase exchange term similar to the one of the momentum equations is not possible due to the missing set of equations for turbulence in the gas flow. Nevertheless, implementing additional production terms in k- and ε- equations can capture the influence of bubbles on turbulence. The term G_α models the production of turbulence by the local shear forces in the continuous phase. It is imaginable that the wakes behind rising bubbles cause additional stresses, which influence the turbulence intensity. The advanced approach is defined as

$$G_a = \mu_{a,eff} (\nabla u_a + \nabla u_a^T) : \nabla u_a + G_{a,BIT} \quad \ldots(12)$$

in which the velocity gradients of the first term model the shear-induced production. The energy input of the bubble wakes results from the forces acting between a gas bubble and the surrounding liquid and the local slip velocity

$$G_{\alpha,BIT} = C_{k/\varepsilon}\left|M_{\alpha,\beta}\right|.\left|u_{\beta} - u_{\alpha}\right| \quad \ldots(13)$$

Since only the drag force is acting in the recent modeling approach, the bubble-induced turbulence term is proportional to the interphase exchange term $M_{\alpha,i}$ and is represented by Eq. (7). The constants $C_{k/\varepsilon}$ corresponds either to the *k*- or ε- equation and are combined with RNG *k*- ε constants. The settings are $C_k = C_{\varepsilon 1} = 1.44$ and $C_{\varepsilon} = C_{\varepsilon 2} = 1.92$. Similar approaches for bubble-induced turbulence are published[17, 18].

CFD Simulation setup

The first step in developing the computer simulation was to create a 3-D model and a two-dimensional axisymetric of the bubble column reactor. For this reason, Gambit Fluent's preprocessor is used, that permit both; geometry creation and meshing as shown in Fig. 1.

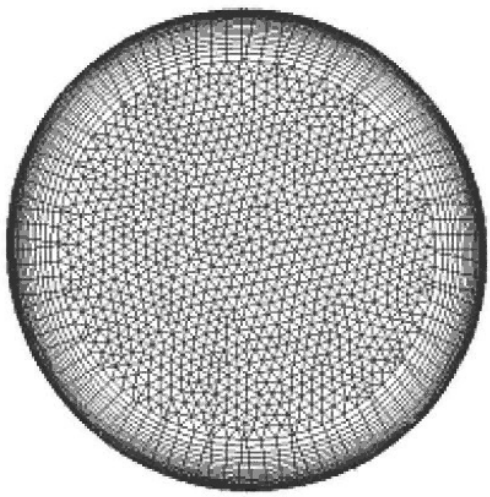

Fig. 1: Computational mesh (structured grid)

The geometry of the column, as shown in Fig. 2 was basically a vertical cylinder with a velocity inlet at the bottom and an outflow at the top that was simple to create. After that the Gambit software generated the mesh. The next step is imposed the boundary conditions for the problem. The bubble column is divided into grids of different resolutions

to evaluate grid (in) dependence. The grids consist of cell numbers between 6100 and 62, 500. The standard tri grid is represented by only 33000 cells with a boundary computational grid. The geometry is represented in three dimensions through Cartesian coordinates (Fig. 2).

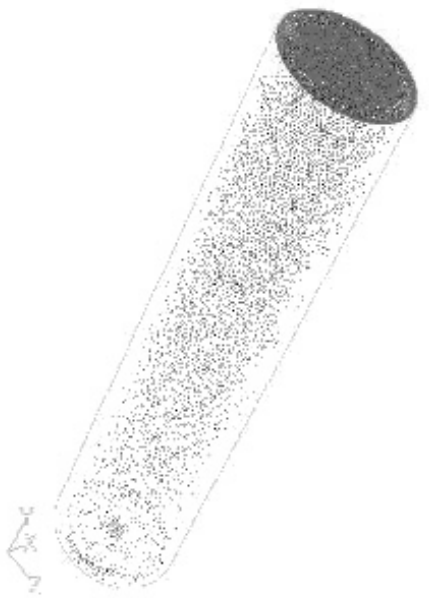

Fig. 2: Geometry and computational domain

The circular cross-section is divided into a central circular with 2-rim zone with the standard tri grid. The latter ones fill one-cylindrical of a circle between the circular wall boundary and the center circle. The axial direction is split up into 5000 cells with grading to the gas sparger modeled by an inlet boundary condition and the free surface modeled by condition with a degassing sink. The standard tri grid and boundary grid subdivision are chosen after tests in the tension between the exactness of simulation and requirements of CPU time. The two-dimensional axisymetric computational mesh is uniform grid. The solution of the equation system is carried out using the SIMPLEC procedure. The application of a higher order differencing schemes like total variation diminishing (TVD) is necessary to obtain accurate solutions which are well known for Eulerian-Eulerian multiphase models[7]. The overall calculation of the 150 min real time increment needs Dual (CPU, 3.00 GHz) processor.

RESULTS AND DISCUSSION

To get a better understanding of gas-liquid flow structure, the experimental data, with reference to the works literature experimental data of Dudukovic and Chang[19] that was obtained via Computer Automated Radioactive Particle Tracking System (CARPT) and Pfleger et al.[20] works literature that was obtained via particle image velocimetry, is applied.

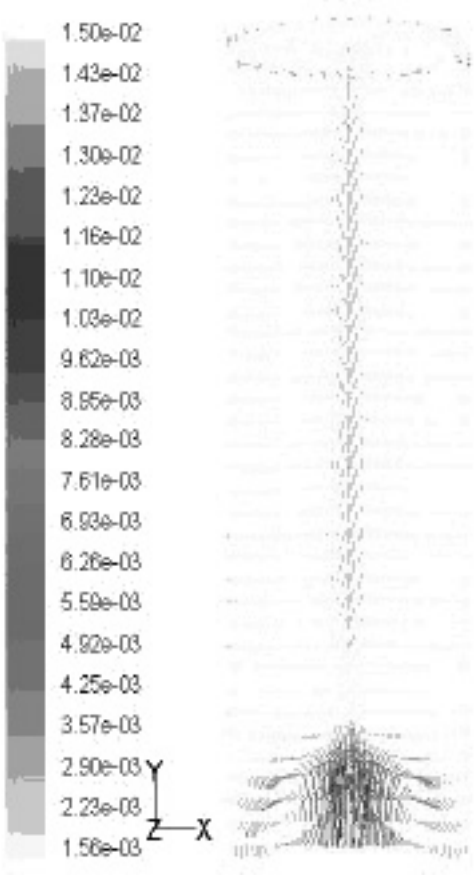

Fig. 3: Contour of velocity vectors (5th time step)

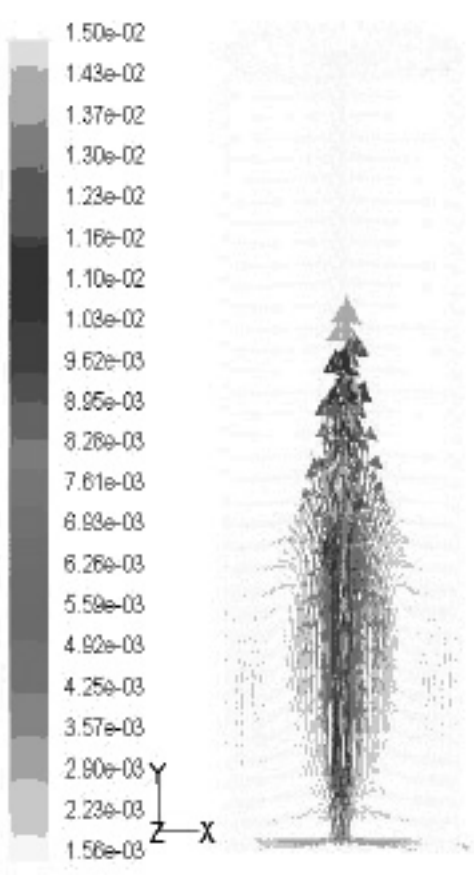

Fig. 4: Contour of velocity vectors (20th time step)

The experimental results were compared with the numerical simulation results. One main simulated evolution of variable is investigated. It consists in the evolution of pressure drop and local axial velocity. The local axial velocity is a fundamental quantity in

the description and analysis of multiphase flow, since it affects the flow regime; pressure drop, heat transfer and mass transfer characteristics.

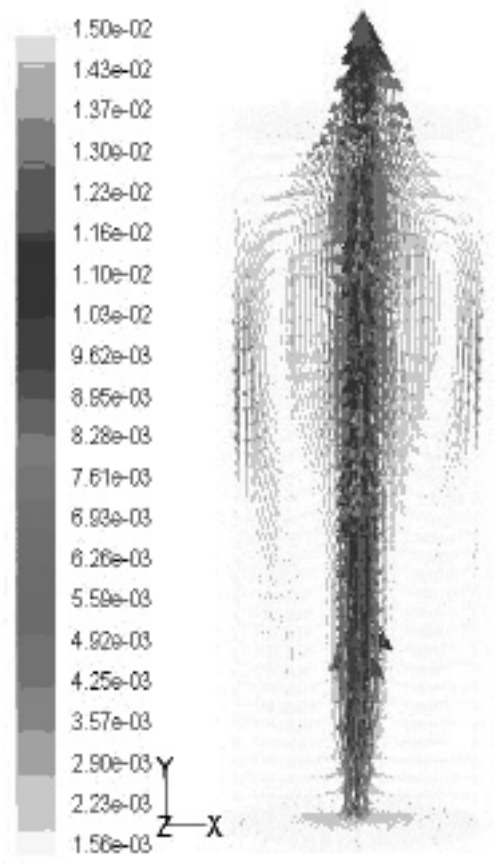

Fig. 5: Contour of velocity vectors (100th time step)

Fig. 6: Contour of full three dimensional velocity vectors (100th time step)

Generally, its distribution is influenced mainly by the gas and liquid flow rates, but also by the fluid properties of column geometry. The evolution of axial velocity with superficial gas velocity (as shown in Fig. 7 and Fig. 8) and mean gas holdup profile are compared to the experimental values (Fig. 9) and shows a good prediction of the experimental data.

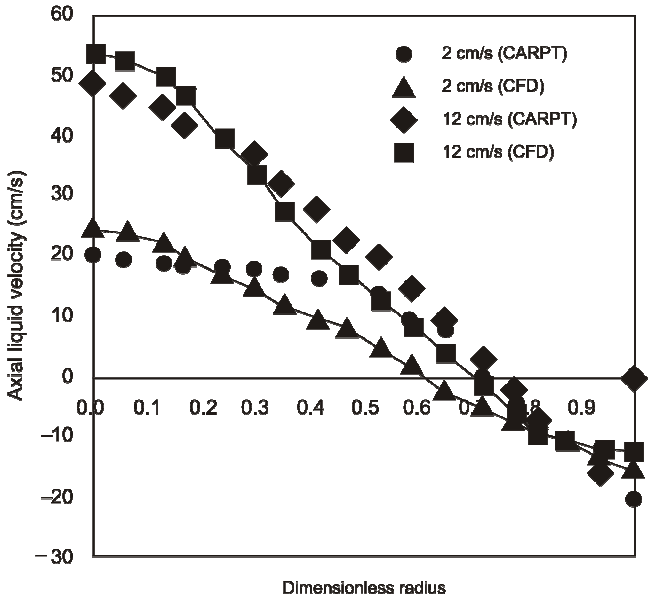

Fig. 7: Comparison between experimental data (CARPT data) and CFD simulation

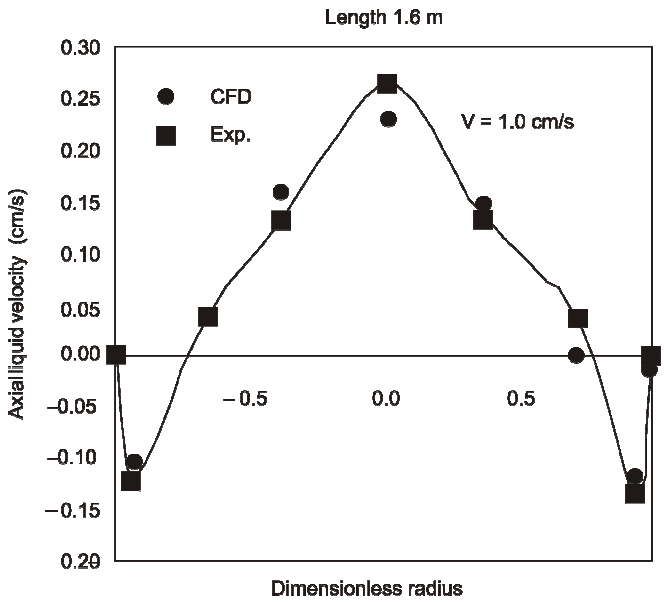

Fig. 8: Comparison between experimental data (D. Pfleger et al.[3]) and CFD simulation (with all enhancement effects, full 3D)

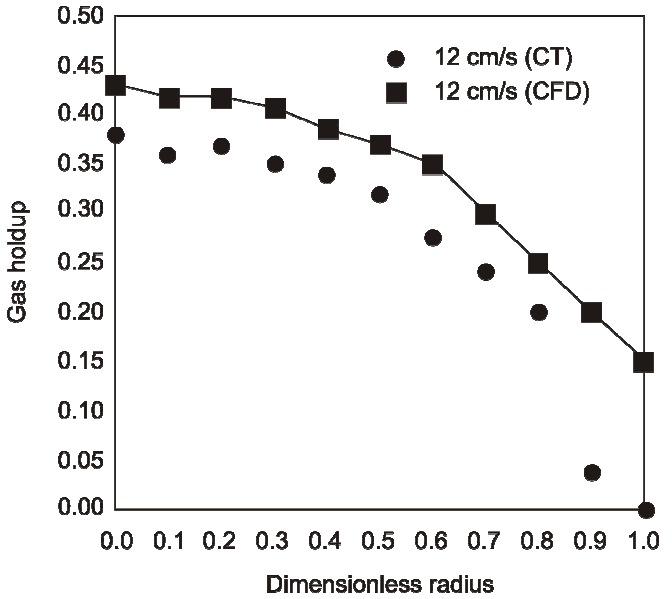

Fig. 9: Comparison between experimental data (CARPT data) and CFD simulation

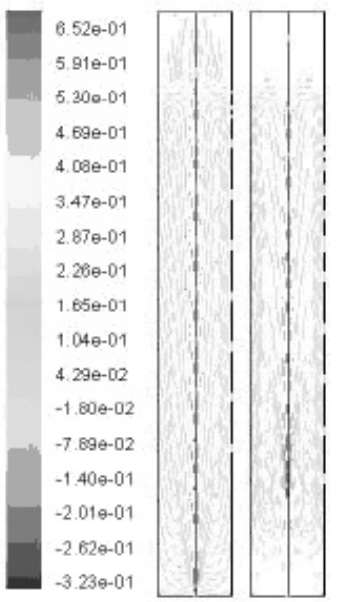

Fig. 10: Path line of gas axial velocity (Slip flow assumption)

Figs. 3, 4, 5 and 6 in 3D model and Fig. 10 in 2D column shows the evolution of local axial velocity and gas holdup with radial distance, which in these cases, it can seen that the results are reasonable and have good quality trend.

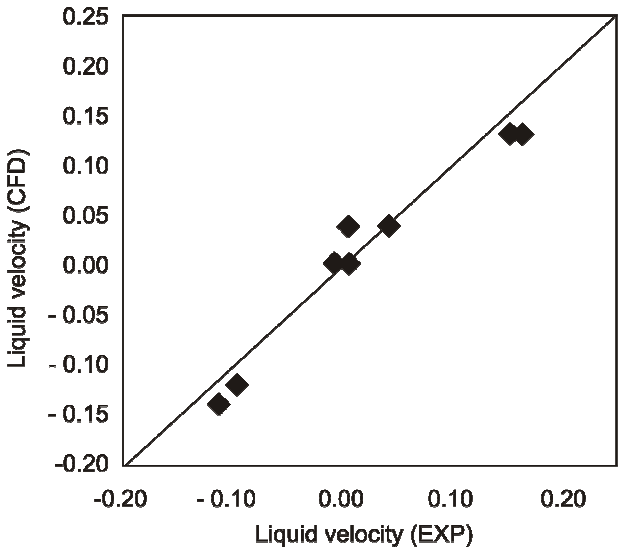

Fig. 11: Error comparison between experimental liquid velocity (D. Pfleger) and calculated liquid velocity (Full 3D)

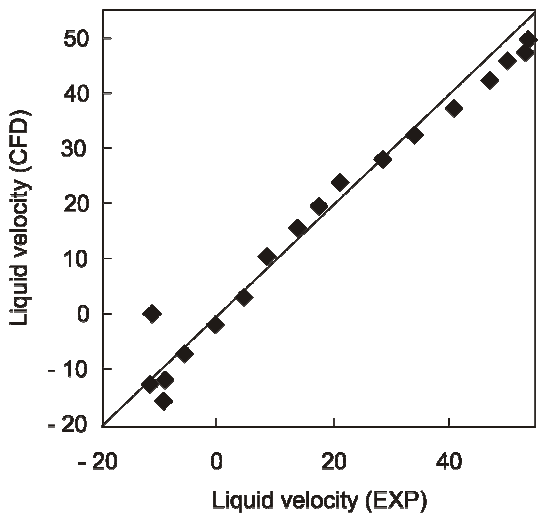

Fig. 12: Error comparison between experimental liquid velocity (CREL) and calculated liquid velocity (2D, axis)

Figs. 11 and 12 show the error comparison between experimental and calculated liquid velocity for both the models, which have good correlations and less than 10% error. Thus the CFD simulation enables the estimation of local axial velocity and pressure drop with these models. It can be seen with difference models. Computational fluid dynamics can apply easily to estimate and predicate of the other important parameters.

CONCLUSIONS

In summary, the usefulness of two-dimensional axisymetric models has to be acknowledged. They provide good engineering descriptions, and can be used reliably for approximately predicting the time-averaged flow and velocity patterns in bubble columns. We have validated the models in different flow regimes, as well as with different fundamental modeling approaches to describe the flow pattern (i.e. comparison of wall effects and slip flow). We have also shown that a reasonable choice of turbulence description is able to predict the holdup profiles, and must do so in a self-consistent model. Further improvements in the turbulence model, or in description of two point correlations, is likely to improve the description of the other turbulence parameters such as shear stress and turbulent diffusivities. Also we make a fully transient three dimensional model, which is necessary to capture the transient flow structure in the bubble column that is in general, not asymmetric and have a significant azimuthal component. It would be interesting to examine the relative importance of these phenomena in determining the overall flow pattern, and more importantly, the overall reactor performance. A satisfactory answer to this issue can only be determined through a detailed comparison of flow, turbulence and reactor performance variables between experiment and simulation. For $k - \varepsilon$ model, the effect of mesh size needs to be investigated further. Finer mesh size will bring out further details in the flow structure. In addition, flow near the wall needs simulation for understanding the transport phenomena, which is of great interest. The progress in CFD will continue with the development in computers and now, there is a need to simulate the relation between flow patterns and design. Presently, work is in progress in this area and we hope to present some of our results in this field in a subsequent communication.

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