CFD Simulation of Bubbly Flow Through a Bubble Column

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Abstract- In this investigation, CFD simulation is presented to study the hydrodynamic of bubbly flow and mass transfer in bubble column using Eulerian- Eulerian Multifluid approach with a standard k- ε turbulence model. unsteady state method for modeling the multiphase flow and mass transfer from air to de-aerated water and the column hydrodynamics. Understanding the complexity of the fluid dynamics and mass transfer in bubble column and is important due to its application in the chemical and bioprocess industries. Numerical simulation was carried out using COMSOL multiphysics software. The results were presented for various hydrodynamics parameters such as phase dynamics, phase velocity profile contours of fluid velocity in chosen cross-section planes of the column and concentration of gas in liquid phase .

Index Terms—CFD, bubble column, multiphase flow, aeration, agitation, bubbly flow, gas dispersion

1.INTRODUCTION

In multiphase contactors, the dispersed phase is either bubbles, drops, particles, or combinations thereof. The continuous phase is either liquid or gas. The governing features of the dispersed phase are its size and velocity distributions, both of which have a major impact on the performance of these equipments. The other governing parameters include column diameter, column height, sparger design, and internal design. Bubble column reactors belong to the general class of multiphase reactors which consist of three main categories namely, the trickle bed reactor (fixed or packed bed), fluidized bed reactor, and the bubble column reactor. A bubble column reactor is basically a cylindrical vessel with a gas distributor at the bottom. The gas is sparged in the form of bubbles into either a liquid phase or a liquid-solid suspension. These reactors are generally referred to as slurry bubble column reactors when a solid phase exists(Vinay Mahajan 2010). Bubble columns are used especially in chemical processes involving reactions such as oxidation, chlorination, alkylation, polymerization and hydrogenation, in the manufacture of synthetic fuels by gas conversion processes and in biochemical processes such as fermentation and biological wastewater treatment (Kantarci et al., 2005). Gas-liquid flow in bubble column reactors is characterized by a combination of inherently unsteady complex processes with widely varying spatial and temporal scales.
Understanding the complexity of the fluid dynamics in bubble column and airlift reactors is important due to their application in the chemical and bioprocess industries The two most common approaches to modeling bubble columns are the Euler-Euler or two-fluid approach and the Euler-Lagrange or discrete bubble approach. In the Euler-Euler approach, both phases (the continuous liquid phase and the dispersed gas phase) are modeled as two inter-penetrating continua. In the Euler-Lagrange approach on the other hand, the volume averaged Navier-Stokes equations are used to describe the motion of the liquid phase and each bubble is tracked on basis of a balance of forces acting upon (Mousavi et al., 2007). In the present work an attempt has been made to understand the hydrodynamic behavior multiphase flow and mass transfer mass transfer of a concurrent gas(air)-liquid(water) up-flow bubble column by CFD analysis.
CFD simulation of bubble column reactor:
Bubble columns are gas-liquid reactors where liquid forms a continuous phase and gas flows in the form of dispersed bubbles, the bubbles are injected from the center of the inlet surface in the simulation domain . The bubble trajectory is tracked from the inlet to the outlet of the domain.
The motion of the bubbles are tracked using the discrete phase model which in embedded in Comsol multiphysics. CFD simulation of bubble columns is a very demanding task, there are several reasons for this. First of all, the hydrodynamics of bubble columns is very complex. The rising bubbles carry liquid with them upwards in the direction of liquid flow. The liquid upflow then returns downwards at the column wall. This upflow at the centre and downflow at the wall periodically breaks down to form large turbulent vortices. The flow in the column is chaotic and turbulent at high gas flow rates.

2.COMPUTATIONAL MODEL

The eulerian-eulerian approach has been used to simulate the multiphase flow of the bubble column hydrodynamics. The standard k-e mixture turbulence model has been used to account the effect of turbulence. COMSOL multiphysics [10] has been used to simulate the system for various

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hydrodynamics parameters, tidal in the Eulerian multiphase flow model, the phases are treated as interpenetrating continua coexisting in the flow domain. Equations for conservation of mass and momentum are solved for each phase. The share of the flow domain occupied by each phase is given by its volume fraction and each phase has its own velocity, and physical properties. Interactions between phases due to differences in velocity are taken into account via the inter-phase transfer terms in the transport equations.

In an Eulerian multiphase model, the motion of each phase is governed by respective mass and momentum conservation equations.

Continuity equation:

$$\frac{\partial}{\partial t}(\epsilon_k \rho_k) + \nabla(\epsilon_k \rho_k u_k) = 0 \quad (1)$$

where ρk is the density, εk is the volume fraction and uk is the velocity of phase k = L, g, the sum of the volume fractions is equal to unity,

$$\sum_k \epsilon_k = 1 \quad (2)$$

Momentum equation

The conservation of momentum for phase k, liquid or gas are given by Eq. (3)

$$\frac{\partial}{\partial t}(\rho_k \epsilon_k u_k) + \nabla.(\rho_k \epsilon_k u_k u_k) = -\epsilon_k \nabla p + \nabla.\tau_k + \rho_k \epsilon_k g + F_{i,k} \quad (3)$$

where P is the pressure shared by two phases. The term F i,K represent the interface momentum exchange. The term τK is the stress-strain tensors.

2.1 Interphase transport models

There are various interaction forces such as the drag force, the lift force and the added mass force etc. during the momentum exchange between the different phases. But the main interaction force is due to the drag force caused by the slip between the different phases (Panneerselvam et al. 2010). The liquid phase is treated as a continuous phase and the gas phase is treated as a dispersed phase. The interphase forces considered for this simulation is the drag force between liquid and gas and the turbulent dispersion force. The drag force between the gas and liquid phases is represented by Khopkar (Khopkar et al., 2005).

$$F_{D,lg} = C_{D,lg} \frac{3}{4} \rho_l \frac{\epsilon_g}{d_b} |u_g - u_l| (u_g - u_l) \quad (4)$$

where the drag coefficient exerted by the dispersed gas phase on the liquid phase is obtained by the modified Brucato drag model (Khopkar et al., 2003), which accounts for interphase drag by microscale turbulence and is given by

$$\frac{C_{D,lg} - C_D}{C_D} = 6.5 \times 10^{-6} \left(\frac{d_b}{\lambda}\right)^3 \quad (5)$$

where CD is the drag coefficient of single bubble in a stagnant liquid and it's calculated by Schiller-Nauman correlation (Ranade 2002)

$$C_D = \frac{24}{Re_b}(1 + 0.15 Re_b^{0.687}) \quad Re_b \le 1000 \quad (6)$$

$$C_D = 0.44 \quad Re_b > 1000$$

where Reb is the bubble Reynolds number and they are defined by

$$Re_b = \frac{(u_l - u_g) d_b}{\nu_l}$$

2.2Turbulence Modeling

The k-ε turbulence model can use for turbulent flows, and solve for the averaged velocity field. The turbulence model relevant for bubbly flows is similar to the single-phase k-ε turbulence model. However, there are additional source terms in order to account for the extra production of turbulence due to the relative motion between the gas bubbles and the liquid. When we use the k-ε turbulence model, a turbulent viscosity is adds to the physical viscosity in the momentum transport equation. The turbulent viscosity is modeled by

$$\eta_T = \rho_l C_\mu \frac{\kappa^2}{\varepsilon}$$

where Cμ is a model constant.

The transport equation for the turbulent kinetic energy k is given

$$\rho_l \frac{\partial k}{\partial t} - \nabla \cdot \left[\left(\eta + \frac{\eta_T}{\sigma_k}\right)\nabla k\right] + \rho_l \mathbf{u}_l \cdot \nabla k = \frac{1}{2}\eta_T (\nabla \mathbf{u}_l + (\nabla \mathbf{u}_l)^T)^2 - \rho_l \varepsilon + S_k \quad (8)$$

and the evolution of the turbulent energy's dissipation rate ε is governed by

$$\rho_l \frac{\partial \varepsilon}{\partial t} - \nabla \cdot \left[\left(\eta + \frac{\eta_T}{\sigma_\varepsilon}\right)\nabla \varepsilon\right] + \rho_l \mathbf{u}_l \cdot \nabla \varepsilon = \frac{1}{2} C_{\varepsilon 1} \frac{\varepsilon}{k} \eta_T (\nabla \mathbf{u}_l + (\nabla \mathbf{u}_l)^T)^2 - \rho_l C_{\varepsilon 2} \frac{\varepsilon^2}{k} + \frac{\varepsilon}{k} C_\varepsilon S_k \quad (9)$$

The term Sk accounts for the bubble induced turbulence and is given by

$$S_k = -C_k \epsilon_g \nabla p . u_{slip}$$

For the gas phase's velocity field, a drift velocity is added:

$$\mathbf{u}_g = \mathbf{u}_l + \mathbf{u}_{slip} + \mathbf{u}_{drift}$$

Where

$$u_{drift} = -\frac{\eta_T \nabla \epsilon_g}{\rho_l \epsilon_g}$$

Dissolution of gas

dissolution of gas can be calculated using two-film theory, then calculates the mass transfer rate according to

$$m_{gl} = k\left(\frac{p+p_{ref}}{H} - c\right) M_a \quad (10)$$

$$a = (4n\pi)^{1/3}(3\epsilon_g)^{2/3}$$

Where a is interfacial are ,which depends on the volume fraction of gas and the number of bubbles per volume, n (1/m3). In two-film theory model, the application mode automatically also solves for n. It assumes that bubbles cannot split or merge, while the size of each bubble can vary:

$$\frac{\partial n}{\partial t} + \nabla(n\, u_g) = 0 \quad (11)$$

Convection and Diffusion mode

The transport equation for dissolved gas is

$$\frac{\partial c}{\partial t} + \nabla c\, u_l = \nabla.(D\nabla c) + \frac{m_{gl}}{M} \quad (12)$$

where D is the diffusion coefficient (m2/s). When you use a turbulence model for the flow field, the diffusion coefficient is

$$D = \frac{\eta_T}{\rho_l}$$

Solving the concentration of the dissolved gas due to mass transfer convection and diffusion mode Eq. (12).

3. Numerical Methodology

The finite volume method [Patankar et al.1980] was used to discretize the governing equations. The convection and diffusion terms in all equations were discretized by central differencing scheme and this differencing scheme was also used for discretization of the convection and diffusion terms in the simulation method. The geometry of the simulation model is shown in Figure (1) schematically. The geometry consists of 2D tube with 0.2m width and 0.75 m height. A uniform grid was used to simulate the mass transfer process. An unsteady simulation was performed with the time step size of 2 sec. The simulations were done until steady state was achieved, So that the average of transport component mass fraction did not change with time. 2D segregated 2nd order implicit unsteady solver is used. Standard κ-ε mixture multiphase model is used to model turbulence with standard wall functions. The constants of simulate model are listed in Table 1.

Table 1 constants of simulated model.

Cμ	0.09
C1ε	1.44
C2ε	1.92
TKE Prandtl Number (σκ)	1
TDR Prandtl Number (σε)	1.3
Dispersion Prandtl Number	0.75
Energy Prandtl Number	0.85
Wall Prandtl Number	0.85
Turb Schmidt Number	0.7

3.1 Boundary conditions

The application of appropriate boundary conditions is one of the most important factors in a successful CFD analysis, and one of the more challenging since there are many different approaches. The difficulty faced in this problem was that the flow in the raceway is driven by various factors involving the air bubbles in the riser tube.

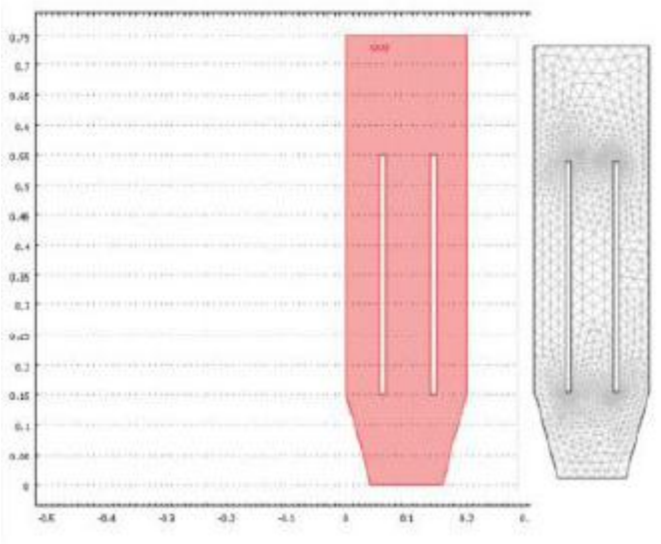

Figure 1: Geometry of bubble column and meshing.

The displacement of water at depth caused by the introduction of air into the system induces hydraulic head developed by gas hold-up in the tube, which contributes to gravity driven flow along the raceway. Also, the buoyancy of the bubbles causes them to rapidly rise to the surface of the tube, and this momentum is transferred to the water by friction and wake effects in the bubbles. While these interactions are complex, they can be resolved and accounted for in the CFD solver with the appropriate boundary conditions and initial setup, including a reasonable estimate of the final flow velocity.

In two-phase flow simulation, the reactor is initially full with liquid. Gas is feeder from the bottom region of the reactor. The bottom region contains gas inlet holes with velocity inlet boundary condition. A pressure boundary condition is applied to the top of the reactor with an average static reference pressure of 0 Pa. The rest of the boundaries for reactors walls (i.e., front, back and others) and riser walls are standard no-slip boundary condition where velocity increases from zero at the wall surface to the free stream velocity away from the surface for both phases.

4. Results and Discussion

A gas-liquid bubble column of diameter 0.2 m and height 0.75 m has been simulated using Comsol multiphysics, The simulated results have been presented graphically. While simulating the column profile changes with time. But after some time no significant change in the profile is observed. This indicates that the column has come to a quasi steady state.

4.1 Gas and liquid holdup

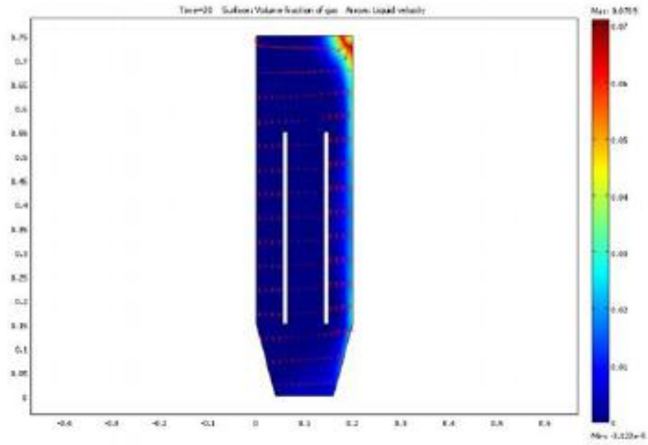

Fig. 2 Contour of volume fraction of gas and arrows is liquid velocity pattern.

The gas holdup values are obtained from CFD simulation at sufficient points in the bubble column. Fig. 2 represents the variation of gas holdup in the two phase with constant gas velocity 0.001 m/s. It is seen from the figure the values of gas mole fraction rounds between 0 to 0.07 along the height of the column, with increasing liquid velocity, the gas holdup decreases, due to the fact that at higher liquid velocity and vise versa. The bubbles are fast driven by the liquid. The residence time of the bubbles decreases with the liquid velocity and hence the gas holdup is likely to decrease.

4.2 Gas volume fraction

Contours of volume fraction of gas for air velocity of 0.001 m/s until quasi-steady state is reached is shown in Fig. 2. The volume fraction of gas in the column is similar throughout the column for 20 sec which indicates the column has achieved the quasi-steady state. Gas volume fraction or gas holdup is obtained as mean area-weighted average of volume fraction of air at sufficient number of points in the bubble column..

4.3 Mass transfer rate

Gas holdup plays a very important role in gas-liquid mass transfer. The rate of mass transfer depends on the gas holdup of the column. It is found that higher the gas holdup higher is the mass transfer rate of gas. This indicates that the gas holdup decreases with increase in liquid velocity. Fig. 3 shows the variation of gas holdup with water velocity for a constant air velocity 0.001 m/s. Figure indicates that the gas holdup decreases with increase in liquid velocity due to dissolving of gas into liquid . Because the liquid circulates in the tank, the dissolved species is rapidly distributed within the entire tank.

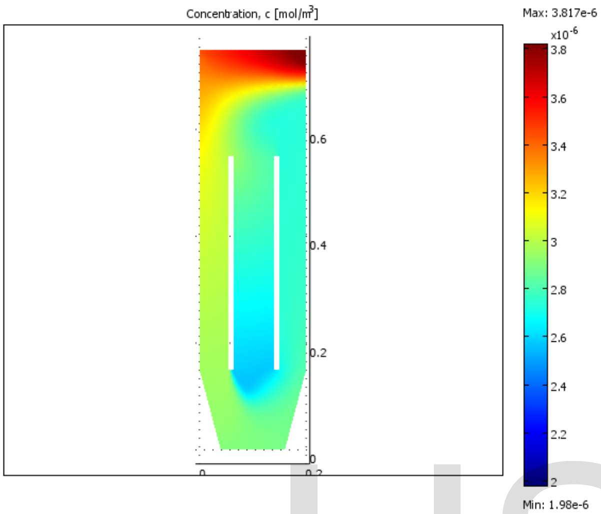

Fig. 3. Contours of concentration of gas for air velocity of 0.001 m/s.

4.1 Liquid and gas velocities

In gas-liquid bubble column, the velocities of gas and liquid vary with time and location in the column. Vectors of velocity magnitude of water and air in the column obtained at inlet air velocity of 0.001m/s after the quasi steady state is achieved are shown in Figs. 4. These vectors show velocity magnitude with direction and thus are helpful in determining flow patterns in bubble column.

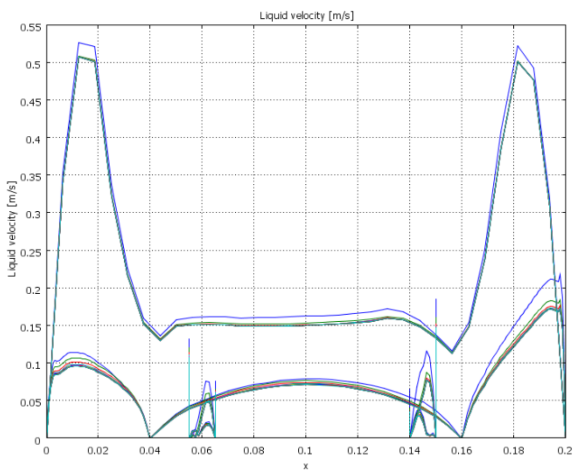

Fig. 4 Velocity distribution inside bubble column along radial distance.

The radial velocity profiles, from 2D simulations, of liquid phase at selected location in the whole reactor is shown in Figure 4. Liquid velocity increases from zero at the wall surface to the free stream velocity away from the surface due to no-slip BC for low liquid velocities, can be considered to be virtually in plug flow. With increasing superficial liquid velocities, liquid phase loses their plug flow character and the velocity profile assume a parabolic shape. The parabolic velocity profile becomes more prominent with increasing superficial liquid velocities , radial velocity profiles for both phases are almost axi-symmetric. The lower part of the graph represent the distribution in the bottom of the column (entire cross-section) and the upper part the top of the column. Contour the turbulent viscosity and circulation motion of liquid phase as shown in Fig.5

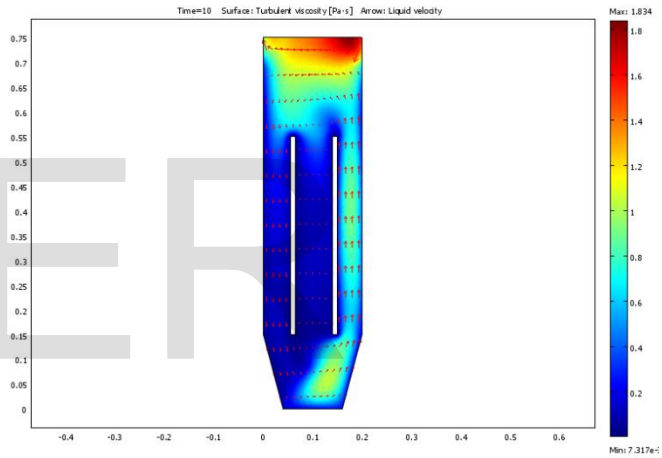

Fig. 5 Contour of turbulent viscosity and arrows of liquid velocity pattern

main factor to variation of the liquid velocity profile in the column. The intensity of the circulation along the column axis varies due to the variation of energy distribution. The energy distribution of course is a function of the phase physical properties. Along the core region of the column, the velocity is higher than the other radial position due to the dilution of interfacial stress between wall of the column and the liquid

Due to this variation of the liquid velocity, the fluid gets circulates at different intensity along the column. Also due to the variation of the circulation velocity the momentum exchange results in distribution in kinetic energy for which the flow pattern and the gas holdup will change radically.

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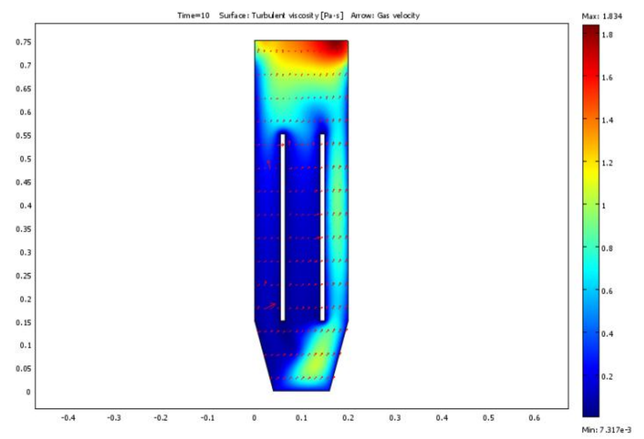

Fig. 6 Contour of turbulent viscosity and arrows of gas velocity pattern.

The radial distribution of gas holdup, εg, in bubble column, obtained from 2D simulations are shown in Figure 6. It exhibits that the gas holdup shows a pronounced increase in the gas holdup inside whole reactor with increasing Ug values, in this case the liquid recirculation tend to move gas towards the right side of the column. Also, there is an increment in gas holdup near the riser wall. The reason for this is that the larger sized liquid circulation at the riser bottom tends to move the gas towards the wall.

5. Conclusion

CFD simulation of hydrodynamics of gas-liquid bubble column(0.1 m ID and 0.75 m height) has been simulated using Comsol multiphysics by employing the Eulerian-Eulerian multiphase approach. The hydrodynamic parameters studied are gas hold up, and operating variables varied are gas and liquid velocity. The standard k−ε model has been used to model turbulence and segregated solver has been used. The gas holdup has been found to increase with increase in gas velocity but decreases with increase in liquid velocity. A similar trend has been observed for the liquid phase with the corresponding phase velocities. The gas holdup has been found to vary from 0.0 to 0.07 for constant gas velocity 0.001 m/s. It has been observed that the local gas velocity depends on the physical flow time. Also the volume fraction of gas is decreases due to dissolved species of gas into circulation liquid.

6. Nomenclature

a interfacial area per volume (m2/m3)
C_D : drag coefficient
C_{D0} : drag coefficient in stagnant water
C_ω : constant
c the concentration of gas dissolved in liquid (mol/m3)
D : column diameter, m
d_b : bubble diameter, m
Fq : interphase momentum exchange term
F_D : interphase drag force, N/m3
g : acceleration due to gravity, m/s2
G : turbulence generation rate
H Henrys constant (Pa·m3/mol)
K : constant
k mass transfer coefficient (m/s)
Qg : volumetric gas flow rate, m3/s
t : time, s
U : axial velocity, m/s
V : radial velocity, m/s

Subscripts
k phase
l liquid phase
g gas phase
eff effective
Greek letters
α phase volume fraction
ϵ holdup
ρl Density of water (kg/m3)
ρg Density of gas (kg/m3)
κ Turbulent kinetic energy (m2/s3)
ε Turbulent dissipation rate (m2/s3)
λ Kolmogorov length scale (m)
μ Viscosity (kg/m. s)
μ_{tm} Turbulent viscosity of mixture (kg/m. s)
μ_{tq} Viscosity of turbulence (kg/m. s)
σ surface tension (N/m)
T Shear stress (N/m)

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References

1.COMSOL multiphysics chemical engineering software V3.5.
2.Han, L., Al-Dahhan, M. H., 2007. Gas-liquid mass transfer in a high pressure bubble column reactor with different sparger designs. Chemical Engineering Science. 62, 131-139
3.Gimbun, J., Rielly, C. D., Nagy, Z. K., 2009. Modelling of Mass Transfer in Gas-Liquid Stirred Tanks Agitated by Rushton Turbine and CD-6 Impeller. 13th European Conference on Mixing. London
4.Kantarci, N., Borak, F., Ulgen, K. O., 2005. Bubble column reactors (Review). Process Biochemistry. 40, 2263-2283.

5.Khophkar, A. R, Rammohan, A. R., Ranade, V. V., Dudukovic, M.P., Gas-Liquid Flow Generated by a Rushton Turbine in Stirred Tank Vessel: CAPRT/CT Measurements and CFD Simulations, Chemical Engineering Science, 60, 2215 (2005).

6.Khopkar, A. R., Kasat, G. R., Pandit, A. B. and Ranade, V. V., Computational fluid dynamics simulation of the solid suspension in stirred slurry reactor. Ind. Chem. Res. Des., 2006, 45, 4416.
7.Khopkar, A.R., Aubin, J., Xureb, C., Le Sauze, N., Bertrand, J. and
8.Han, L., Al-Dahhan, M. H., 2007. Gas-liquid mass transfer in a high pressure bubble column reactor with different sparger designs. Chemical Engineering Science. 62, 131-139.

9.Mousavi, S.M., Jafari, A., Yaghmaei, A., Vossoughi, A., Turunen, I., 2007. Proceedings of the World Congress on Engineering and Computer Science (WCECS 2007), San Francisco, USA.
10.Panneerselvam Ranganathan and Sivaraman Savithri Computational Flow Modeling of Multiphase Mechanically Agitated Reactors pp. 420, January 2010, India
11.Patankar S.V., Numerical Heat Transfer and Fluid Flow, Taylor and Francis, Philadelphia, 1980.
12.Ranade, V. V, Computational Flow Modeling for Chemical Reactor Engineering, Academic Press, New York (2002).
13.Ranade, V.V., 2003. Gas– liquid flow generated by a pitched blade turbine: PIV measurements and CFD simulations. Industrial and Engineering Chemistry Research, 42, 5318–5332.
14.Vinay Mahajan "CFD Analysis of Hydrodynamics and Mass Transfer of a Gas-Liquid Bubble Column" Indea 2010