CFD ANALYSIS OF A TRICKLE BED WITH AIR-CMC SYSTEM

A THESIS SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE DEGREE OF

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Submitted by

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Under the guidance

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CERTIFICATE

This is to certify that the thesis entitled, "**CFD ANALYSIS OF A TRICKLE BED WITH AIR-CMC SYSTEM**", submitted by Subhashree Sahoo, Roll no. 110CH0086, in partial fulfilment of the requirements for the award of degree of Bachelor of Technology in Chemical Engineering at National Institute of Technology, Rourkela is an authentic work carried out by her under my supervision and guidance.

To the best of my knowledge, the matter embodied in the report has not been submitted to any other University / Institute for the award of any Degree or Diploma.

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ABSTRACT

Trickle Bed Reactors have wide scale application in chemical process industries mainly in petrochemical and refinery process because of their flexibility and simplicity of operation. Pressure drop and liquid holdup are the basic parameters for design, scale up and operation of trickle bed reactors. However multiphase flow in trickle bed reactor is known to be extremely complex and depends on various effects including the physico-chemical properties of gas, liquid and solid phases, ratio of column diameter to particle diameter and most importantly gas and liquid superficial velocities. Since most of the fluids encountered in industrial processes are non Newtonian, simulations have been carried out for air- Carboxy Methyl Cellulose system. In the present work an attempt has been made to study the hydrodynamics of a co-current gas-liquid-solid trickle bed reactor. CFD simulations have been done using Eulerian-Eulerian approach for a trickle bed system. The contours of volume fraction for the different phases are shown. Also the effect of liquid and gas velocity on the phase hold up and pressure drop are represented in graphical form and studied. The results obtained from simulations have been compared with the experimental data available in literature and there is a close agreement between the two.

Keywords: Trickle bed reactor, Computational Fluid Dynamics, Hydrodynamics

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NOMENCLATURE

g= Acceleration due to gravity, m/s^2

ρ_q = Density of phase, kg/m^3

ε= Dissipation rate of turbulent kinetic energy, m^{2}s^{-3}

μ_{eff} = Effective viscosity, kg/m-s

α_q = Volume fraction of phase (dimensionless)

v_q = velocity of phase q, m/s

m_{pq} = mass transfer rate from pth to qth phase, kg/s

m_{qp} = mass transfer rate from qth to pth phase, kg/s

S_q = Source term, J/K

τ_q = stress-strain tensor for qth phase, Pa

p = Pressure, Pa

t= Time, s

F_q = External body force, N

$F_{lift,q}$ = Lift force, N

$F_{vm,q}$ = Virtual mass force, N

R_{pq} = Interaction force between phases, N

h_q = Specific enthalpy of qth phase, J/kg

q_q = Heat flux, W/m^2

Q_{pq} = Intensity of heat exchange between pth and qth phase, W

h_{pq} = Interphase enthalpy, J/kg

k= Turbulent kinetic energy, J

U= Velocity of phase, m/s

D = Diameter of the column, m

D_p = Diameter of particle, mm

ϵ = void fraction (dimensionless)

C_2 = Inertial Resistance term, m^{-1}

CMC = Carboxy Methyl Cellulose

TBR = Trickle Bed Reactor

CHAPTER 1

INTRODUCTION AND LITERATURE REVIEW

1.1 TRICKLE BED REACTORS

In trickle bed reactors, the gas and liquid flow co-currently downward over a fixed bed of catalyst. Upward flow of gas and liquid trickling downward over the catalyst particles is in principle possible, but this can occur only with very coarse packing or at very low velocities. Hence nearly all commercial TBRs operate with downward flow of liquid and gas so that in practice trickle flow is similar to co-current gas-liquid downflow over a fixed or moving bed of catalyst. Trickle bed reactors are used in petroleum, petrochemical and chemical industries, in waste water treatment and biochemical and electrochemical processing. The schematic diagram of a trickle bed reactor is shown below:

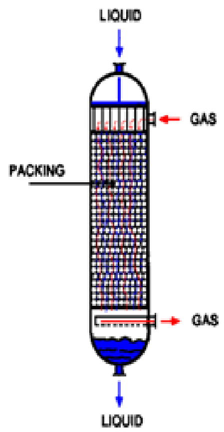

Figure 1.1: Schematic diagram of a trickle bed (Aydin, 2008)

The design and scale up of TBR depend on key hydrodynamic variables such as liquid volume fraction, particle scale wetting and overall gas-liquid contact. Important aspects for design of TBR are:

a) Pressure drop
b) Liquid and Gas holdups
c) Axial and radial distribution of liquid and gas
d) Catalyst contacting
e) Thermal stability
f) Heat transfer
g) Mass transfer

Performance of TBR depends on various factors such as:

a) **Porosity**: liquid and gas holdup, pressure drop, mal-distribution factor and wetting deficiency decreases with increase in porosity, however gas-liquid mass transfer rate, liquid solid mass transfer rate and axial dispersion of fluid increases with increase in porosity.

b) **Surface tension**: pressure drop increases with increase in surface tension of liquid but gas-liquid mass transfer and wetting efficiency decreases.

c) **Liquid superficial velocity**: liquid holdup, pressure drop, mass-transfer, wetting efficiency and axial dispersion increases with liquid superficial velocity but mal-distribution of liquid decreases.

d) **Gas superficial velocity**: liquid holdup and mal-distribution decreases with increase in gas superficial velocity but pressure drop, mass transfer and wetting efficiency increases.

e) **Particle size**: liquid and gas holdup, pressure drop, mass transfer rate and wetting efficiency decreases with increase in particle size but axial dispersion and mal-distribution factor increases.

f) **Liquid density**: pressure drop increases with increase in liquid density and performance in mass transfer and wetting efficiency becomes poor.

g) **Liquid viscosity**: holdup, pressure drop, gas-liquid mass transfer and wetting efficiency increases with increase in liquid viscosity but axial dispersion of liquid decreases.

h) **Gas viscosity**: holdup, pressure drop, liquid-gas mass transfer rate increases with increase in gas viscosity.

i) **Pressure** (gas density): liquid holdup, liquid-solid mass transfer rate and liquid mass transfer rate decreases with increase in pressure but pressure drop, gas-solid mass transfer rate and wetting efficiency increases.

1.2 ADVANTAGES OF TRICKLE BED REACTORS

The advantages of trickle bed reactors include (Saroha et al., 1996):

a) The absence of moving parts in trickle bed reactors results in lower maintenance cost.

b) Plug flow operation and effective catalyst wetting result in higher reaction conversions.

c) Liquid holdup is less i.e, ratio of liquid to solid is less, which reduces the possibility of homogeneous side reactions.

d) Trickle bed reactors have large capacities.

e) The liquid flows over the fixed bed of catalyst particles in the form of thin film due to which higher gas-liquid interfacial area is obtained. Trickle bed reactors can be operated at higher pressure and temperature.
f) In concurrent down flow operation of gas and liquid, uniform partial pressure of the gas phase can be achieved due to low pressure drop in the reactor. The gas is in contact with the solid particles throughout the reactor.
g) The trickle bed reactor can be operated as a partially or completely vapour phase reactor, by varying the liquid flow rate according to catalyst wetting efficiency and heat and mass transfer resistances. This reduces the operating cost as heat required for reactant vaporisation is substantially reduced.
h) The problem of flooding is not encountered in concurrent downflow operation.
i) The catalyst loss is low; costly catalyst like Pt. can be used.

1.3 DISADVANTAGES OF TRICKLE BED REACTORS

The disadvantages of trickle bed reactors include (Saroha et al., 1996):

a) The catalyst effectiveness is reduced due to large catalyst size particles.
b) Incomplete catalyst welting at low liquid flow rates and due to liquid maldistribution considerably reduces the reactor yield.
c) Continuous removal of heat is difficult. This can cause damage to the catalyst in highly exothermic reactions.
d) Trickle bed reactors are less effective with viscous and foaming systems.

1.4 APPLICATIONS OF TRICKLE BED REACTORS

The major processes carried out in a trickle bed reactor include hydrotreating, hydrodenitrogenation, hydrocracking, hydrodewaxing, hydrodesulfurisation, hydrofinishing and hydrometallisation. Trickle Bed Reactors also find application in chemical and biochemical industries. In effluent treatment plants, trickling filters are used for removal of organic matter from waste water streams by aerobic bacterial actions. In this process, biological growths are allowed to attach themselves to a bed of stone or other support over which the waste water is allowed to trickle in contact with air. The typical processes using TBRs are (Sai et al., 1998):

a) Hydro-de-nitrogenation of gas-oil and vacuum gas-oil.
b) Hydro-desulfurization of gas-oil, vacuum gas-oil and residues.

c) FCC feed hydro-treating.
d) Hydrocracking of catalytically cracked gas-oil and vacuum gas-oil.
e) Hydro-cracking of residual oil.
f) Hydro-metallization of residual oil.
g) Hydro-processing of shale oils
h) Hydro-cracking/Hydro-fining of lubeoils
i) Oxidative Treatment of Waste water.
j) Paraffin Synthesis by Fischer-Tropsch.
k) Synthesis of diols.

1.5 HYDRODYNAMICS OF TRICKLE BED REACTORS

Hydrodynamics of TBR is quantified in terms of hydrodynamic parameters like pressure drop, liquid or gas hold up, liquid maldistribution, which are related to gas-liquid-solid contacting efficiency and operational efficiency of reactor column. Pressure drop and liquid hold up depends both on operation condition and flow history of the bed. Flow distributions are closely related to studies of hysteresis in TBR, which is attributed to change in flow distribution and related flow patterns with flow history.

1.5.1 Flow Regimes:

In a TBR, various flow regimes are distinguished depending on gas/ liquid flow rates (most influential), fluid properties and packing characteristics. These flow regimes are (Saroha et al., 1996):

a) Trickle Flow (gas continuous): it occurs at low liquid and gas flow rates. Liquid flows down the reactor on the surface of the packing in the form of rivulets and films while the gas travels in the remaining void space. There is very little interaction between gas and liquid in this regime.
b) Pulse Flow (unstable regime with partly gas continuous and partly liquid continuous): it occurs at relatively high gas and liquid input flow rates. It refers to pulsing behaviour of gas and liquid slugs traversing the reactor alternately. It is also called rippling or slugging.
c) Dispersed Bubble Flow: this occurs at high liquid flow rate and low gas flow rates. Entire bed is filled with the liquid and the gas phase is in the form of slightly elongated bubbles.

d) Spray Flow (gas continuous, highly dispersed liquid): this occurs at high gas flow rates and low liquid flow rates. Liquid phase moves down the reactor in the form of droplets entrained by the continuous gas phase.

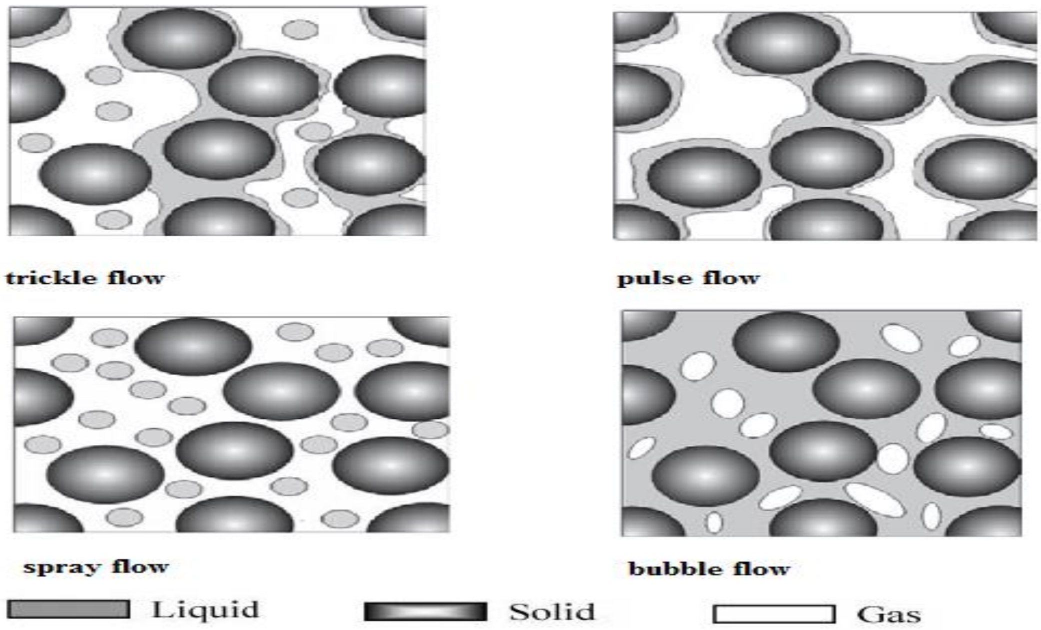

Figure 1.2: Various flow regimes in a trickle bed (Boelhouwer, 2001)

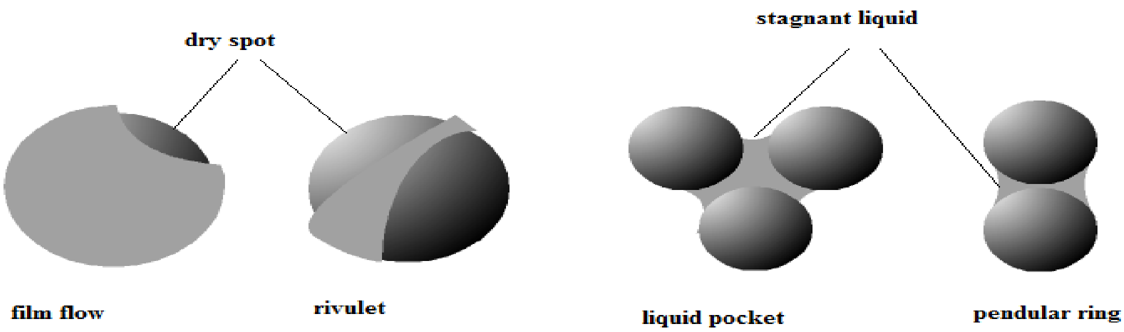

Figure 1.3: Schematic illustration of the several liquid flow textures during trickle flow operation (Boelhouwer, 2001)

1.5.2 Pressure Drop

Pressure drop in trickle beds is one of the most important design parameters as it governs the energy required to move the fluids through the bed. It is often used as a correlating parameter for prediction of other design parameters such as gas-liquid, liquid-solid mass transfer coefficient, wetting efficiency and heat transfer coefficient. The energy is required against the gas-liquid flow resistance in porous media. The resistance to flow in trickle regime is mainly because of shear and capillary forces. Two phase pressure drop along the length of the bed is a function of reactor hardware such as column diameter, particle size and shape and internals, operating parameters such as gas-liquid flow rates and fluid properties like density and viscosity of flowing fluid surface tension and surface characteristics. Operating pressure and temperature indirectly affect the pressure drop through fluid properties.

According to the literature data available in the thesis of Aydin (2008): Ellman et al. (1988) proposed two pressure drop correlations for the low interaction (trickle flow) and high interaction (pulse, dispersed bubble and spray flow) regimes.

Wammes et al. (1991) also proposed a theoretical correlation to estimate the two-phase pressure drop by making the following assumptions: the trickle bed reactor operates under stationary and isothermal conditions, the gas density is constant, the gas-liquid surface tension does not play a role. However the validity of the correlation of Wammes et al. (1991) was more limited than that of Larachi et al. (1991), as it was based on a narrower range of operating conditions. Moreover, it needed prior evaluation of the liquid holdup.

Al-Dahhan et al. (1994) extended the model of Holub et al. (1992) to describe the effect of high pressure on pressure drop and liquid holdup in trickle flow regime. The effect of gas density at constant superficial gas velocity on two-phase pressure drop was studied by Al-Dahhan et al. (1994) using hexane-nitrogen- helium systems. Helium pressure about seven times higher than that of nitrogen yields helium density equal to nitrogen density. It was observed that for a given value of gas density and liquid mass velocity both systems have approximately the same pressure drop. This showed that the effect of high pressure operation is due to the increase in gas density.

Simulation of the trickle bed reactor at high pressure with different spherical particle shows that decreasing the diameter of particle, liquid holdup and pressure drop of the bed increases (Lopes et al., 2008). The increase in pressure drop is more pronounced in two-phase flow because of enlargement of liquid holdup which decreases the available void space for the gas in the trickle bed reactor. Al-Naimi et al. (2011) studied the hydrodynamics of trickle bed reactor in non-ambient condition with air–water and air–acetone (pure organic liquid of low surface tension) systems. They reported that the pressure drop tends to increase with increase superficial gas and liquid velocities whereas it tends to decrease with increasing bed temperature.

Giri et al. (2014) have made an attempt to study the flow regime map in TBR with air-Newtonian and air-non-Newtonian liquid systems, the influence of dynamic variables with Newtonian and non-Newtonian liquid systems on pressure drop, analyze the pressure drop by a mechanistic model and analyze the degree of pressure reduction in a trickle bed reactor. A bed of height 0.6 m and diameter 0.08 m has been used having 3 mm diameter glass beads as solid packing. Polyethylene oxide has been used as the pressure reducing agent. It is observed that percentage of pressure drop reduction increases with increasing surfactant concentration. However there is a critical concentration (30 ppm) above which no more reduction can be obtained.

1.5.3 Liquid Holdup

Liquid holdup in trickle bed is expressed in two ways: total liquid holdup defined as volume of liquid per unit bed volume and liquid saturation defined as volume of liquid per unit void volume. Liquid holdup varies with reactor hardware such as column diameter, particle shape and size and internals, operating parameters such as gas and liquid flow rates and physico-chemical properties of fluids. It is considerably sensitive to particle diameter than bed diameter due to higher specific area of solid particles for smaller sized particles which lead to higher liquid phase retention and holdup.

Again from the thesis of Aydin (2008): Ellman et al. (1990) derived two correlations for liquid holdup, one for the high and the other for the low interaction regimes. Wammes et al. (1991) investigated static and non-capillary liquid holdups by the stop-flow technique and bed drainage for the same operating conditions as used in the two-phase pressure drop studies. They reported that liquid holdup decreased when the pressure was increased for given gas and liquid superficial velocities. Such a decrease was interpreted as due to a shift in the reactor fluid dynamics from a state predominantly controlled by gravity (trickle flow with zero gas flow rate) to a state controlled by gas-liquid shear stress (or pressure drop). The Specchia et al. (1977) correlation for the low interaction regime described correctly their two-phase flow liquid holdup data.

Al-Dahhan et al. (1994) measured liquid holdups using the stop-flow technique and bed drainage for the same conditions as for the pressure drops, *i.e.* trickle flow regime. Their high pressure data were well described with the parameter-free phenomenological model of Holub et al. (1992).

The experimental reported results of Larachi et al. (1991) confirm observations made by Wammes et al. (1991), but over a wider range of operating conditions: at very low gas velocities, the total liquid holdup is independent of pressure regardless of the type of gas-liquid system. However for larger gas superficial velocities, the influence of pressure has to be taken into account.

Moreover, Larachi et al. (1991) found that at given gas and liquid mass flow rates, the total liquid holdup increases with pressure, owing to the lower superficial gas velocity as a consequence of the increase in gas density. The total liquid holdup is reduced when the liquid viscosity decreases. The total liquid holdup is much smaller for foaming liquids, regardless of the operating pressure, owing to the high stability of fine gas bubbles adhering to the solid particles.

In brief, the external liquid holdup is an increasing function of liquid velocity, viscosity and particle diameter. It is a decreasing function of the gas superficial velocity and of the liquid surface tension. Liquid holdup reduces as the gas density increases, except for very low gas velocities, where it is insensitive to gas density. Non-coalescing liquids exhibit much smaller holdups than coalescing liquids. Gas viscosity appears to have a marginal effect on the liquid holdup.

1.5.4 CFD Prediction of Pressure Drop and Liquid Holdup

Gunjal et al. (2005) proposed an Euler–Euler CFD model to predict hydrodynamic parameters in TBRs. Using this model, parametric analysis of the hysteresis phenomena in pressure drop and liquid holdup was performed at various operating conditions. The CFD model predictions were compared with three different data sets in the literature (Specchia and Baldi, 1977; Rao et al., 1983; Szady and Sundaresan, 1991). The model predictions generally showed good agreement with the experimental data on pressure drop and liquid saturation.

Aydin et al. (2005) carried out hydrodynamic measurements that concerned flow regime changeover from trickle to pulse flow, two phase pressure drop, liquid holdup and liquid axial dispersion coefficient using air as the process gas and water and 0.25% CMC solution (inelastic pseudoplastic behaviour) as the process liquid. They observed that the transition boundary was more distinct for air-CMC system and shifts to higher fluid velocity with increasing temperature. Two phase pressure drop and liquid holdup values were higher for air-CMC system as compared to air-water system due to higher viscosity and the values decrease with increase in temperature. Thus both Newtonian and power law non-Newtonian fluids behaved qualitatively similarly regarding the effect of temperature.

Iluita et al. (2006) analysed the transition between trickle and pulse flow regimes in trickle bed reactor involving gas-non-Newtonian liquid system using a stability analysis of the solution of a transient trickle bed, two-fluid hydrodynamic model around the equilibrium state of trickle flow. Special solution for plastic Bingham, power law shear thinning and thickening and Newtonian can be derived from this. They found that increasing temperature and pressure promote pulse flow at increasing superficial liquid and gas velocity. Conversely an increase in yield stress, flow consistency index or power law index was found to induce pulse flow at lower liquid velocity.

Atta et al. (2007) developed a 2 phase Eulerian CFD model based on porous media concept based on porous media concept to simulate gas-liquid flow through packed beds. The porous media model is advantageous to handle gas-liquid interaction terms due to its ability to lump the adjustable parameter as compared to conventional k-fluid CFD treatment of the problem. The two phase Eulerian model describing the flow domain as a porous region has been used to simulate the macroscale multiphase flow in trickle bed operating under trickle flow regime using FLUENT 6.2 software. While being simple in structure, this CFD model is flexible and predictive for large body of experimental data. They also developed a 3-D CFD simulation in pilot scale TBR using porous media flow, for predicting the meso-scale liquid maldistribution. Numerical simulation were carried out for air-water system with several initial liquid distribution and over the liquid and gas superficial velocity range of 0.001-0.006 m/s and 0.02-0.154 m/s, respectively. It was found that for low liquid and gas velocity, the details of particle wetting phenomenon seems to have more significant effect in case of large diameter column rather than in a smaller diameter column. For higher velocity, better accuracy is obtained.

Rodrigo et al. (2008) developed a 3-dimensional Euler-Euler model to study the hydrodynamic behaviour of TBR at high pressure (30 bar) in terms of pressure drop and liquid hold up. TBR operation was found to be more sensible to pressure drop than to liquid hold up results when performing same deviation scale in the cell number. It is found that as particle size of packing decreases, specific surface area of bed increases and therefore liquid hold up and pressure drop also increases. Deviation of local velocity near solid surfaces were observed which showed existence of stagnant zones near points of approximation retained from the packing spheres which enables the unsteady state behaviour exhibited by TBR in trickling flow condition.

1.6 SCOPE OF THE PRESENT WORK:

Aside from air and water, most of the fluids encountered in physical and industrial processes are non-Newtonian. TBR with downward flow of gas and liquid have wide applications in the petroleum and petrochemical industries. Many petroleum products like kerosene, naphtha, diesel fuels and lubricating oils have foam forming tendency during processing and behave as non-Newtonian fluid. Moreover TBR is also used in biochemical processes and the initial liquid behaving like a Newtonian fluid could turn into a non-Newtonian fluid after various biochemical processes. Hence it is essential to study TBR hydrodynamics with non-Newtonian systems. Here CMC (carboxyl methyl cellulose) is used as the liquid phase, which is a Non-Newtonian (pseudoplastic) fluid.

1.7 OBJECTIVE OF THE PRESENT WORK

The aim of the present work can be stated as follows:

a) To study the hydrodynamic parameters in a trickle bed reactor for air-CMC system.
b) To determine liquid holdup and pressure drop in a gas-liquid-solid cocurrent trickle bed system.
c) To examine the effect of superficial liquid and gas velocity on the individual phase holdup and pressure drop.
d) To study the variation of hydrodynamic properties with column height and also along the radial direction.

The present work is concentrated on understanding the phase holdup and pressure drop behaviours in a three phase Co-current Trickle bed. Trickle bed of height 0.6 m with diameter of 0.08 m has been used having glass beads of diameter 3 mm as the solid packing. Gas (air) is taken as the continuous phase. Liquid (CMC) and gas (air) are injected at the top with different superficial velocities. In all the cases the solid (glass bead) volume fraction has been taken to be 0.63. CFD simulations have been carried out using ANSYS FLUENT 13.0.

CHAPTER 2

CFD MODELING AND SIMULATION OF TRICKLE BED SYSTEM

CFD is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyse problems that involve fluid flow. Computers are used to perform the calculations required to simulate the interaction of liquids and gases with surface defined by boundary conditions. The fundamental basis of almost all CFD problems are the Navier-Stokes equation, which define any single phase fluid flow. These equations can be simplified by removing terms describing viscous actions to yield the Euler equation. Vorticity terms can then be removed to get full potential equations. They can be linearised to yield the linearised potential equation. CFD is used in a variety of disciplines and industries, including aerospace, automotive, power generation, chemical manufacturing, polymer processing, petroleum exploration, pulp and paper operation, medical research, meteorology and astrophysics.

2.1 CFD MODELING

2.1.1 ELEMENTS OF CFD CODES

All CFD codes consist of three main elements:

a) A pre-processor which is used to generate the grid, input the problem geometry, define the flow parameters and the boundary conditions to the code.
b) A flow solver (for example: FLUENT, CFX, POLYFLOW, etc.) which is used to solve the governing equations of the flow subject to the conditions provided. There are four different methods used as a flow solver: finite difference method, finite element method, finite volume method and spectral method.
c) A post processor which is used to interpret the data and show the results in graphical and easy to read format.

2.1.2 ADVANTAGES OF CFD

The main advantages of CFD include:

1. CFD is very much helpful in cases when it is not possible to design a working model and test its performance.

2. There is no size and scale restriction in CFD simulation. So it avoids pilot scale simulation and the difficulties of upgrading pilot scale plant to large scale plant.
3. It provides the much needed flexibility in changing design parameters without the expense of onsite changes.
4. It gives results faster as compared to the practical experiment.
5. It reduces the cost of experiment very effectively by allowing changes to variable parameter such as flow rates, temperature.

2.1.3 MULTPHASE FLOW: Eulerian Model

In the Euler-Euler approach, the different phases are treated mathematically as interpenetrating continua. Since the volume of a phase cannot be occupied by the other phases, the concept of phase volume fraction is introduced. These volume fractions are assumed to be continuous functions of space and time and their sum is equal to one. Conservation equations for each phase are derived to obtain a set of equations, which have similar structure for all phases. These equations are closed by providing constitutive relations that are obtained from empirical information, or, in the case of granular flows, by application of kinetic theory. In ANSYS FLUENT, three different Euler-Euler multiphase models are available: the volume of fluid (VOF) model, the mixture model, and the Eulerian model. In the present work, the Eulerian model has been used for carrying out the simulations.

The Eulerian model is the most complex of the multiphase models in ANSYS FLUENT. It solves a set of n momentum and continuity equations for each phase. Coupling is achieved through the pressure and interphase exchange coefficients. The manner in which this coupling is handled depends upon the type of phases involved; granular (fluid-solid) flows are handled differently than non-granular (fluid-fluid) flows. For granular flows, the properties are obtained from application of kinetic theory. Momentum exchange between the phases is also dependent upon the type of mixture being modeled. ANSYS FLUENT's user-defined functions allow you to customize the calculation of the momentum exchange. Applications of the Eulerian multiphase model include bubble columns, risers, particle suspension, and fluidized beds.

2.1.4 CONSERVATION EQUATIONS IN EULERIAN MODEL

Conservation of Mass:

$$\frac{\partial}{\partial t}(\alpha_q\rho_q) + \nabla\,.\,(\alpha_q\rho_q v_q) = \sum_{p=1}^{n}\ (m_{pq} - m_{qp}) + S_q \qquad (1)$$

where v_q is the velocity of phase q and m_{pq} characterises the mass transfer from p^{th} to q^{th} phase and S_q is the source term.

Conservation of Momentum:

$$\frac{\partial}{\partial t}(\alpha_q\rho_q v_q) + \nabla\,.\,(\alpha_q\rho_q v_q v_q) = -\,\alpha_q\nabla p + \nabla.\tau_q + \alpha_q\rho_q g + \sum_{p=1}^{n}(R_{pq} + m_{pq}v_{pq} - m_{qp}v_{qp})$$

$$+\,(F_q + F_{lift,q} + F_{vm,q}) \qquad (2)$$

where τ_q is the q^{th} phase stress-strain tensor, F_q is an external body force, $F_{lift,q}$ is a lift force, $F_{vm,q}$ is a virtual mass force, R_{pq} is an interaction force between phases and p is the pressure shared by all phases.

Conservation of Energy:

$$\frac{\partial}{\partial t}(\alpha_q\rho_q h_q) + \nabla\,.\,(\alpha_q\rho_q u_q h_q) = \alpha_q\frac{\partial}{\partial t}p + \tau_q : \nabla u_q - \nabla.\,q_q + S_q +$$

$$\sum_{p=1}^{n}(Q_{pq} + m_{pq}h_{pq} - m_{qp}h_{qp}) \qquad (3)$$

where h_q is the specific enthalpy of the q^{th} phase, q_q is the heat flux, Q_{pq} is the intensity of heat exchange between p^{th} and q^{th} phases and h_{pq} is the interphase enthalpy.

2.1.5 TURBULENCE MODELING

To account for turbulence modeling, the standard k-ϵ model is used. It is a semi-empirical model based on model transport equations for the turbulence kinetic energy (k) and its dissipation rate (ϵ). The model transport equation for k is derived from the exact equation while the model transport equation for ϵ was obtained using physical reasoning.

Table 2.1: Model Constants used for turbulence modeling

C-mu	0.09
C1-ϵ	1.44
C2-ϵ	1.92
C3-ϵ	1.3
TKE Prandtl Number	1
TDR Prandtl Number	1.3
Dispersion Prandtl Number	0.75

2.1.6 FLOW MODEL

A two–dimensional Eulerian three phase model is for simulation in the present work where gas (air) is treated as the continuous phase, inter-penetrating and interacting everywhere within the computational domain. The liquid flow velocity is in trickle flow regime. The motion of liquid and gas phase is governed by the respective mass and momentum balance equations. The momentum equation for the solid phase is not solved as it is a packed bed and each particle in the bed is assumed to be stationary. The velocity of solid phase is fixed to zero via a user interface command.

2.1.7 ASSUMPTIONS

a) Both fluids are incompressible.

b) The inertial, viscous and Reynolds terms are neglected as compared to the drag force terms (momentum exchange terms)

c) Bed porosity is constant and uniform.

d) Reactor is operating under trickling flow regime.

e) Capillary pressure is neglected.

f) There is no inter-phase mass transfer and heat transfer.

2.1.8 PROBLEM DESCRIPTION

The problem is based on a three phase solid-liquid-gas Trickle Bed in which both liquid and gas are flowing co-currently downward. Solid phase consists of glass bead of uniform diameter of 3 mm and having a constant porosity of 0.37. The primary phase consists of air and the secondary phase consists of CMC (concentration= 1 kg/m^3). The gas and liquid velocities are taken such that the flow lies in the trickle flow regime. The schematic of the setup used in the problem is shown in the figure below:

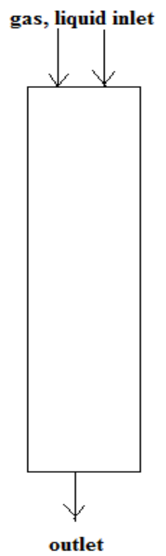

Figure 2.1: Schematic of the set-up

The properties of gas, liquid and solid phases are shown in the following table.

Table 2.2: Properties of air, CMC and glass beads

	Density (kg/m^3)	Viscosity (kg/m s)
Air	1.225	1.789*10^{-5}
CMC (1 kg/m^3 conc.)	1000.8	0.023
Glass beads	2470	1.789*10^{-5}

2.1.9 POROUS MEDIA CONDITIONS

The porous media model can be used for a wide variety of single phase and multiphase problems, including flow through packed beds, filter papers, perforated plates, flow distributors and tube banks. In this model a cell zone is defined in which the porous media model is applied and the pressure loss in the flow is determined via inputs in the momentum equations for porous media.

Porous media are modelled by the addition of a momentum source term to the standard fluid flow equations. The source term is composed of two parts: a viscous loss term and an inertial loss term.

User inputs for porous media:

- The porous zone is defined.
- The fluid material flowing through the porous medium is identified.
- The relative velocity resistance formulation is enabled.
- The viscous resistance term ($1/\alpha$) and the inertial resistance term C_2 are set and the direction vectors in which they apply are specified.
- The porosity of the porous medium is specified.

The viscous resistance coefficient and inertial resistance coefficient are derived from the Ergun equation and given by:

$\alpha = [D_p^2/150]*[\epsilon^3/(1-\epsilon)^2]$

$C_2 = [3.5/D_p]*[(1-\epsilon)/\epsilon^3]$

where D_p is the mean particle diameter and ϵ is the void fraction.

2.2 CFD SIMULATION

2.2.1 GEOMETRY AND MESH

A two dimensional rectangular geometry of width 0.08 m and height 0.6 m is made. Fine particle size is used for better accuracy. Uniform quadrilaterals having element size 0.005 m are used for the construction of the mesh. The mesh contains 2074 nodes and 1936 elements.

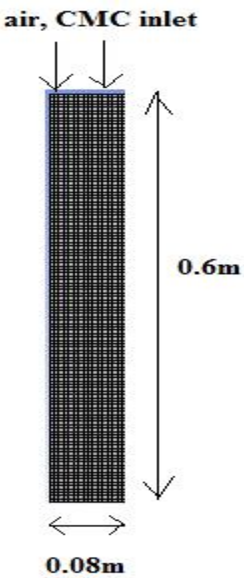

Figure 2.2: Mesh used in the problem

2.2.2 SOLUTION

In this problem, the gas phase is treated as primary phase and liquid phase is considered as secondary phase. Unsteady state simulations are carried out with the time step of 0.005 s for 30 seconds (or 6000 number of time steps). Drag coefficients are considered to account for the force interaction among phases. The models used for these, the solution methods and the solution control parameters are shown in the tables below.

Table 2.3: Models used for considering force interactions among phases

INTERACTIONS	MODEL
CMC-Air	Schiller-Naumann
Glass bead-Air	Schiller-Naumann
Glass bead-CMC	Schiller-Naumann

The Schiller-Naumann model is the default model and it is acceptable for general use for all fluid-fluid pairs of phases (ANSYS FLUENT 12.0 Theory Guide). The drag function f is given by:

$$f = C_D Re/24 \tag{4}$$

where $C_D = 24\,(1 + 0.15Re^{0.687})/Re$ for $Re < 1000$

$= 0.44$ for $Re > 1000$

C_D is the drag coefficient and Re is the Reynolds Number.

Table 2.4: Solution Method

PV Coupling Scheme	Phase Coupled SIMPLE
Gradient	Least Square Cell Based
Momentum	First Order Upwind
Volume fraction	First Order Upwind
Turbulent Kinetic Energy	First Order Upwind
Turbulent Dissipation Rate	First Order Upwind
Transient Formulation	First Order Implicit

Table 2.5: Solution Control Parameters

Pressure	0.3
Density	1.0
Body Forces	1.0
Momentum	0.7
Volume Fraction	0.5
Turbulent Kinetic Energy	0.8
Turbulent Dissipation Rate	0.8
Turbulent Viscosity	1.0

2.2.3 CELL ZONE CONDITIONS AND BOUNDARY CONDITIONS:

The cell zone (interior of the body) is defined as fluid, through which the gas-liquid mixture flows. Porosity is specified to be 0.37 which remains constant throughout. For the gas and liquid phases, source terms in the form of viscous and inertial resistance terms are specified as described in section 2.1.9. Inlet boundary conditions are specified in terms of inlet velocity of air and CMC and the volume fraction of CMC. At the outlet, the gauge pressure is specified to zero by default. No slip boundary condition for the wall is specified.

CHAPTER 3

RESULTS AND DISCUSSIONS

Simulation has been carried out for three-phase trickle bed system of height 0.6 m and diameter 0.08 m. 3 mm glass beads have been used as the packing material and bed porosity has been considered to be constant at 0.37. The simulations have been carried out until quasi steady state is reached and no further change in average bed parameters in the form of volume fraction of air is observed as shown in figure 3.1.

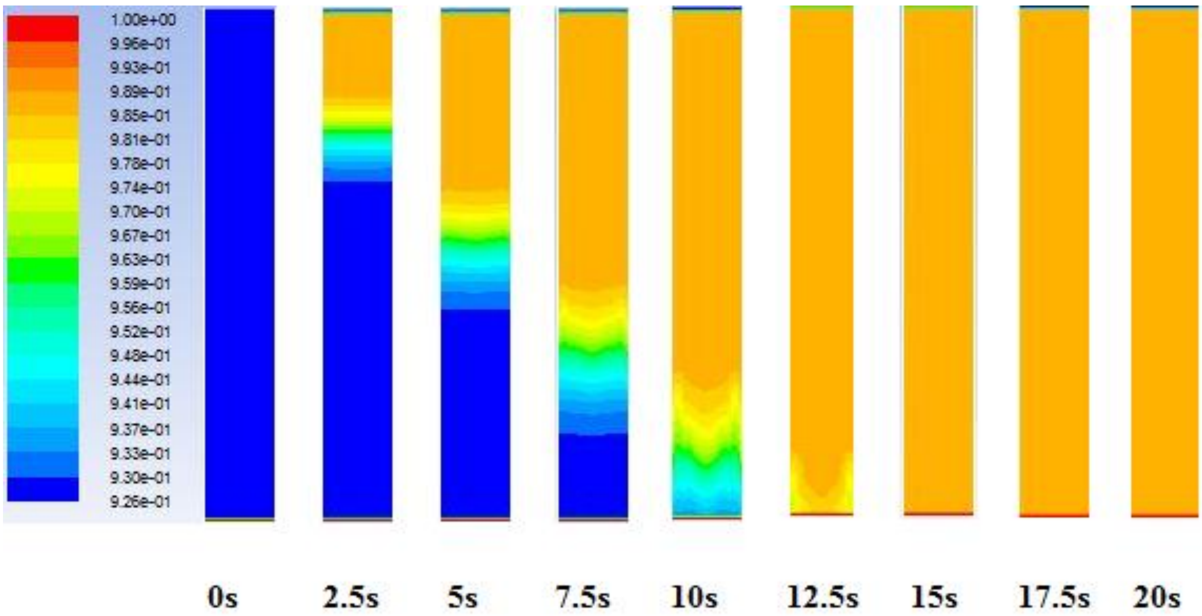

Figure 3.1: Contours of volume fraction of air for air velocity 0.05 m/s and liquid velocity 0.004 m/s

Figure 3.1shows the contours of volume fraction of air at different times for air velocity 0.05 m/s and liquid velocity 0.004 m/s. As air begins to flow from the top, initially variation in the volume fraction is observed in the upper section of the bed. Gradually steady state is reached after 15 sec and no further change in the volume fraction of air in the bed is observed.

Figure 3.2 shows the contours of volume fraction of air, CMC and glass beads after the attainment of steady state for air velocity 0.06 m/s and liquid velocity 0.006 m/s. The contours indicate that most of the porous region in the bed is occupied by the gas phase. This is because gas phase is the continuous phase and liquid flow is in the trickle flow regime

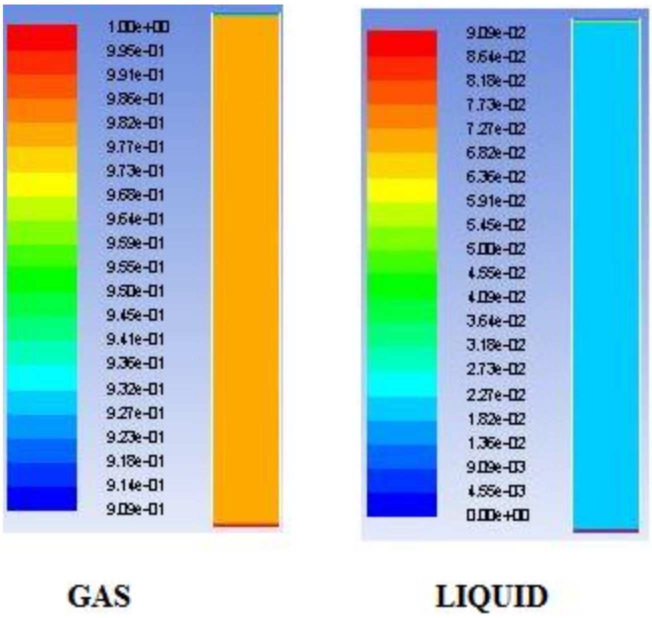

Figure 3.2: Contours of volume fraction of gas and liquid phases at air velocity 0.06 m/s and liquid velocity 0.006 m/s

3.1 LIQUID HOLDUP

Liquid holdup is an important hydrodynamic parameter in the study of Trickle Bed Reactors. It is defined as the volume fraction of liquid, referred to total bed volume that remains in the bed after complete draining. Many other design parameters of trickle bed like wetting efficiency, heat and mass transfer coefficients, are dependent on liquid holdup. The prevailing liquid holdup in the bed also controls the liquid phase residence time and therefore conversion of the reactants. Hence it is important to understand how liquid holdup varies with operating parameters such as gas and liquid flow rates.

The variation of liquid holdup with liquid velocity and gas velocity are shown in figures 3.3 and 3.4, respectively. It is observed that liquid holdup increases with liquid velocity and decreases with increase in gas velocity. The liquid holdup increases with liquid velocity because of displacement of gas phase by the liquid. In a trickle flow regime, this displacement occurs till liquid occupies maximum possible region. Decrease in liquid holdup with increase in gas velocity can be attributed to increase in shear between gas and liquid phases. A similar pattern was observed by Aydin et al. (2005) at higher temperature and pressure.

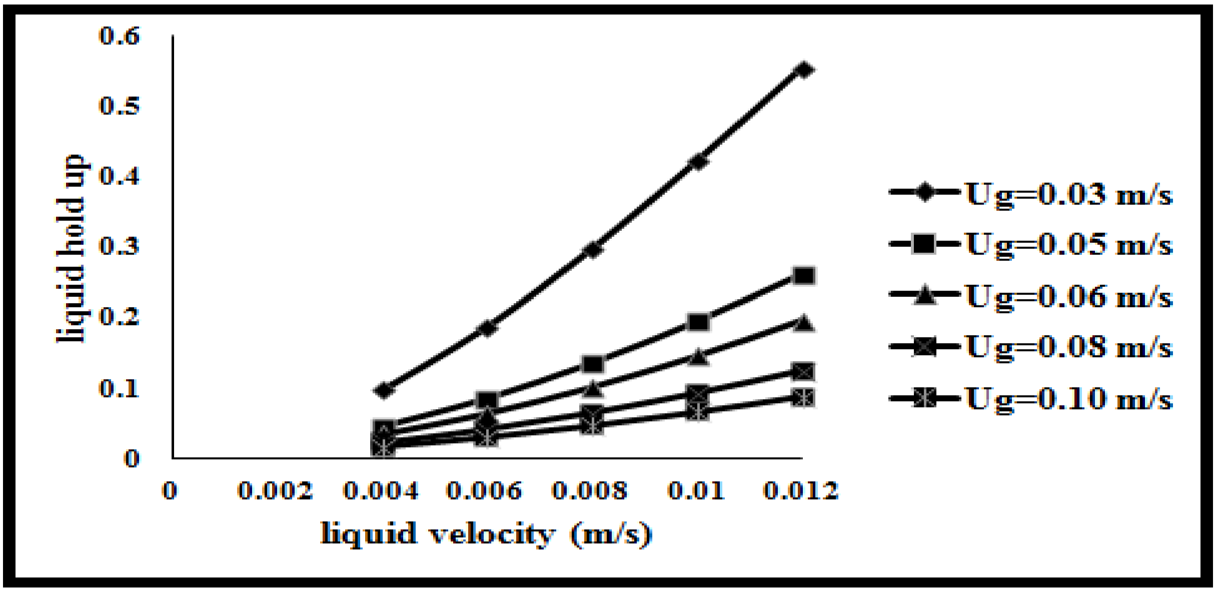

Figure 3.3: Variation of liquid holdup with liquid velocity

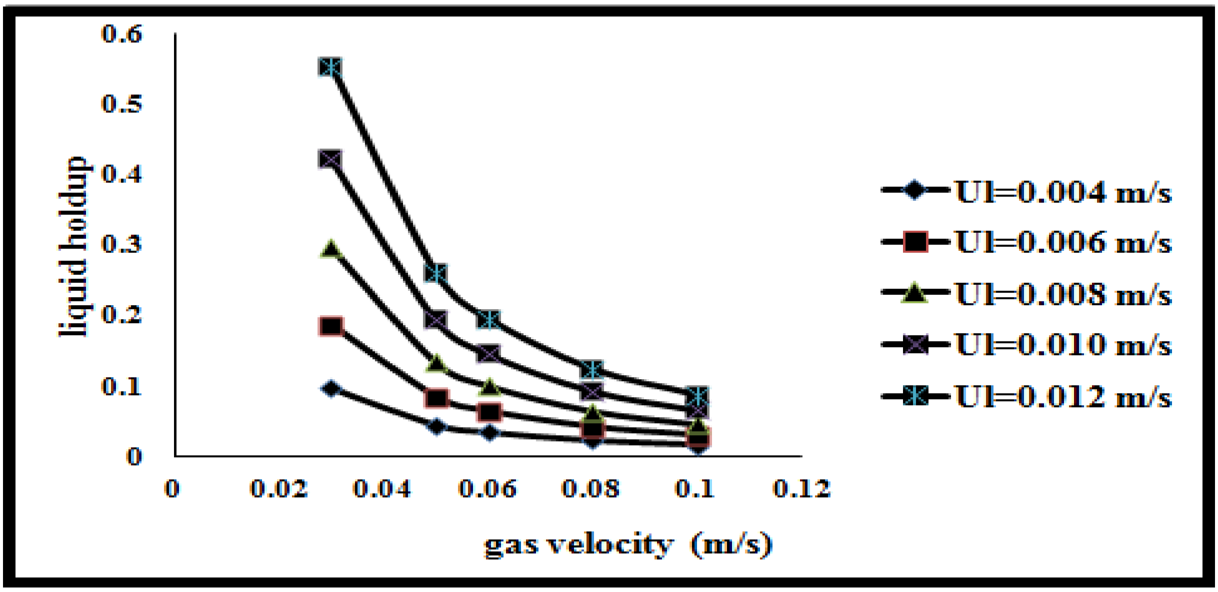

Figure 3.4: Variation of liquid holdup with gas velocity

Figure 3.5 and 3.6 show the variation of liquid holdup with column height at gas velocity 0.08 m/s and liquid velocities 0.004 m/s and 0.006 m/s, respectively. It is observed that liquid holdup is very small at the bottom of the column, remains constant for a certain height and then increases with column height. It is maximum at the top of the column. The gradient is more prominent at lower liquid velocities and a flat profile is observed at higher liquid velocities.

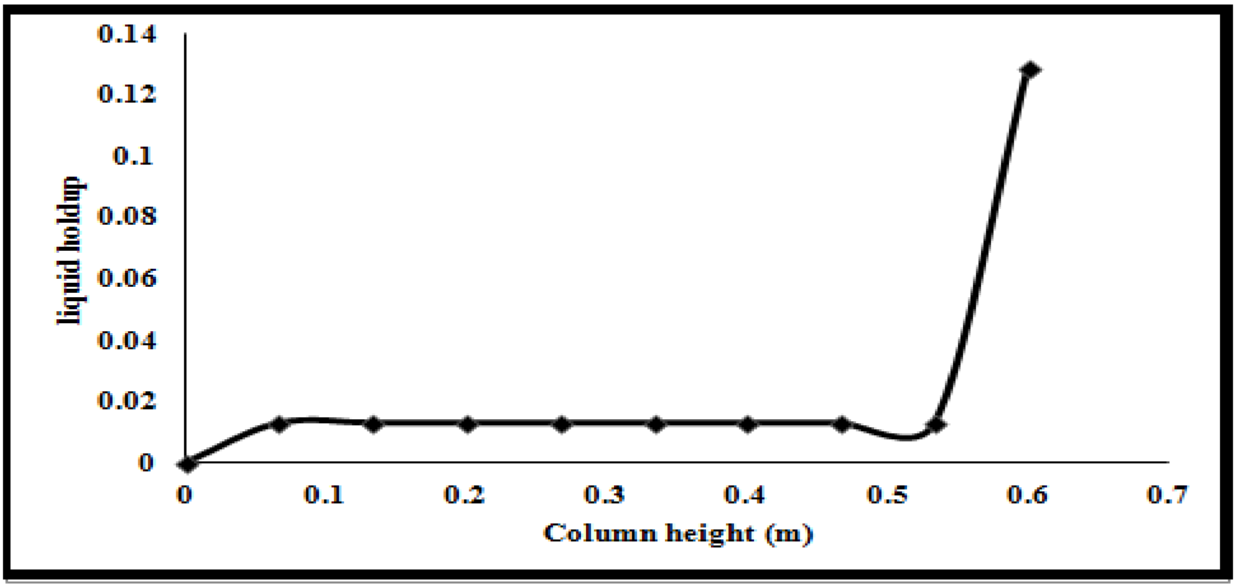

Figure 3.5: Variation of liquid holdup with column height for air velocity 0.08 m/s and liquid velocity 0.004 m/s

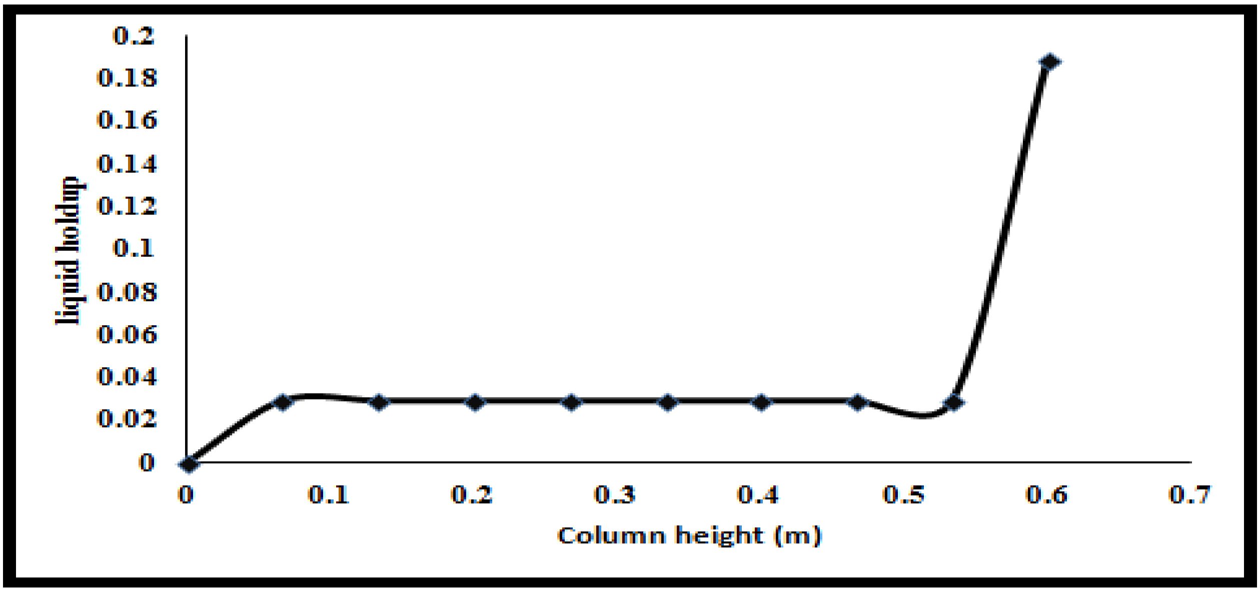

Figure 3.6: Variation of liquid holdup with column height for air velocity 0.08 m/s and liquid velocity 0.006 m/s

Figure 3.7 and 3.8 show the radial variation of liquid holdup at a particular bed height for air velocity 0.1 m/s and liquid velocities 0.004 m/s and 0.006 m/s, respectively. It is observed that in both cases, the liquid holdup is initially low near the wall, then increases and remains nearly constant in the central part of the column and then again decreases at the other end of the wall. This may be due to high porosity near the wall. However a more flat profile is observed at higher liquid velocity.

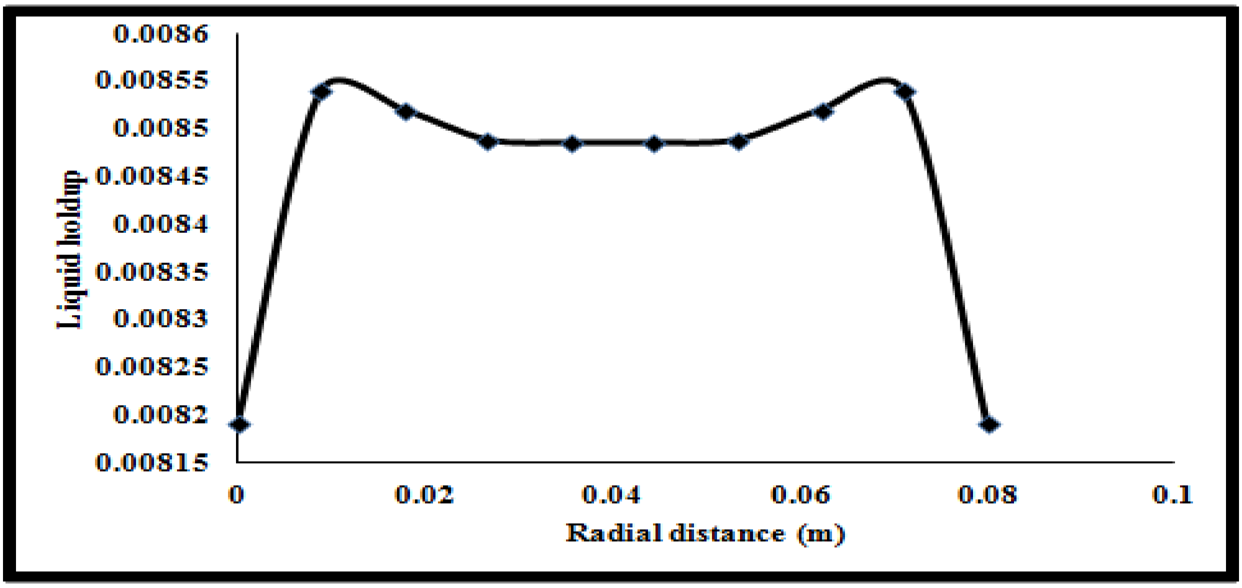

Figure 3.7: Radial variation of liquid holdup at bed height 0.2 m for air velocity 0.1 m/s and liquid velocity 0.004 m/s

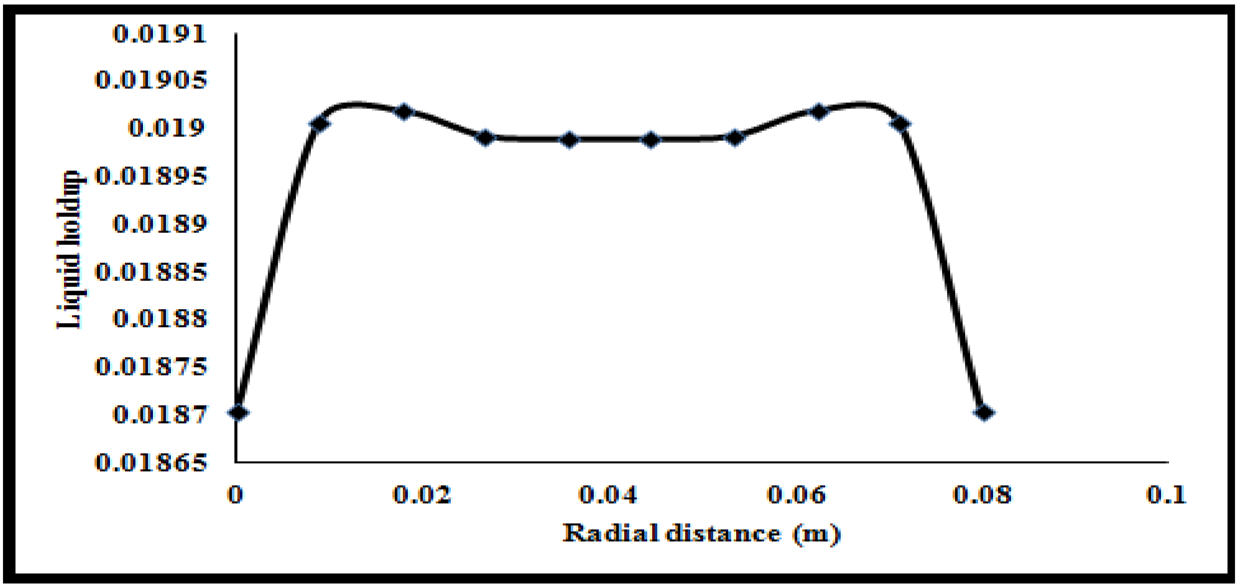

Figure 3.8: Radial variation of liquid holdup at bed height 0.2 m for air velocity 0.1 m/s and liquid velocity 0.006 m/s

3.2 GAS HOLDUP

Since the volume fraction of solid phase is constant throughout the bed, the volume fractions of the liquid and gaseous phase are interdependent. Hence gas holdup is obtained from the liquid holdup data. Figure 3.9 and 3.10 show the variation of gas holdup with liquid velocity and gas velocity, respectively.

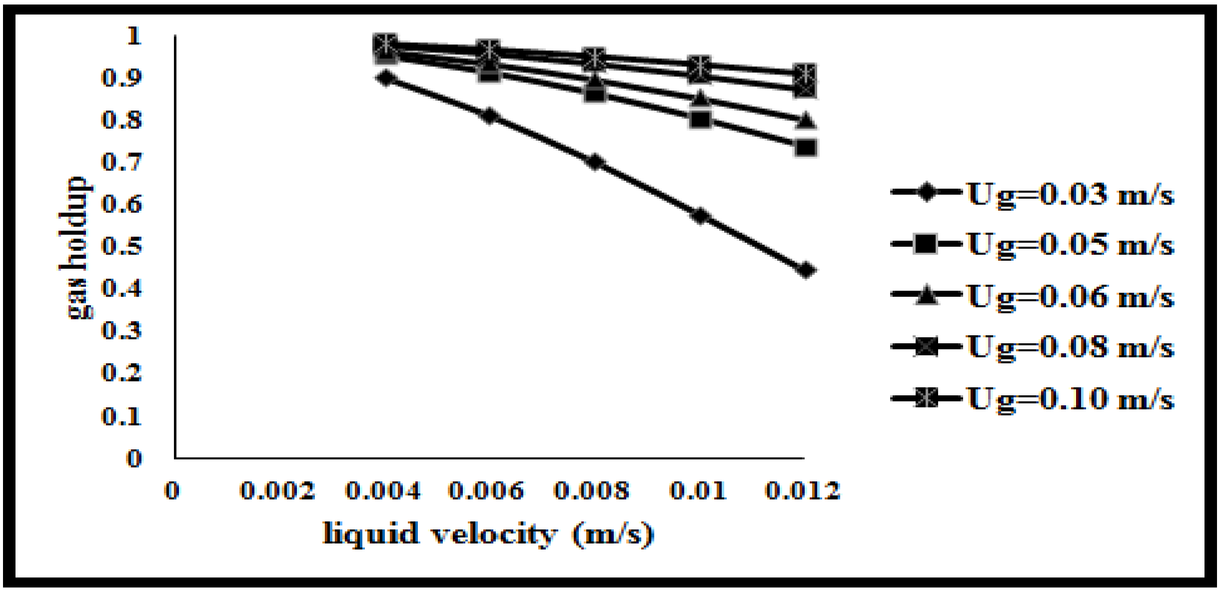

Figure 3.9: Variation of gas holdup with liquid velocity

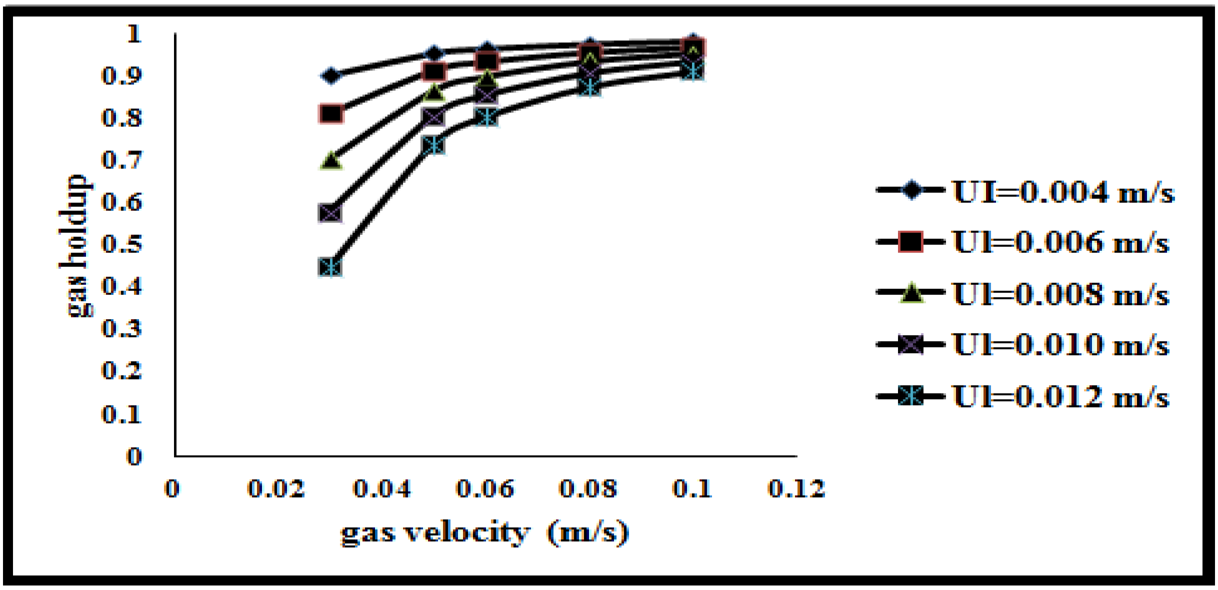

Figure 3.10: Variation of gas holdup with gas velocity

From figure 3.9 it is observed that gas holdup decreases with increase in liquid velocity and at a particular liquid velocity, gas holdup is higher for higher gas velocity. Similarly from figure 3.10 it is observed that gas holdup increases with increase in gas velocity and at a particular gas velocity, gas holdup is higher for lower liquid velocity.

Figure 3.11 and 3.12 shows the variation of gas holdup along the column height for gas velocity 0.1 m/s and liquid velocities 0.004 m/s and 0.006 m/s, respectively. It is observed that gas holdup decreases with increase in column height.

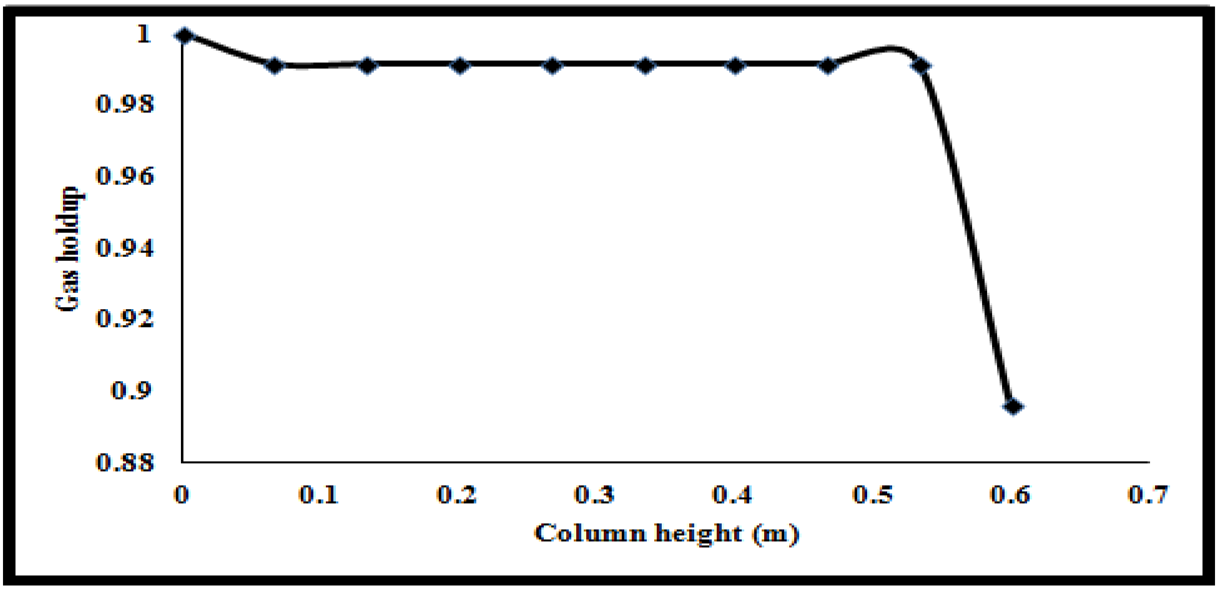

Figure 3.11: Variation of gas holdup with column height for air velocity 0.1 m/s and liquid velocity 0.004 m/s

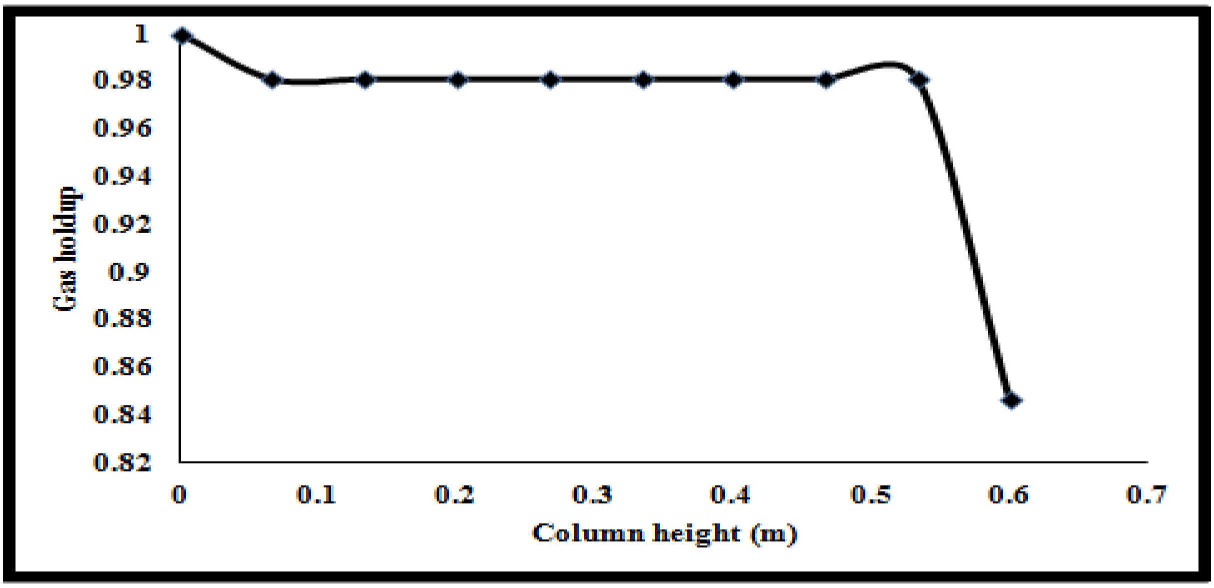

Figure 3.12: Variation of gas holdup with column height for gas velocity 0.1 m/s and liquid velocity 0.006 m/s

Figure 3.13 and 3.14 shows the radial variation of gas holdup at a particular bed height for gas velocity 0.06 m/s and liquid velocity 0.004 m/s and 0.006 m/s, respectively. It is observed that variation of gas holdup is more prominent at low liquid velocity than the corresponding higher velocity.

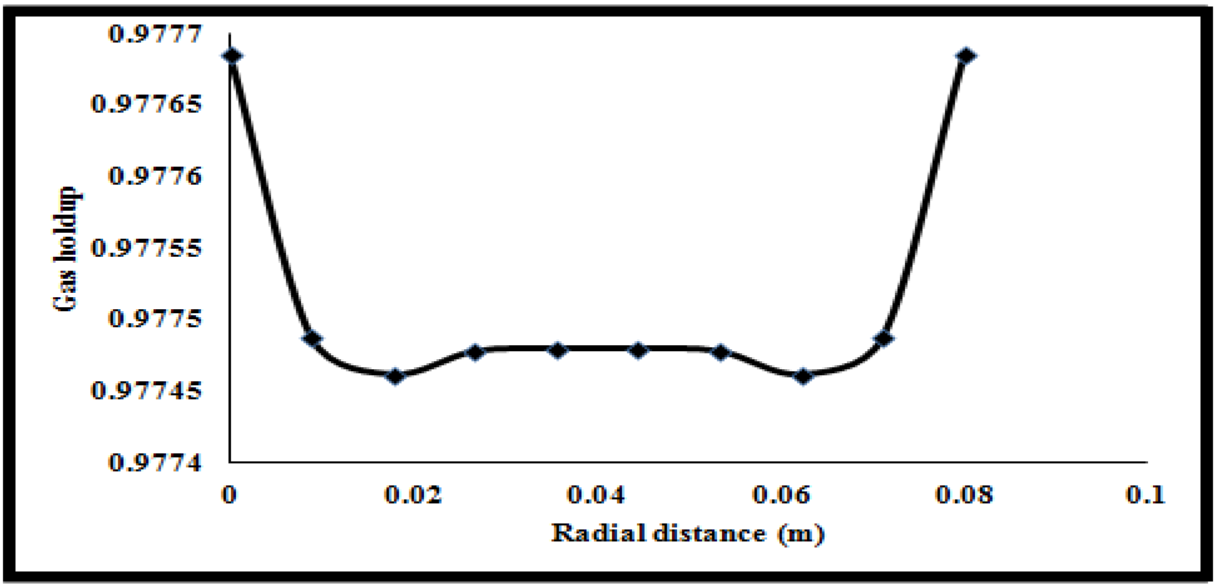

Figure 3.13: Radial variation of gas holdup at column height 0.4m for gas velocity 0.06 m and liquid velocity 0.004 m/s

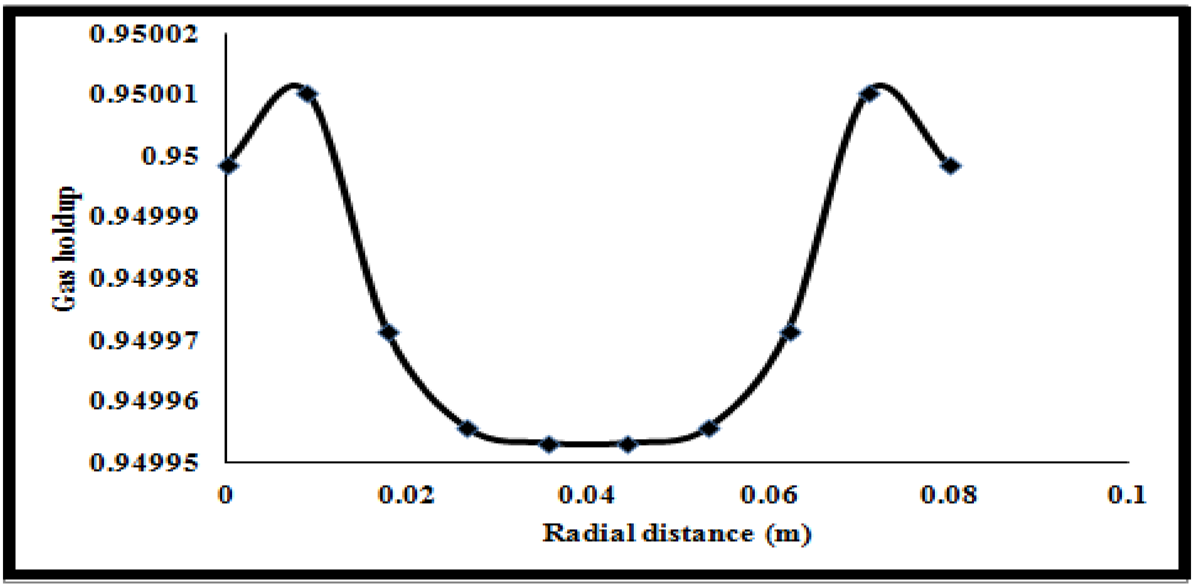

Figure 3.14: Radial variation of gas holdup at column height 0.4m for gas velocity 0.06 m/s and liquid velocity 0.006 m/s

3.3 PRESSURE DROP

Pressure drop is yet another important hydrodynamic parameter in the study of trickle bed system. Two- phase pressure drop is one of the driving forces acting on the system which plays an important role on energy dissipation in packed bed systems. Energy dissipation in porous media is mainly caused by friction forces due to fluid viscosity at the gas-liquid, gas-solid and liquid-solid interfaces. In the trickling regime, the resistance to flow is essentially controlled by shear and capillary forces. The liquid and gas phase experience pressure in trickle bed because of friction at the gas-liquid, liquid-solid and solid-gas interfaces. The pressure is more for liquid of high surface tension and high solid-liquid interaction. Figures 3.15 show the variation of pressure drop with liquid velocity.

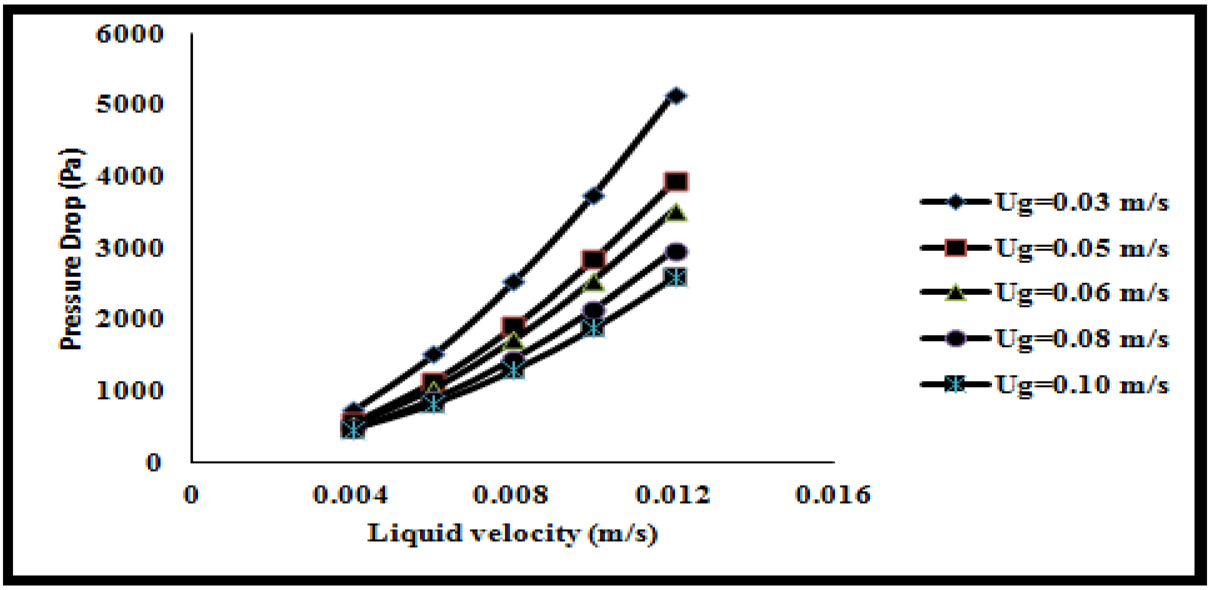

Figure 3.15: Variation of pressure drop with liquid velocity

From figure 3.15 it is observed that pressure drop increases with increase in liquid velocity and at a particular liquid velocity it is higher for lower gas velocity. Pressure increases with increase in liquid velocity due to blocking of void space because of high liquid holdup that leads to high gas-liquid interfacial friction.

Figures 3.16 and 3.17 show the variation of pressure drop along the height of the column for gas velocity 0.03 m/s and liquid velocity 0.01 m/s and 0.012 m/s, respectively. It is observed that there is linear variation in pressure drop along the column height. This indicates that there is uniform channelling in the column. Slope of this linear variation can be used to represent the pressure drop per unit length. As the flow proceeds from top to bottom, gradually increasing resistance leads to drop in pressure. Moreover as outlet gauge pressure is specified to be zero, hence pressure is maximum at the top of the column.

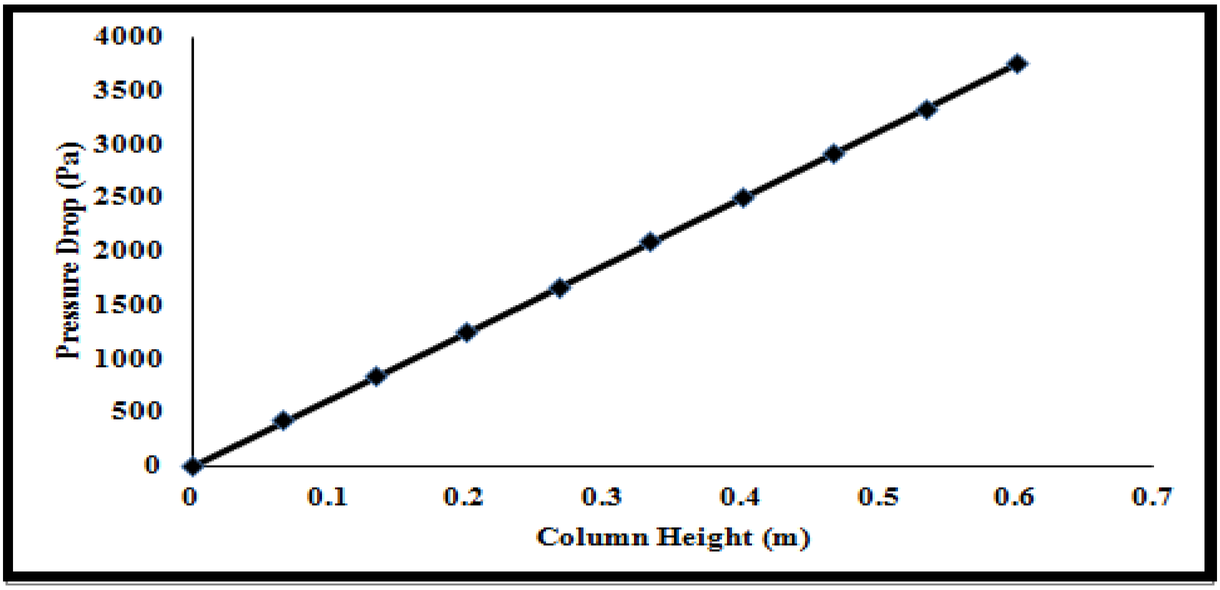

Figure 3.16: Variation of pressure drop along column height for gas velocity 0.03 m/s and liquid velocity 0.01 m/s

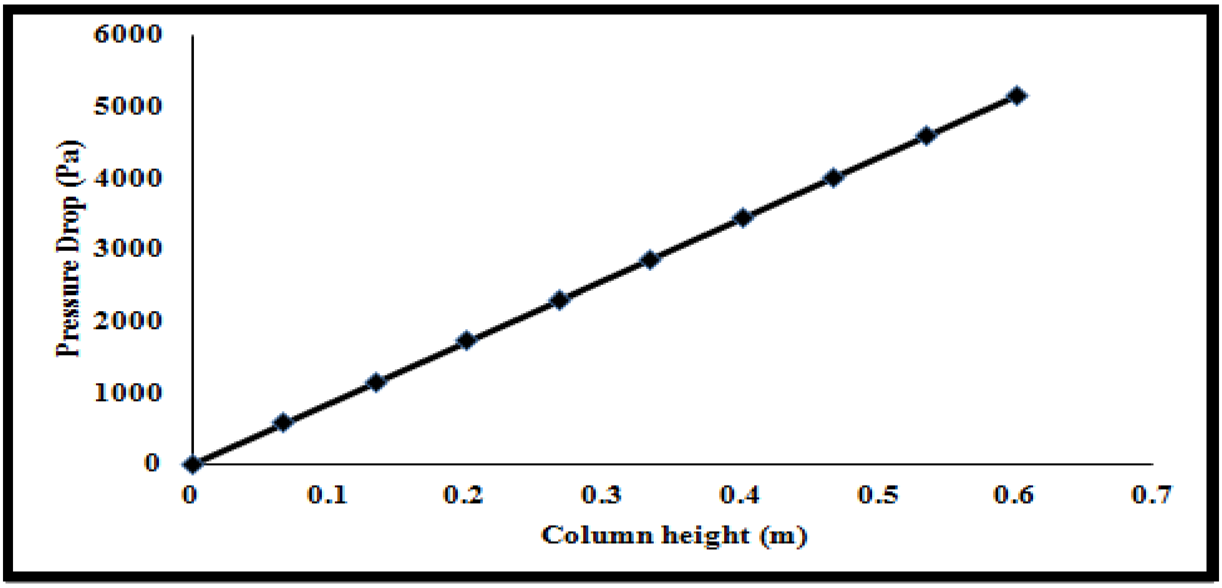

Figure 3.17: Variation of pressure drop along column height for gas velocity 0.03 m/s and liquid velocity 0.012 m/s

Figures 3.18 and 3.19 show the radial variation of pressure drop at different bed heights for gas velocity 0.03 m/s and liquid velocity 0.01 m/s and 0.012 m/s, respectively.

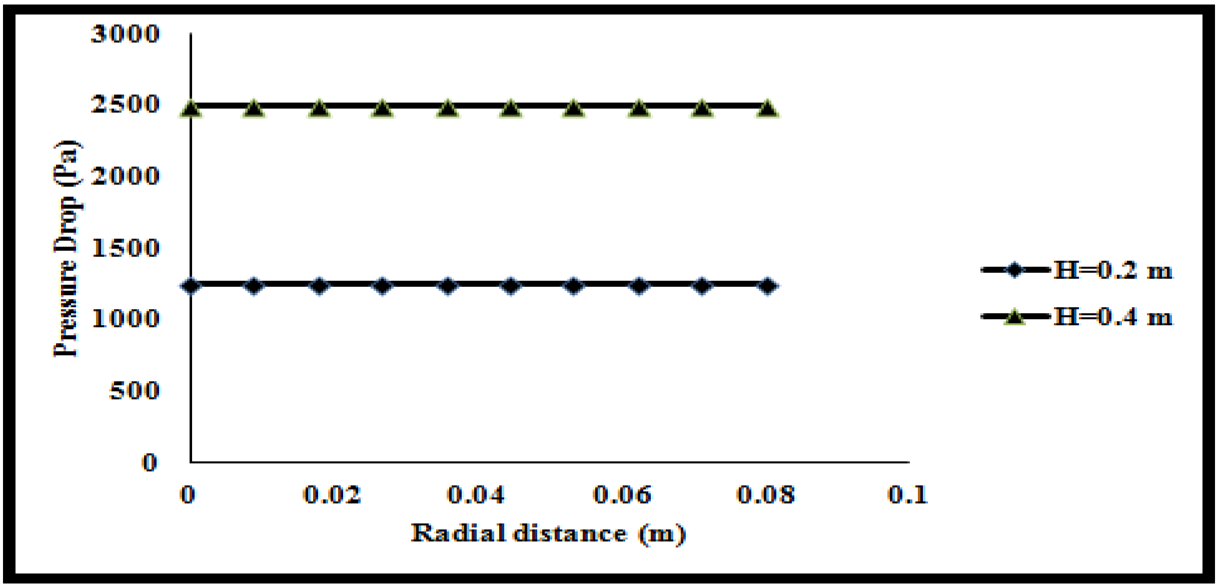

Figure 3.18: Radial variation of pressure drop at bed heights 0.2m and 0.4m for gas velocity 0.03 m/s and liquid velocity 0.01 m/s

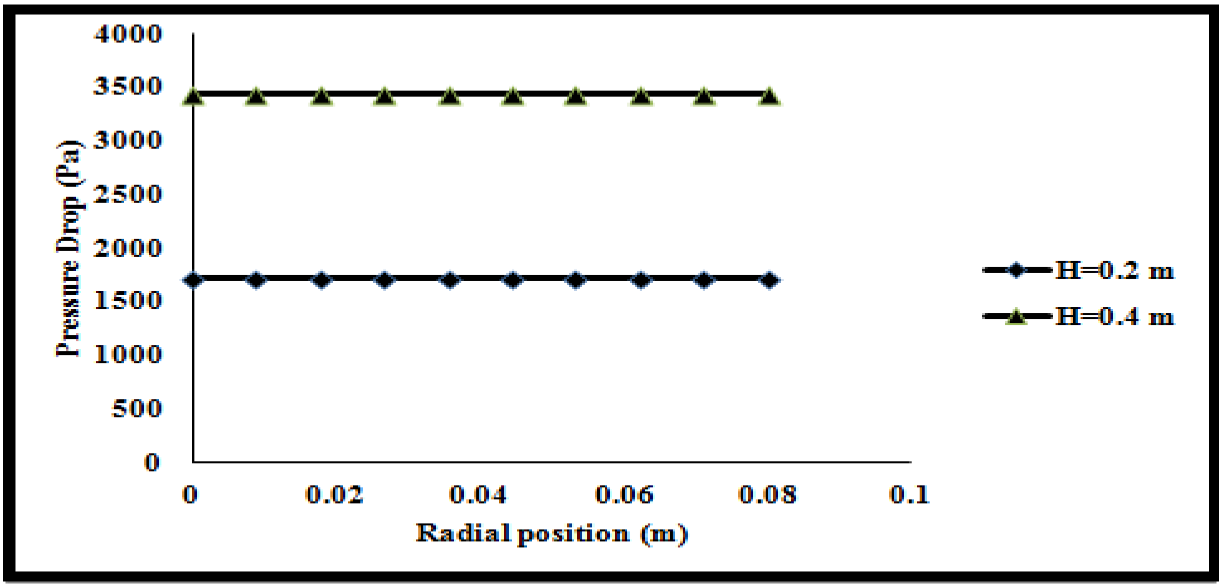

Figure 3.19: Radial variation of pressure drop at bed heights 0.2m and 0.4m for gas velocity 0.03 m/s and liquid velocity 0.012 m/s

It is observed that in both cases, pressure drop is constant along the radial direction (because of hydrostatic equilibrium) and it increases with increase in bed height. This is due to the same reason as mentioned in the previous paragraph.

3.4 COMPARISON WITH LITERATURE DATA

Since comparatively less literature data is available for air-CMC simulations, the present CFD work is compared with the experimental work carried out by Giri et al. (2014).

The pressure drop values have been compared as shown in the following table and figure:

Table 3.1: Comparison of Pressure Drop Data

Sl no.	Gas velocity (m/s)	Liquid velocity (m/s)	Pressure Drop (Pa) **Giri et al. (2014)**	Pressure Drop (Pa) **Present work**
1	0.033	0.00796	1000	2285
2	0.033	0.00947	2200	3157.98
3	0.033	0.01194	4000	4872

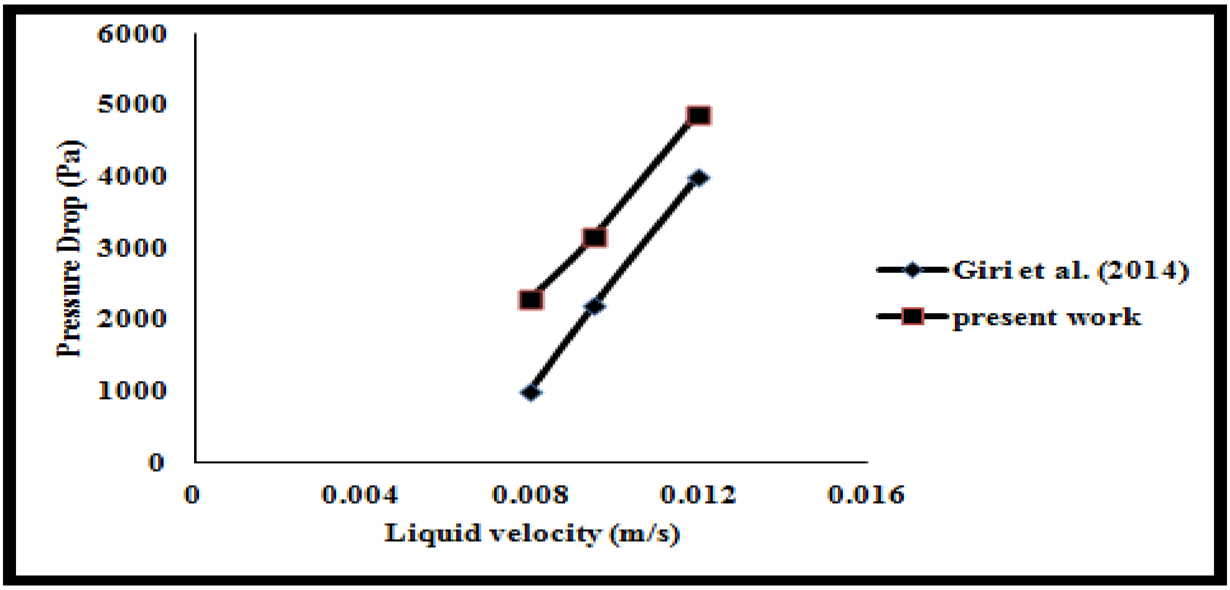

Figure 3.20: Comparison of pressure drop with literature data

The data is found to agree well with the present work. However variation is present since the available data is based on experiment and the present work is based on CFD analysis.

CHAPTER 4

CONCLUSIONS

CFD simulations of three phase trickle-bed reactor have been carried out by using Eulerian-Eulerian approach for different flow conditions. Air, CMC and glass beads are used as the gas, liquid and solid phase, respectively. Important hydrodynamic parameters such as pressure drop, liquid holdup and gas holdup have been studied. The results obtained are represented in graphical form and analysed.

The main conclusions that can be drawn are:

- Liquid holdup increases with increase in liquid velocity and decreases with increase in gas velocity.
- Liquid holdup is very small at the bottom of the column, remains constant for a certain height and then increases with column height. It is maximum at the top of the column.
- The gradient is more prominent at lower liquid velocities and a flat profile is observed at higher liquid velocities.
- The radial variation of liquid holdup is somewhat parabolic in nature. It is relatively lower near the walls and remains constant in the central region of the column.
- Gas holdup increases with increase in gas velocity and decreases with increase in liquid velocity.
- Gas holdup decreases with increase in column height and radial variation of gas holdup is more prominent at low liquid velocity than the corresponding higher velocity.
- Pressure drop increases with increase in liquid velocity and decreases with increase in gas velocity.
- There is linear variation of pressure drop along the column height which indicates that there is uniform channeling. Slope of this linear variation can be used to represent the pressure drop per unit length.
- Pressure drop is constant along the radial direction and it increases with increase in bed height.
- The results obtained from simulations have been compared with the experimental data as obtained from the work of Giri et al. (2014) and there is a close agreement between the two.

Scope for Future Work

In the present work, CFD simulations have been carried out for air-CMC system at ambient conditions. However, high temperature and pressure conditions are encountered in most industrial processes. Hence simulations can be carried out at higher operating conditions for better understanding of the performance of trickle bed reactors. Moreover bed porosity has been considered to be constant and uniform throughout. Simulations can be done to study the effect of porosity distribution on hydrodynamic parameters such as pressure drop and phase holdup. Effect of change of packing material and particle size on various hydrodynamic properties can also be analysed.

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