HYDRODYNAMIC CHARACTERISTIC STUDY OF A THREE PHASE CO-CURRENT TRICKLE-BED REACTOR: CFD ANALYSIS

A thesis submitted in partial fulfillment of the requirements for the degree of
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In

Chemical Engineering

By

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CERTIFICATE

This is to certify that the thesis entitled "**Hydrodynamic Characteristic Study of a Three Phase Co-current Trickle-Bed Reactor: CFD analysis**" being submitted by **Bidhu Bhusan Meher (107CH032)** as an academic project in the Department of Chemical Engineering, National Institute of Technology, Rourkela is a record of bonafide work carried out by him under my guidance and supervision.

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ABSTRACT

Trickle-bed has been extensively used in chemical process industries mainly in petrochemical and refinery process since it provide flexibility and simplicity of operation as well as high throughputs. The basic parameter for design, scale-up and operations of a trickle bed reactor are the pressure gradient and liquid saturation. Knowledge of these hydrodynamics parameters and prevailing flow regime is essential for design and performance evaluation of the reactor. But hydrodynamics of trickle bed reactor involve complex interaction of gas and liquid phase with packed solid which is very difficult to understand. Many computational models have been developed and extensive CFD study of hydrodynamics parameters has been done is last few decades to understand the behaviour of trickle bed reactor.

In the present work an attempt has been made to study the hydrodynamics of a co-current gas-liquid-solid trickle bed reactor using FLUENT 6.3.26. CFD simulations has been done using Eulerian-Eulerian approach for a trickle bed system with column of height 1 m and diameter 0.194 m containing glass beads of diameter 6mm as solid packing. GAMBIT 2.3.16 has been used to generate a 2D coarse grid. The phase holdup and pressure drop behaviours have been studied and their axial and radial distributions have been illustrated. The results show that liquid holdup increases with increase in liquid velocity and decrease with increase in gas velocity. The trend is reverse for gas holdup i.e. it increases with increase in gas velocity and decrease with increase in liquid velocity. Pressure drop increases with increase in both gas and liquid velocity. Quantification of this behaviour has been done. The results have been compared with previous literature data available and found to agree well.

Keywords: Hydrodynamics, Trickle-bed reactor, Liquid holdup, Pressure Drop, CFD

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NOMENCLATURE

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

ρ_k = Density of phase k= g (gas), l (liquid), kg/m^3

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

μ_{eff}= Effective viscosity, kg/m-s

Mi,g= Interphase force term for gas phase

Mi,l= Interphase force term for liquid phase

P= Pressure, Pa

t= Time, s

k= Turbulent kinetic energy, J

U_k= Velocity of phase k= g (gas), l (liquid), s (solid), m/s

α_k= Volume fraction of phase k= g (gas), l (liquid), such that $\alpha_L+\alpha_G=1$

D = Diameter of the column, m

x = Radial Position in the column, m

Z= Height of the column, m

CHAPTER 1

INTRODUCTION

1.1 Trickle Bed Reactor:

Trickle bed reactor is a packed bed of stationary particle that are subjected to co-current gas and liquid flow at relatively low fluid superficial velocities. It is considered to be the simplest reactor type for performing catalytic reactions. TBRs find widespread use in petroleum refining, chemical and process industries, pollution treatment and biochemical industries. Design and scale up of TBRs continues to be a major challenge for chemical engineers. A rigorous and fundamentally exhaustive mathematical description of trickle flow dynamics has not been achieved. The design and scale-up of trickle bed reactors depend on key hydrodynamic variables such as liquid volume fraction (liquid saturation), particle scale wetting and overall gas–liquid distribution. Some of the important chemical engineering aspects for design of Trickle-bed reactor are: (Sie and Krishna, 1998)

1. Pressure Drop
2. Liquid and Gas Holdups
3. Catalyst Contacting
4. Axial and Radial Dispersion of liquid and gas
5. Mass Transfer
6. Heat Transfer
7. Thermal stability

These variables are difficult to determine experimentally and interactions between these are as yet poorly understood. Even though numerous experimental studies have been reported in measurement of these variables, predicting them from first principle hydrodynamic simulations is difficult as yet and no coherent and conclusive methodology for doing so has yet been espoused. In order to explain the hydrodynamics of trickle bed reactor many models and approaches has been proposed by the authors.

In trickle bed reactor Hydrodynamics is quantified in terms of hydrodynamics parameter like pressure drop, liquid holdup, gas holdup, liquid mal-distribution which are related in some way to the gas-liquid-solid contacting effectiveness and operational efficiency of the reactor column. A phenomenon that greatly complicates the mathematical description of trickle bed reactor is that these hydrodynamic variables are path variable, which depend on the history of the operation. This phenomenon manifests itself in the form of hysteresis loops or multiple hydrodynamics state.

Factors that affect the performance of a trickle bed reactor are:

- Porosity: increase in porosity decreases liquid and gas holdup, pressure drop, wetting deficiency and mal-distribution factor, however it increases gas-liquid mass transfer rate, liquid solid mass transfer rate and axial dispersion of fluid.(Kundu et al, 2001)
- Particle size: increase in particle size decreases liquid and gas holdup, pressure drop, mass transfer rate and wetting efficiency but increases axial dispersion and mal-distribution factor. .(Kundu et al, 2001)
- Liquid density: increase in liquid density increases pressure drop and give poor performance in mass transfer and wetting efficiency.
- Liquid viscosity: it promotes holdup, pressure drop, gas-liquid mass transfer and wetting efficiency but decrease axial dispersion of liquid.
- Surface tension: increase in surface tension of liquid increases pressure drop but decreases gas-liquid mass transfer and wetting efficiency.(Saroha et al, 2008)
- Liquid superficial velocity: this promotes liquid holdup, pressure drop, mass-transfer, wetting efficiency and axial dispersion and decreases mal-distribution of liquid.

- Gas superficial velocity: this decreases the liquid holdup and mal-distribution but increases pressure drop, mass transfer and wetting efficiency.
- Gas viscosity: increase in gas viscosity promotes holdup, pressure drop, liquid-gas mass transfer rate.(Wang et al, 1997)
- Pressure (gas density) : increase in pressure decrease liquid holdup, liquid-solid mass transfer rate and liquid mass transfer rate but increases pressure drop, gas-solid mass transfer rate and wetting efficiency.(Al-Dahhan et al 1997)

1.2 Hydrodynamics of trickle flow:

The hydrodynamics of trickle flow are related someway to the performance of the trickle flow column. We will come across some frequently used parameters like liquid holdup ($\alpha_{L)}$ and pressure drop ($\Delta P/Z$), the liquid holdup is a roughly indicative of liquid-solid contact efficiency. High holdup also indicates good radial spreading of liquid and large mass transfer areas. Pressure drop is an indicative of the overall operating cost, sometimes it is an indication of degree of gas-solid interaction. Wetting efficiency is also proportional to the external liquid-solid mass transfer area (Satterfield, 1975)

1.2.1 Flow Regimes

Co-current gas-liquid flow in packed beds adopts a variety of flow morphologies depending on the bed properties and operating conditions. The normal regime of trickle flow is mainly determined by superficial velocities of liquid and gas. For co-current downward flow of liquid and gas through a bed of solid particles flowing four types of regime can be distinguished (Sie & Krishna, 1998).

1. Trickle flow (gas continuous)
2. Pulse flow (unstable regime with partly gas continuous and partly liquid continuous)
3. Dispersed bubble flow
4. Spray flow (gas continuous, highly dispersed liquid)

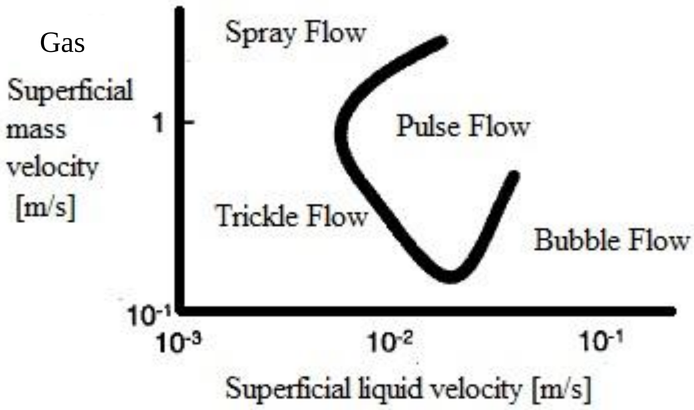


Figure 1.1 Co-current down flow regime in a trickle bed

The precise location of boundary is dependent upon the properties of the fluids and operating conditions. Shift between the trickle-flow and pulse-flow regime caused by increase of operating pressure (Wammes et al, 1990). The region of stable trickle flow also extends to higher velocity as the pressure increases. In trickle flow the catalyst particle tends to be covered by a film of liquid of varying thickness, whereas gas tends to flow through interstitial space which is not occupied by liquid. In the figure 1.2. It demonstrates the tendency of fluid flow in a catalyst bed, where the contact point between the adjacent catalyst particles form pocket for stagnant liquid.

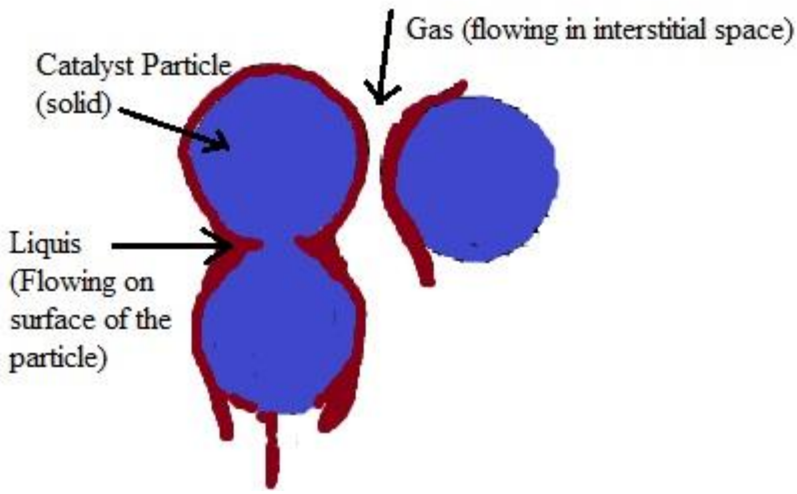


Figure 1.2. Gas and liquid flow pattern in a Trickle-Flow

1.3 Advantages and Dis-advantages of Trickle-Bed Reactor:

The main advantages of trickle-bed reactors are as follows:

- The flow inside a trickle-bed reactor is close to plug flow of gas and liquid phase.
- Small liquid phase holdup compared to slurry or ebulliating-bed reactor; thus suitable for minimizing homogenous liquid phase reactions. (Sie & Krishna, 1998)
- Because of co-current flow of gas and liquid there is no problem of flooding as occurs in counter-current flow.
- The construction of Trickle bed is simple and easy to operate with fixed adiabatic beds. In case of exothermic reaction, the excessive rise in temperature can be limited by liquid or gas recycle.

The main Dis-advantages of trickle-bed reactors are as follows:

- At low liquid velocities mal-distribution, channelling and incomplete catalyst wetting occurs.
- Particle diameter cannot usually be smaller than 1mm because of pressure drop considerations; (Sie & Krishna, 1998)
- Counter-current operation is a preferred mode of operation for high gas-liquid interaction, but not possible at practical velocities due to flooding.
- In trickle-bed, the radial dispersion of heat and mass is a problem. For highly exothermic or endothermic reactions multi-tubular or internally cooled fixed beds are necessary

1.4 Application of Trickle-Bed Reactor:

TBRs have been commonly used in the petroleum industry for many years and are now gaining widespread use in several other fields from bio and electrochemical industries to the remediation of surface and underground water resources, being also recognized for its applications in advanced wastewaters treatments (Rodrigo et al, 2009). Packed bed reactors with multiphase flow have been used in a large number of processes in refinery, fine chemicals and biochemical operations. Effective scale up of bench-scale packed bed reactors in the development of new processes and scale down of the commercial units in the improvement of existing processes have become predominant tasks in the research and development divisions of many companies (Sie & Krishna, 1998). Various processes using trickle bed reactor are:

- Hydro-desulfurization of gas-oil, vacuum gas-oil and residues.
- Hydro-de-nitrogenation of gas-oil and Vacuum gas-oil.
- Hydrocracking of cat-cracked gas-oil and vacuum gas-oil.
- FCC feed Hydro-treating.
- Hydro-metallization of residual oil.
- Hydro-cracking of residual oil.
- Hydro-cracking/Hydro-fining of lubeoils
- Hydro-processing of shale oils
- Paraffin Synthesis by Fischer-Tropsch.
- Oxidative Treatment of Waste water.
- Synthesis of diols.

1.5 Objective of the work:

The aim of the present work could be summarized as follows:

- Study of complex hydrodynamics of Three phase co-current Trickle bed.
- Determining the individual phase holdup in a gas-liquid-solid Trickle bed.
- Analysis of the phase holdup behaviour and various parameters that affect it.
- Examining the effect of superficial gas and liquid velocity on the individual phase holdup.

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 1 m with diameter of 0.194 m has been simulated. Glass beads of diameter 6 mm are used as the solid packing. Gas (Air) is taken as the continuous phase. Liquid (water) and Gas (air) has been injected at the top with different superficial velocities. In all the cases the Solid (Glass bead) volume fraction is taken to be 0.63 with the superficial velocity of gas varying from 0.11-0.22 m/s and that of liquid ranging from 0.003-0.011 m/s. CFD simulations have been carried out using FLUENT 6.3, CFD Software. GAMBIT 2.3.16 has been used to design the Mesh.

CHAPTER 2

LITERATURE REVIEW

2.1 Scope:

A fundamental understanding of the hydrodynamics of trickle-bed reactors is indispensable in their design scale-up and performance. The hydrodynamics are affected differently in each flow regime Three-phase reactors (G-L-S) comprising a fixed bed of catalyst with flowing liquid and gaseous phases have various applications, particularly in the petroleum industry for hydro-processing of oils (e.g. hydro-treating, hydrocracking). Trickle-bed reactors (TBR) are one of the most extensively used three-phase reactors. With a view towards developing more efficient TBR units in the future, for meeting stringent environmental and profitability targets, it is crucial that we develop the know-how for tailoring the flow patterns in them to optimally match the demands made by the kinetics of these reaction processes. One of the critical issues in the efficient use of TBRs is the understanding and prediction of liquid mal-distribution. With current interest in technologies of 'deep' processing, such as Deep-hydrodesulphurization, the need to be able to predict liquid misdistribution accurately is even more important, since small variations in liquid distribution can cause significant loss in activity in trickle-bed reactors operating close to 100% conversion.

In this chapter we will have a comprehensive review of literature related to the various characteristics and factors affecting them in gas-liquid-solid trickle-bed. An overview of the literature relevant to this study is presented next. The first section deals with the experimental works done and the succeeding section deals with the CFD predictions.

2.2 Experimental Review:

Most of the experimental studies on Trickle-bed hydrodynamics were restricted to trickle and pulse flow regimes.

Several aspects of hydrodynamics including flow pattern, gas and liquid holdup, wetting efficiency etc. were thoroughly studied by Satterfield and co-workers.(Satterfield, 1975).

Sundaresan et al (1991) studied the effect of boundary on trickle bed reactor hydrodynamics. They examined the effect of boundaries effect on the hysteresis by taking four different beds with different packing. He studied the effect of superficial liquid and gas velocities on the pressure drop of the column.

Wammes et al (1991) studied the influence of the gas density on the liquid holdup, the pressure drop, and the transition between trickle and pulse flow has been investigated in a trickle-bed reactor at high pressure with nitrogen or helium as the gas phase. Gas-liquid interfacial areas were determined by means of CO, absorption from $C0_2/N_2$ gas mixtures into amine solutions. The gas-liquid interfacial area increases when operating at higher gas densities. They showed that the gas density has a strong influence on the liquid holdup.

Latifi et al (1992) used micro-electrode in a non-conducting wall to determine the flow regime in a trickle bed reactor and analysed the wall wetting by Probability Density Function. He also identified the trickling-pulsing, trickling-dispersed and dispersed-pulsing regime transition.

Wang et al (1995) performed Extensive experimental work with three different gas-liquid systems and three kinds of pickings to examine the influence of various parameters on pressure drop hysteresis, Gas and liquid flow rates, physical properties of liquid and operation modes that influence the behavior of hysteresis in the packed reactor, and liquid flow rate is the most important factor. They found that the hysteresis is not so pronounced for columns packed with large particles and it disappears in the pulsing flow regime and the mechanism responsible for hysteretic behavior resides in the variable uniformity of gas-liquid flow in the packed section. A parallel zone model for pressure drop in the trickling flow regime was established on the basis of experimental facts and analysis of flow structure.

Mao et al (2001) did Extensive experimental work on hysteresis in a concurrent gas–liquid up flow packed bed was carried out with three kinds of packing and the air–water system. Two more liquids with different liquid properties were employed to further examine the influence of parameters on pressure drop hysteresis.

Kundu et al (2001) studied the radial distribution in a trickle bed reactor with five different size of catalytic packing with uniformly distributed liquid inlet.

Trivizadakis et al (2004) worked on two types of catalytic particle packing i. e. spherical and cylindrical extrudes to study co-current down flow in steady state trickling and induced liquid-pulsing mode operation and predicted the mechanical characteristics of trickle bed reactor.

Lange et al (2004) performed experimental and theoretical study of forced unsteady-state operation of trickle-bed reactors in comparison to the steady-state operation. In their study a forced periodic operation of a trickle-bed reactor an unsteady-state technique was used in which the catalyst bed was contacted periodically with different liquid flow rates. The unsteady-state operation was considered as square-waves cycling liquid flow rate at the reactor inlet. They demonstrated that the liquid flow variation has a strong influence on the liquid hold-up oscillation and on the catalyst wetting efficiency.

Gunjal et al (2005) used wall pressure fluctuation measurements to identify prevailing flow regime in trickle beds. Experiments were carried out on two scales of columns (of diameter 10 cm and 20 cm) with two sets of particles (3 mm and 6 mm diameter spherical particles). Effects of pre-wetted and un-wetted bed conditions on pressure drop and liquid holdup were reported for a range of operating conditions.

Maiti et al (2006) made a concise review of the hysteresis in co-current down-flow trickle-bed reactors (TBRs). The effects of several factors on the hysteresis, such as the type of particles (porous/nonporous), the size of the particles, the operating flow ranges, and the start-up conditions (wet/dry) were studied. Also effects of other factors, such as addition of wetting agents (surfactants) and inlet liquid distribution, are also determined. Empirical and theoretical models were developed to predict hysteresis. An attempt was made to understand the comprehensive hysteretic behavior of both porous and nonporous particles with the conceptual framework of hysteresis.

Saroha & Nandi (2008) performed experiment to study the effect of liquid and gas velocity, liquid surface tension, liquid viscosity and particle diameter of the packing in two phase pressure drop hysteresis. An understanding of the hydrodynamics of trickle bed reactors (TBR) is essential for their design and prediction of their performance was made by Saroha et al (2008) on Flow variables, packing characteristics, physical properties of fluids and operation modes influence the behavior of the TBR. The existence of multiple hydrodynamic states or hysteresis (pressure drop, liquid holdup, catalyst wetting, gas--liquid mass transfer) due to the different flow structures in the packed bed was studied. Experiments were performed to study the effect of liquid and gas velocity, liquid surface tension, liquid viscosity and the particle diameter of the packing on two-phase pressure drop hysteresis. He developed the parallel zone model for pressure drop hysteresis in the trickling flow was for analysis of experimental data and flow structure.

2.3 Review of Computational Work

Ellman et al(1988) proposed a new improved correlation for the pressure drop in a trickle-bed reactor derived from fundamental considerations and a wide-ranging data base of some 4600 hydrodynamic experimental results, which can be applicable to industrial trickle-bed reactors since it was based on wide variations of all the important variables, including measurements at high pressures. No other previously derived correlations are applicable to high pressure operations.

Holub et al (1992) developed a phenomenological, pore-scale, hydrodynamic model for representation of the uniform, two-phase, gas-liquid co-current flow in the low interaction regime in trickle bed reactors. The model provided improved predictions for both the pressure drop and liquid holdup using the parameters obtained exclusively for single phase flow data. In addition, a new criterion for prediction of trickle to pulsing flow regime transition was developed based on laminar film stability.

Al-Dahhan et al (1997) reviewed concisely of relevant experimental observations and modeling of high-pressure trickle-bed reactors. He studied flow regime transitions, pressure drop, liquid holdup, gas-liquid interfacial area and mass-transfer coefficient, catalyst wetting efficiency, catalyst dilution with inert fines, and evaluated of trickle bed models for liquid-limited and gas-limited reactions. He discussed the effects of high-pressure operation, which is of industrial relevance, on the physicochemical and fluid dynamic parameters. He developed Empirical and theoretical models to account for the effect of high pressure on the various parameters and phenomena.

Al-Dahhan et al (1998) studied the phenomenological model for pressure drop and liquid holdup at high pressure. They extended the Holub et al (1992) model at atmospheric pressure to under-predict pressure-drop and holdup at high operating pressure.

Attaou and Ferschneider et al. (1999) developed a physical model based on the basic principle to predict the hydrodynamic parameter of steady state trickle-bed reactor operating in trickle flow regime.

Richard et al (2000) worked on equations of flow in porous media such as Darcy's law and the conservation of mass. Their numerical method for solving these equations was based on a total-velocity splitting, sequential formulation which led to an implicit pressure equation and a semi-implicit mass conservation equation. They used high-resolution finite-difference methods to discretize those equations. The solution scheme extended previous work in modeling porous media flows in two ways. First, it incorporate physical effects due to capillary pressure, a nonlinear inlet boundary condition, spatial porosity variations, and inertial effects on phase mobility. They presented a numerical algorithm for accommodating these difficulties, shown the algorithm is second-order accurate, and demonstrated its performance on a number of simplified problems relevant to trickle bed reactor modeling.

Souadnia et al (2001) presented a phenomenological one-dimensional model of a two-phase gas and liquid and gas flow in a trickle bed reactor. Based on some realistic assumptions specific to tickling flow regime, the original equations of continuity and momentum were reformulated in terms of liquid saturation and gas pressure equations. The computational method used was the finite volume technique combined with Godunov's method.

Jiang et al (2001) studied CFD modelling of multiphase flow distribution in packed bed reactor by implementing pseudo-randomly assigned cell porosity within certain constraints.

Gunjal et al (2005) developed a comprehensive CFD model to predict measured hydrodynamic parameters. The model was evaluated by comparing predictions with the experimental data from their previous experiment. The CFD model was then extended to predict the fraction of liquid holdup suspended in the form of drops in the bed. At the end, the CFD model was used to understand hydrodynamics of trickle beds with periodic operation.

Rodrigo et al (2007) has worked on various computational models to describe the hydrodynamics behavior of trickle-bed reactor. Their study incorporate most recent multiphase model in order to investigate the hydrodynamics behavior of a TBR in terms of pressure drop and liquid holdup.

Boyer & Ferschneider (2007) validated the mechanistic model of Attou et al (1999) and improved it with a new formulation for liquid film.

Lappalainen et al (2008) tried to develop a improved hydrodynamic model based on earlier work by Alopaeus et al (2006) for estimating wetting efficiency, pressure drop and liquid holdup in trickle- bed reactor.

Ookawara et al (2007) proposed a high-fidelity DEM-CFD model for process intensification of packed bed reactors. The discrete element method (DEM) was employed for simulating random packing under gravity with hundreds of spheres in a cylindrical tube. It was verified that the DEM is capable of constituting a packed bed according to particle-to-tube diameter ratio. It was shown that the pressure loss through the bed sufficiently agrees with a correlation that was taken into account the particle-to-tube diameter ratio. Subsequently to the validation, the model capability for process intensification was conceptually demonstrated by specifying arbitrary boundary condition on each particle. Particles simulating inert are mixed among hot catalytic particles in laminar and random blending manners. It was confirmed that the blending style significantly affects the temperature distribution in the bed. it was a design to optimize by the high-fidelity DEM-CFD model.

Arnab et al (2007) modelled a three dimensional CFD simulation for two-phase flow in trickle-bed reactor based on porous media concept by describing the flow domain as a porous media to understand the liquid mal-distribution.

Using 3-D Eulerian k-fluid model.(Rodrigo et al, 2007). developed multiphase volume of fluid (VOF) model to provide a more detailed understanding of transient behavior of a laboratory scale trickle bed reactor. (Rodrigo et al, 2010). They also studied the transition from trickle flow regime to pulse flow regime and several parameters that characterize the pulse flow regime by means of a Eulerian CFD method.

The various models proposed for Trickle-Bed reactor can be summarized below:

Table 2.1: Various Models Proposed for Trickle-bed Reactor

Earlier Models	**Adopted by:**	**Work done:**
Diffusion model	Stanek and Szekely (1974)	The model is formulated to solve the equations of flow and diffusion, but effect of gas–liquid interactions is neglected
Model based on concept of relative permeability: The relative permeability model	Saez and Carbonell (1985)	Drag force is calculated by using the concept of relative permeability of each phase
Slit models Single slit model	Holub et al. (1992)	Local flow of liquid and gas around the particles is modeled by assuming flow in rectangular inclined slits of width related to void fraction of the medium
Double slit model	Iliuta et al. (2000)	Holub's model is extended to allow for a distribution of slits that are totally dry in

		addition to slits that have liquid flow along the wall
The interfacial force model The fluid–fluid interfacial force model	Attou et al. (1999)	The drag force on each phase has contribution from the particle–fluid interaction as well as from the fluid–fluid interaction
Recent 'CFD-based' models Porous media model	(1) Anderson and Sapre (1991) (2) Souadnia and Latifi (2001) (3) Atta et al. (2007)	The drag exchange coefficients are obtained from the relative permeability concept developed by Saez and Carbonell (1985)
k-fluid model	(1) Jiang et al. (2002) (2) Gunjal et al. (2003, 2005)	The drag exchange coefficients are obtained from the fluid–fluid interfacial force model

CHAPTER 3

CFD METHODOLOGY IN MULTIPHASE FLOW

3.1 Computational Fluid Dynamics

CFD is a branch of fluid mechanics that deals with the study of fluid flow problems by analysing the problem using Numerical methods and Algorithms. Navier–Stokes equations form the fundamental basis of almost all CFD problems which define any single-phase fluid flow. These equations can be simplified by removing terms describing viscosity to yield the Euler equations. Further simplification, by removing terms describing vorticity yields the full potential equations. They can be linearized to yield the linearized potential equations. Computers are used to perform numerous calculations involved using softwares such as Fluent, CFX. Even with simplified equations and high speed supercomputers, in many cases only approximate solutions can be achieved. More accurate codes are written that can accurately and quickly simulate even complex scenarios such as supersonic or turbulent flows.

3.2 Advantages of CFD

CFD has been used extensively in last few decades because of development of fast processors and memory storage capability of computers. This technology has widely been applied to various engineering applications such as automobile and aircraft design, weather science, civil engineering process engineering, and oceanography. It allows us to design and simulate any real systems without having to design it practically. CFD analysis enables us to virtually sneak inside the design and see how it performs. CFD gives a deep perception into the designs hence it reduces the time of prototype production and testing, leading to a successful glitch free design. Using CFD we can built our own desired design and have a closed look inside it. A key advantage of CFD is that researchers can evaluate the performance of any practical system on the computer without the time, expense, and they can make necessary changes onsite. After our required design is built, we apply the fluid flow physics and chemistry to this virtual model and correspondingly the software will output a prediction of fluid dynamics and related physical phenomena (Kumar., 2009). Once the simulation is done then various parameters like temperature, pressure, mass fraction etc. can be analysed. Some of the main advantages of CFD can be summarized as:

1. It is always not possible to design a working model and test its performance and glitches. CFD is very much helpful in this regard.
2. CFD simulation doesn't have a size and scale restriction. It can simulate large capacity plant. 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. It therefore costs less than laboratory or field experiments, thereby allowing engineers to try and develop something alternate which will be feasible.
4. It gives the results in a very short time 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

3.3 Governing Equations in Computational Fluid Dynamics

For all flows, conservation equations for mass and momentum are to be solved. For flows involving heat transfer or compressibility, an additional equation for energy conservation is solved. They are the mathematical statements of three fundamental physical principles upon which all of fluid dynamics is based (Anderson J. D., 2009):

(1) Mass is conserved;

(2) F = ma (Newton's second law);

(3) Energy is conserved.

3.3.3 Boundary Conditions

For most of the fluid flow problem the basic governing equations remain the same but boundary conditions differs according to the situations and gives shape to the solutions. The boundary conditions as well as the initial conditions set by the user decided the fate of the solution obtained from the governing equations.

3.4 How CFD Code Works

There are three steps for solving a CFD problem:

1. Pre-processing
2. Solver
3. Post-processing

3.4.1 Pre-processing

This is the first step in solving any CFD problem. It basically involves designing and building the domain. It involves the following steps (Bakker. 2002):

- Definition of the geometry of the region: The computational domain.

- Grid generation the subdivision of the domain into a number of smaller, non-overlapping sub domains (or control volumes or elements Selection of physical or chemical phenomena that need to be modelled).

- Definition of fluid properties.

- Specification of appropriate boundary conditions at cells, which coincide with or touch the boundary. The solution to a flow problem (velocity, pressure, temperature etc.) is defined at nodes inside each cell. The accuracy of a CFD solution is governed by the number of cells in the grid. Optimal meshes are often non-uniform: finer in areas where large variations occur from point to point and coarser in regions with relatively little change. Over *50%* of the time spent in industry on a CFD project is devoted to the definition of the domain geometry and grid generation. GAMBIT, T-GRID is some of the software used in pre-processing.

3.4.2 Solver

After the geometry has been made then the next step is to do the flow calculations. CFD solver does the flow calculations and displays the results obtained. FLUENT, FloWizard, FIDAP, CFX and POLYFLOW are some of the types of solvers. Numerous iterations are performed till the solution converges and the results obtained. The first step is the setting of the under relaxation factors which are essential for the solution convergence as wrong or improper under relaxation factors can hamper the convergence. Initialization of the solution is also as important as setting under relaxation factors because it helps the solver to assume some initial values required to solve the governing equations involved.

ANSYS has developed two solvers namely FLUENT and CFX. They are high precision solvers and rely heavily on a pressure-based solution technique for broad applicability. The CFX solver uses finite elements (cell vertex numeric), similar to those used in mechanical analysis, to discretize the domain. In contrast, the FLUENT solver uses finite volumes (cell cantered numeric). CFX software focuses on one approach to solve the governing equations of motion (coupled algebraic multigrid), while the FLUENT product offers several solution approaches (density-, segregated- and coupled-pressure-based methods) (Kumar., 2009).

Navier–Stokes equations form the backbone in CFD codes and its solution usually relies on a discretization method: it means that derivatives in partial differential equations are approximated by algebraic expressions which can be alternatively obtained by means of the finite-difference or the finite-element method. Fluent mainly uses finite volume method for discretization. The governing equations predicted at discrete points in the domain and several iterations are carried till convergence as follows (Ravelli et al., 2008):

(1) Fluid properties are updated in relation to the current solution; if the calculation is at the first iteration, the fluid properties are updated consistent with the initialized solution.

(2) The three momentum equations are solved consecutively using the current value for pressure so as to update the velocity field.

(3) Since the velocities obtained in the previous step may not satisfy the continuity equation, one more equation for the pressure correction is derived from the continuity equation and the linearized momentum equations: once solved, it gives the correct pressure so that continuity is satisfied. The pressure–velocity coupling is made by the SIMPLE algorithm, as in FLUENT default options.

(4) Other equations for scalar quantities such as turbulence, chemical species and radiation are solved using the previously updated value of the other variables; when inter-phase coupling is to be considered, the source terms in the appropriate continuous phase equations have to be updated with a discrete phase trajectory calculation.

(5) Finally, the convergence of the equations set is checked and all the procedure is repeated until convergence criteria are met.

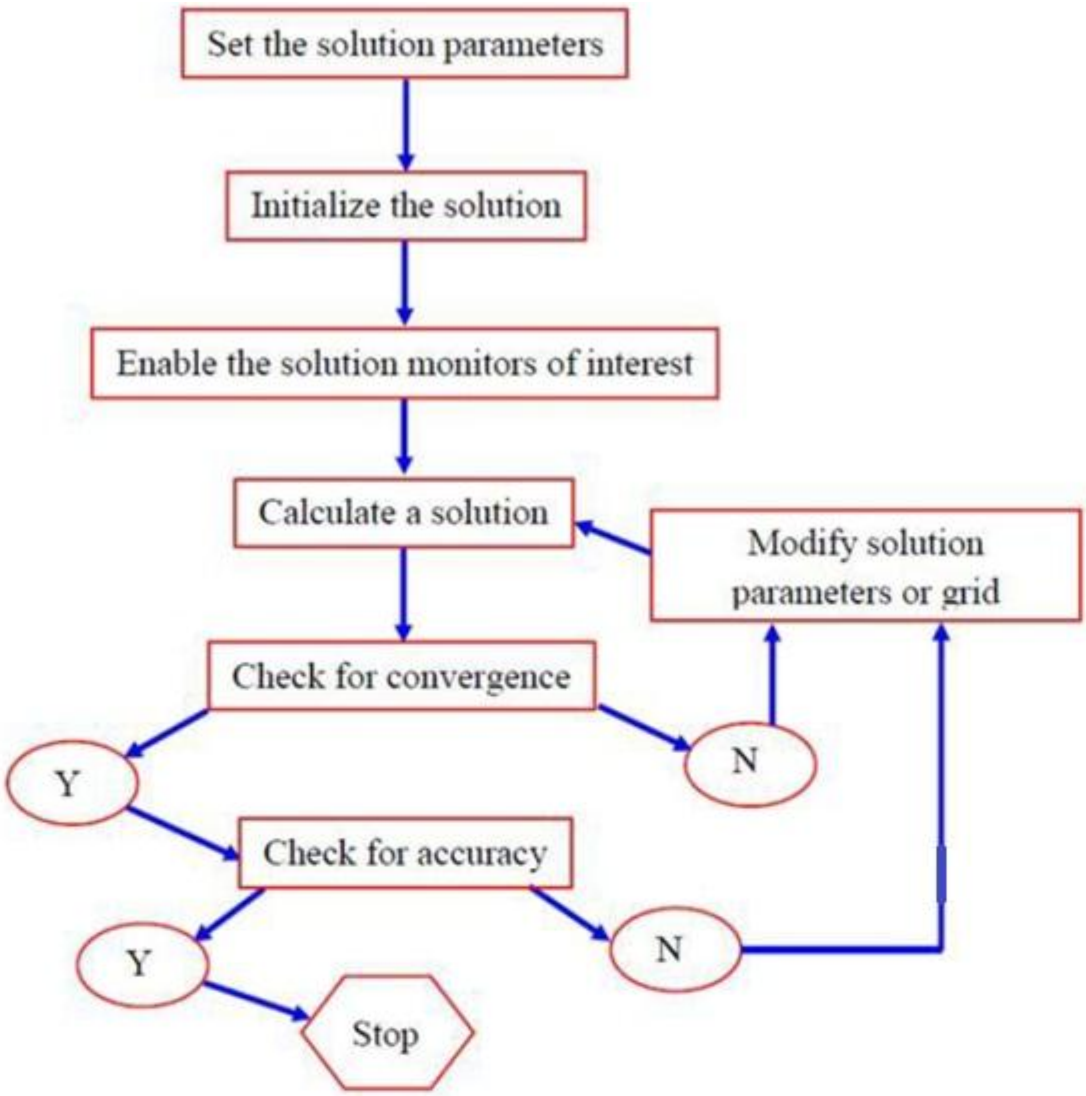


Fig. 3.1 Flowchart showing the general procedure for the simulation using Fluent (Kumar, 2009)

3.4.3 Post- processing

This is the last step and it consists of analysing the data obtained. FLUENT provides all sorts of post processing tools and the simulation results can be interpreted and analysed using various plots and tools. It includes:

- Domain geometry and grid display
- Vector plots
- Line and shaded contour plots
- 2D and 3D surface plots
- Particle tracking
- Animation for dynamic result

3.5 CFD Approaches in Multiphase Flows

Currently there are two approaches for the numerical calculation of multiphase flows: the Euler-Lagrange approach and the Euler-Euler approach.

1. The Euler-Lagrange Approach
2. The Euler-Euler approach

3.5.1 The Euler-Lagrange Approach

The Lagrangian discrete phases model in FLUENT follows the Euler-Lagrange approach. The fluid phase is treated as a continuum by solving the time-averaged Navier-Stokes equations, while the dispersed phase is solved by tracking a large number of particles, bubbles, or droplets through the calculated flow field. The dispersed phase can exchange momentum, mass, and energy with the fluid phase. A fundamental assumption made in this model is that the dispersed second phase occupies a low volume fraction, even though high mass loading ($m_{particles} \geq m_{fluid}$) is acceptable. The particle or droplet trajectories are computed individually at specified intervals during the fluid phase calculation. This makes the model appropriate for the modelling of spray dryers, coal and liquid fuel combustion, and some particle-laden flows, but inappropriate for the modelling of liquid-liquid mixtures, fluidized beds, or any application where the volume fraction of the second phase is not negligible (Fluent. 2006).

3.5.2 The Euler-Euler Approach

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 FLUENT, three different Euler-Euler multiphase models are available: the volume of fluid (VOF) model, the mixture model, and the Eulerian model (Fluent. 2006).

1. The VOF Model

The VOF model is a surface-tracking technique applied to a fixed Eulerian mesh. It is designed for two or more immiscible fluids where the position of the interface between the fluids is of interest. In the VOF model, a single set of momentum equations is shared by the fluids, and the volume fraction of each of the fluids in each computational cell is tracked throughout the domain. Applications of the VOF model include stratified flows, free-surface flows, filling, sloshing, the motion of large bubbles in a liquid, the motion of liquid after a dam break, the prediction of jet breakup (surface tension), and the steady or transient tracking of any liquid-gas interface.

2. The Mixture Model

The mixture model is designed for two or more phases (fluid or particulate). As in the Eulerian model, the phases are treated as interpenetrating continua. The mixture model solves for the mixture momentum equation and prescribes relative velocities to describe the dispersed phases. Applications of the mixture model include particle-laden flows with low loading, bubbly flows, sedimentation, and cyclone separators. The mixture model can also be used without relative velocities for the dispersed phases to model homogeneous multiphase flow.

3. The Eulerian Model

It is the most complex of the multiphase models in 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 modelled. 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.

3.6 Some Multiphase Systems

Some examples of multiphase flow systems are as follows:

- Fluidized bed examples: fluidized bed reactors, circulating fluidized beds.
- Trickle-bed Reactor
- Slurry flow examples: slurry transport, mineral processing.
- Particle-laden flow examples: cyclone separators, air classifiers, dust collectors, and dust-laden environmental flows.
- Stratified/free-surface flow examples: sloshing in offshore separator devices, boiling and condensation in nuclear reactors.
- Pneumatic transport examples: transport of cement, grains, and metal powders.

3.7 Choosing a Multiphase Model

The multiphase models vary for variety of the problems. Some guidelines for deciding the multiphase models are (Fluent., 2006):

- Discrete phase model is used for bubbly, droplet, and particle-laden flows in which the dispersed-phase volume fractions are less than or equal to 10%.
- Mixture model or the Eulerian model is used for bubbly, droplet, and particle-laden flows in which the phases mix and/or dispersed-phase volume fractions exceed 10%.
- For slug flows VOF model is used.
- For stratified/free-surface flows VOF model is used.
- For pneumatic transport, use the mixture model for homogeneous flow or the Eulerian model for granular flow.

CHAPTER 4

CFD SIMULATION OF THREE PHASE CO-CURRENT TRICKLE-BED

4.1 Computational Flow Model

A two–dimensional Eulerian three phase model is implemented in the present work where gas phase is treated as continuous, inter-penetrating and interacting everywhere within the computational domain. The pressure field is assumed to be shared predominantly by air as the liquid flow velocity is in trickle flow regime and it flow under the influence of gravity and shear force exerted by the flowing gas. The motion of liquid and gas phase is governed by the respective mass and momentum 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 fixed to zero via a user interface command.

4.1.1 Equation Reformulation:

4.4.1.1 The Mass Conservation Equation

The equation for conservation of mass, or continuity equation, can be written as follows:

$$\frac{\delta}{\delta t}(\alpha_k \rho_k) + \nabla(\alpha_k \rho_k U_k) = 0$$

Where ρ_k is the density and α_k is the volume fraction of phase k=g, l

and the volume fraction of the two phases satisfy the following condition:

$$\alpha_g + \alpha_l = 1$$

4.4.1.2 Momentum Equations

For liquid phase

$$\frac{\delta}{\delta t}(\rho_l \alpha_l U_l) + \nabla(\rho_l \alpha_l U_l u_l) = -\alpha_l \Delta P + \nabla(\alpha_l \mu_{eff,l} (\nabla U_l + U_l^T)) + \rho_l \alpha_l g + M_{i,l}$$

For gas phase

$$\frac{\delta}{\delta t}(\rho_g\, \alpha_g U_g) + \nabla(\rho_g\, \alpha_g U_g U_g) = -\, \alpha_g \Delta P + \nabla(\alpha_g\, \mu_{eff,g}\, (\nabla U_g + U_g^{T})) + \rho_g\, \alpha_g g + M_{i,g}$$

P is the pressure and μ_{eff} is the effective viscosity. The terms $M_{i,l}$ and $M_{i,g}$ of the above momentum equations represent the interphase force term for liquid, gas and solid phase, respectively.

4.1.2 Turbulence Modeling:

Standard k-ε model is used which include standard version of two equation model that involves transport equations for the Turbulent Kinetic Energy k, and its dissipation rate ε. The exact turbulence modeling equation can be derived by simplifying Navier- Stokes equation. The k - epsilon model consists of the turbulent kinetic energy equation. Its popularity in industrial flow and heat transfer simulations is because of robustness, economy, and reasonable accuracy for a wide range of turbulent flows. It is a semi-empirical model, and the derivation of the model equations relies on phenomenological considerations and empiricism (Fluent. 2006).

Table 4.1: The model constants used for turbulence modeling

Cmu	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

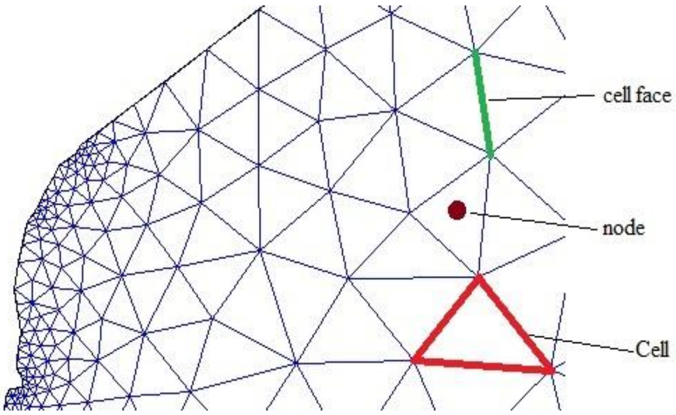
4.2 Problem description for the Simulation:

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 6 mm in this case. The gas and liquid are sent co-currently downward from the top with different superficial velocities. The gas velocities vary from 0.11m/s to 0.22 m/s and liquid velocities varies from 0.003 m/s to 0.011 m/s. The velocity of both the phases lies in the trickle flow regime.

Table 4.2 Properties of air and Water

Phases	**Density, Kg/m^3**	**Viscosity, kg/m-s**
Air	1.225	1.789*10-05
Water	998.2	0.001003

4.3 Geometry and Mesh



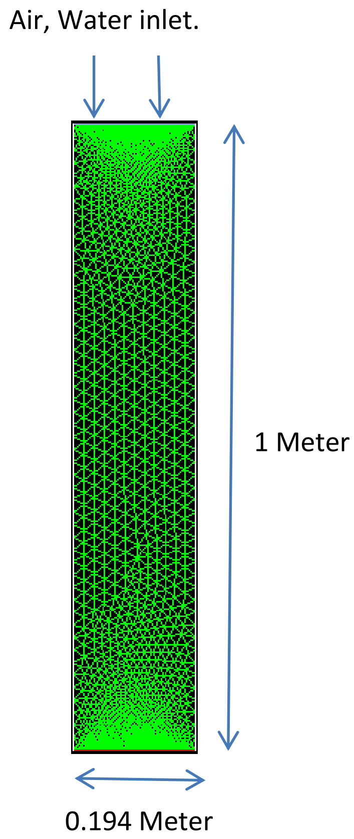


Figure 4.1 The unstructured grid developed for the simulation

GAMBIT 2.2.30 was used for making 2D rectangular geometry of width of 0.194m and height 1m. Coarse triangular unstructured mesh size is used for the whole geometry for better adoptability to the geometry. It consists of 3258 triangular cells, 100 -2D wall faces, 4787 -2D interior faces with 1730 nodes.

4.4 Assumptions:

- Both the fluids are incompressible
- The trickling flow regime is considered, i.e. the gas-liquid interaction are low, so capillary pressure force can be neglected. We assume same pressure for both phases at any time and space.
- There is no inter-phase mass transfer
- The pressure drop across the bed is due to gas phase only, as liquid undergo trickle flow and play a little role here.
- The inertial, viscous and pseudo-turbulence terms are neglected compared to the drag force terms.
- The porosity is uniform and constant.

4.5 Solution:

The above sets of equations were solved using commercial software FLUENT 6.3.26 (of ANSYS Inc., USA) with a two-dimensional Eularian three-phase model considering the flow domain as granular. The gas phase was treated as primary phase and liquid phase was considered as secondary phase. At the inlet, flat velocity profile for gas and liquid phases was assumed and implemented. No slip boundary condition was set for all the impermeable reactor walls. At the bottom of the column, an outlet boundary condition was specified. With mixture gauge pressure at 0 Pascal and back flow volume fraction for air is 0.Unsteady state simulations were carried out with the time step of 0.001 s. Many workers adopted different models and drag force formulation mentioned in table 2.1. In the present work Granular multiphase flow is adopted and the drag force adopted between the three phases are mentioned in table 4.2 (Fluent, 2006).

Table 4.3: Models used for considering Force interactions among phases.

Interactions	**Model**
Solid-Air	Gidaspow
Solid-Water	Gidaspow
Air- Water	Schiller-Naumann

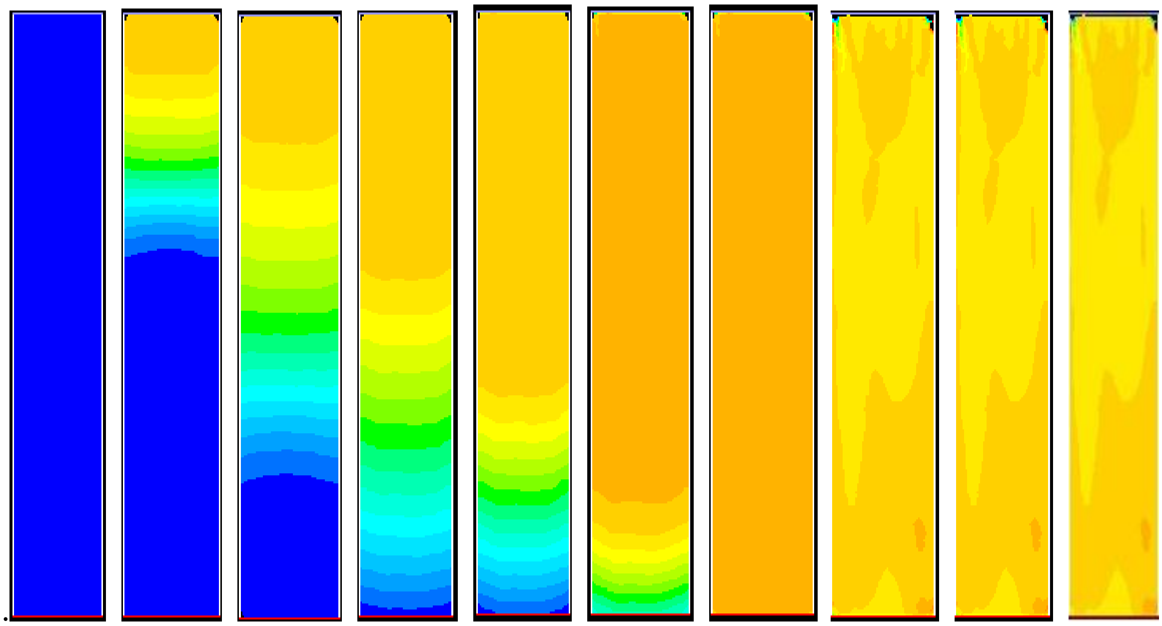
Table 4.4 Solution Control Parameters:

Discretization Scheme	First Order UPWIND
Pressure-Velocity coupling	SIMPLE algorithm
Relaxation Parameters: Pressure Density Momentum Volume fraction Body force Turbulent Kinetic Energy Turbulent Dissipationa Rate	 0.6 1 0.2 0.2 1 0.2 0.2

CHAPTER 5

RESULTS & DISCUSSION

Simulation has been carried out for three-phase Trickle Bed Reactor of 1 m height and 0.194 m diameter as described in chapter-4. 6 mm glass beads have been used as the packing material. At the top of the column uniform fluid distribution was taken considering an ideal distributor. The simulations were performed until a quasi-steady state is reached and no further change in the bed was observed.



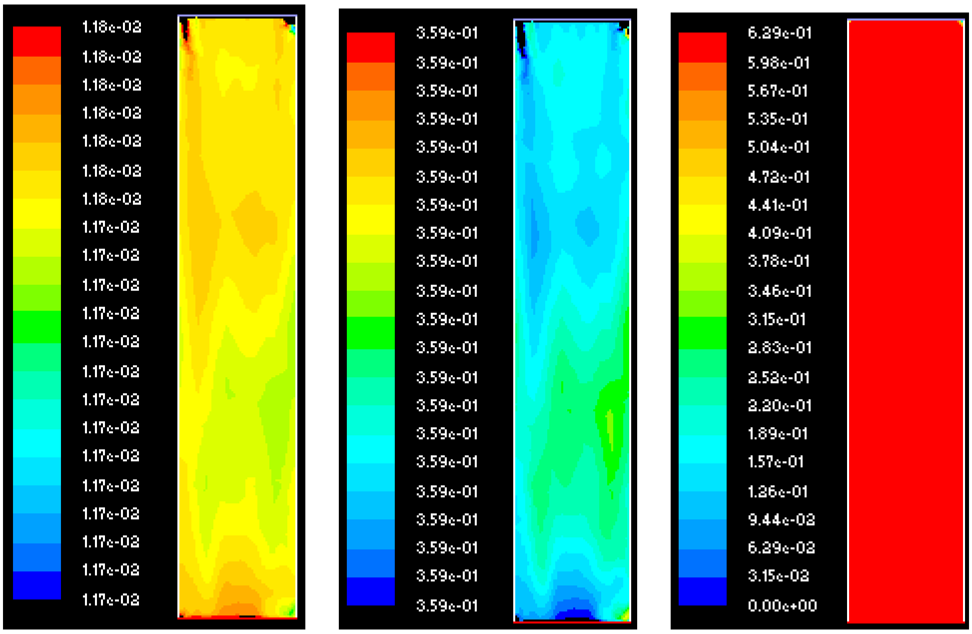
0 sec 5 sec 10 sec 20 sec 30 sec 40 sec 50 sec 60 sec 70 sec 80 sec

Figure 5.1: Contour of volume fraction of air for air velocity 0.14 m/s and liquid velocity 0.009 m/s.

Figure 5.1 shows the change in gas phase volume fraction with time until quasi steady state is reached. Initially an abrupt change in the volume fraction of all the gas and liquid phase were observed. The quasi steady state was reached after 60 sec and no further change in the contour were observed in the bed

5.1 Phase Dynamics:

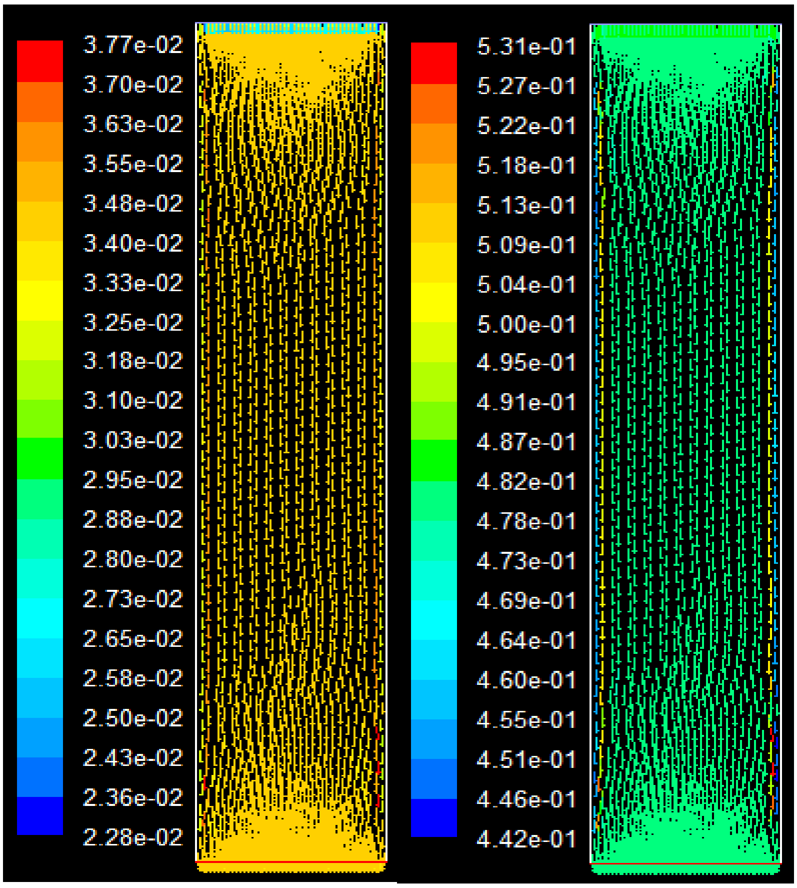
Figure 5.2 shows the contour of all the three phases in the bed volume after reaching the quasi steady state. The contour shows the volume fraction of respective phases and their distribution. The figures indicate that most of the porous region is occupied by the gas phase. Here gas phase is the continuous phase and liquid phase undergo a trickle flow over the particle surface. The contour for solid phase demonstrates the uniform distribution of particle through the bed maintaining a uniform porosity.



Liquid Gas Solid

Figure 5.2: Contour of volume fraction of liquid, gas and solid phase at gas velocity of 0.11m/s and liquid velocity of 0.005m/s.

The figure 5.3 shows the velocity vector of liquid and gas at liquid velocity of 0.009m/s and gas velocity of 0.18m/s. The color of the vector shows the velocity magnitude. The density of the vector is more near the inlet and outlet according to the grid density. The reddish appearance of velocity vector near the wall show slight increase in velocity of fluid may be due to increase in porosity near the wall; however it again decreases may be due to wall effect.



Water Air

Figure 5.3: velocity vector of water and Air

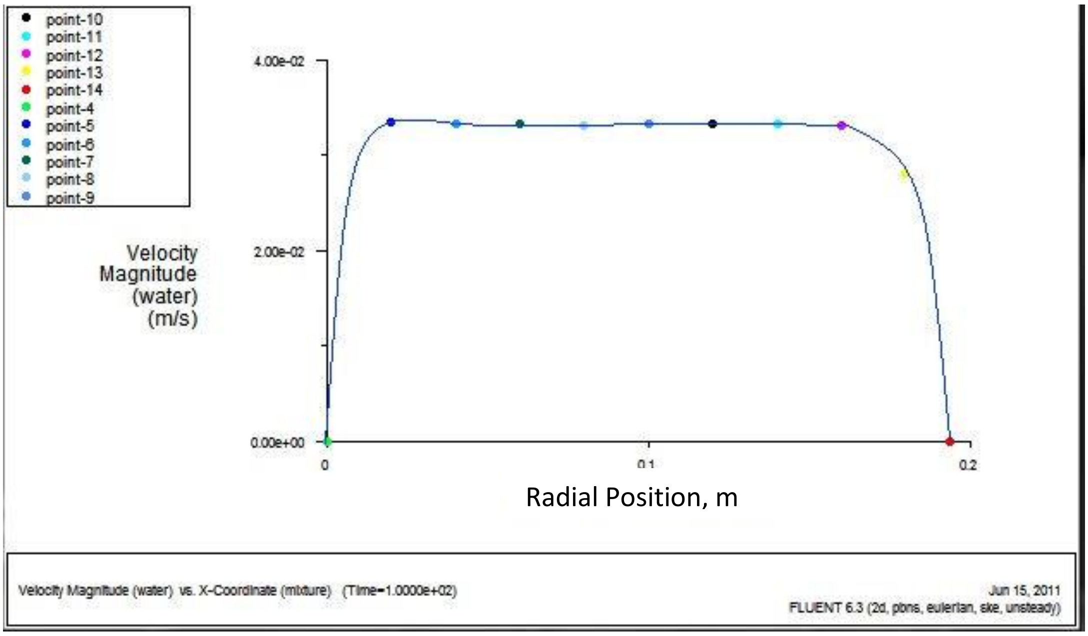


Figure 5.4 Radial variation of velocity of liquid at a height of Z=0.5 m at gas velocity of 0.2m/s

The plot in figure 5.4 shows the velocity profile of liquid along the radial direction at gas velocity of 0.2m/s. Although uniform porosity is assumed throughout the bed still porosity near the wall is always higher than the bulk porosity. For the same reason fluid velocity tends to increase in that region.

5.1.1 Liquid holdup:

Liquid holdup is an important parameter in the hydrodynamics study of Trickle Bed Reactor. With increase in liquid velocity an increase in liquid holdup is observed, however it decreases with gas velocity. The variation of liquid holdup behavior with change in liquid velocity and gas velocity is shown in figures 5.5 and 5.6 respectively.

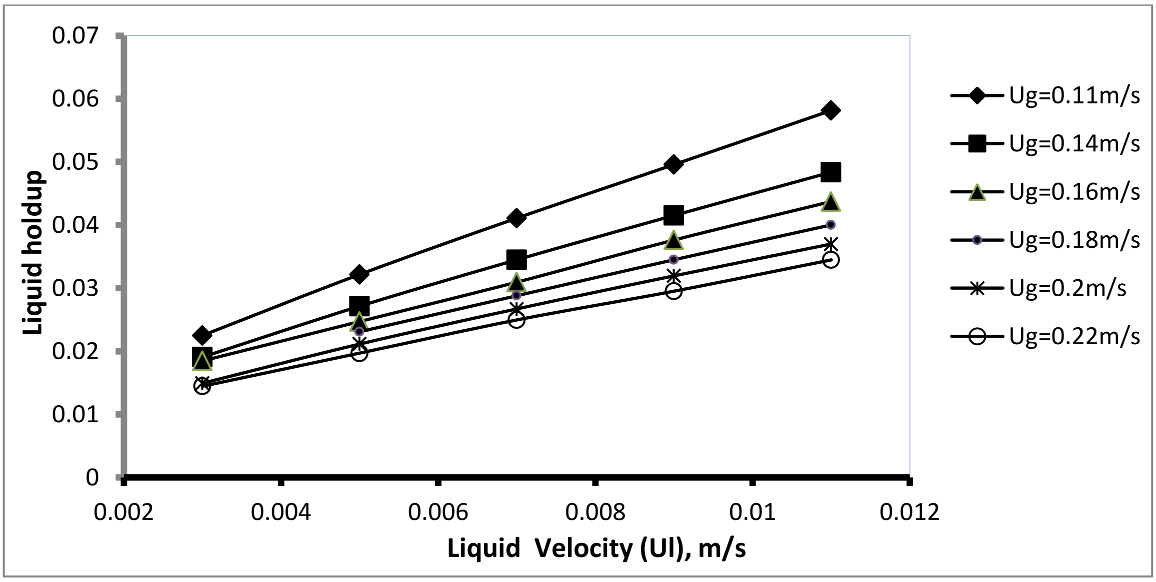


Figure 5.5: liquid holdup for different liquid velocity.

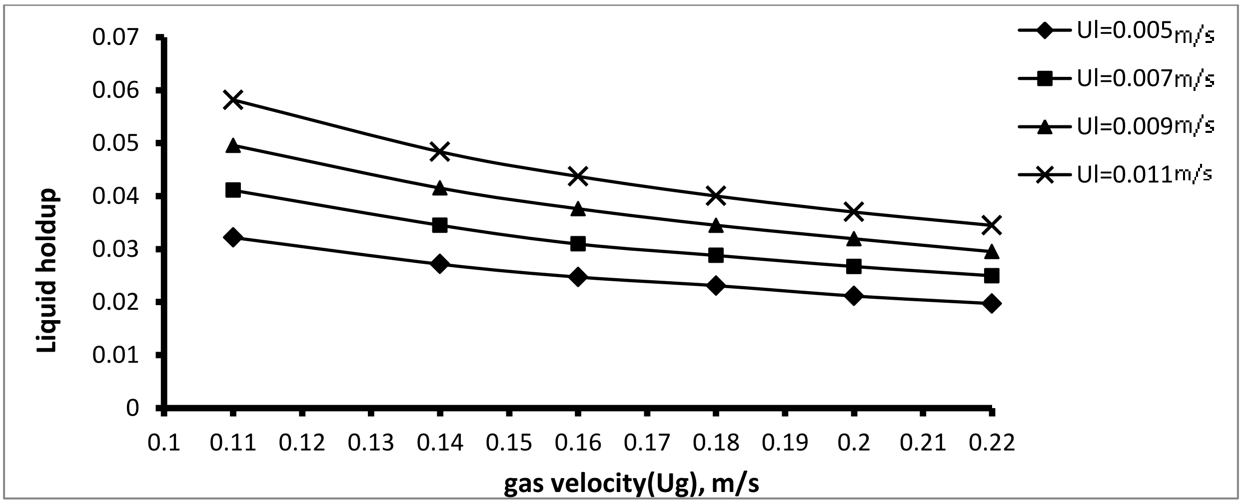


Figure 5.6: liquid holdup for different gas velocity.

Radial averaged liquid holdup was calculated at ten different heights across the bed and their cumulative averages were plotted with various flow conditions. It is an obvious observation that liquid holdup increases with increase in liquid velocity, but it decrease with increase in gas velocity, which is clearly observed in the figure 5.6.

The Figure 5.7 shows the liquid saturation along the length of the column. Radial averaged liquid holdup were calculated at each 0.1 meter interval of height and plotted in the graph. The variation of liquid holdup behavior along the height of the column for two different liquid velocities was shown in the figure 5.7.

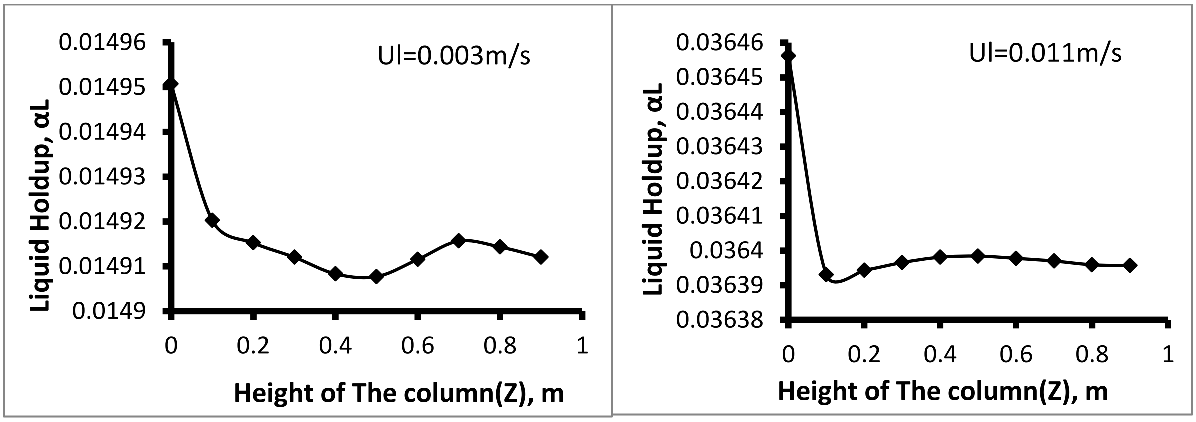


Figure 5.7: Liquid Holdup variation with Height of the column at liquid velocity of 0.003m/s and 0.011m/s.(gas velocity= 0.2m/s)

In both cases the liquid holdup is more at the bottom part of the column. The gradient is more prominent for lower liquid velocities and almost equal distribution is observed at higher liquid velocities. The liquid saturation shows a gradient when operated at lower liquid velocity of 0.003m/s however it shows a flat profile along the length of the column when the velocity is increased to 0.011m/s.

figures 5.8(a) and 5.8 (b) show the radial distribution of liquid at different height of the column. Liquid holdup along the cross section were observed at three different height i.e 0.25m, 0.5m, 0.75m for two different gas velocities. In both the cases the liquid saturation is uniform at the distributor and gradually the liquid saturation increases at the center and tends to decrease near the wall.

Comparison of the two sets of figure revels that the variation in liquid saturation along the diameter is more in case of lower gas velocity i.e. 0.11m/s but the variation is not so prominent at higher gas velocity i.e. 0.20 m/s.

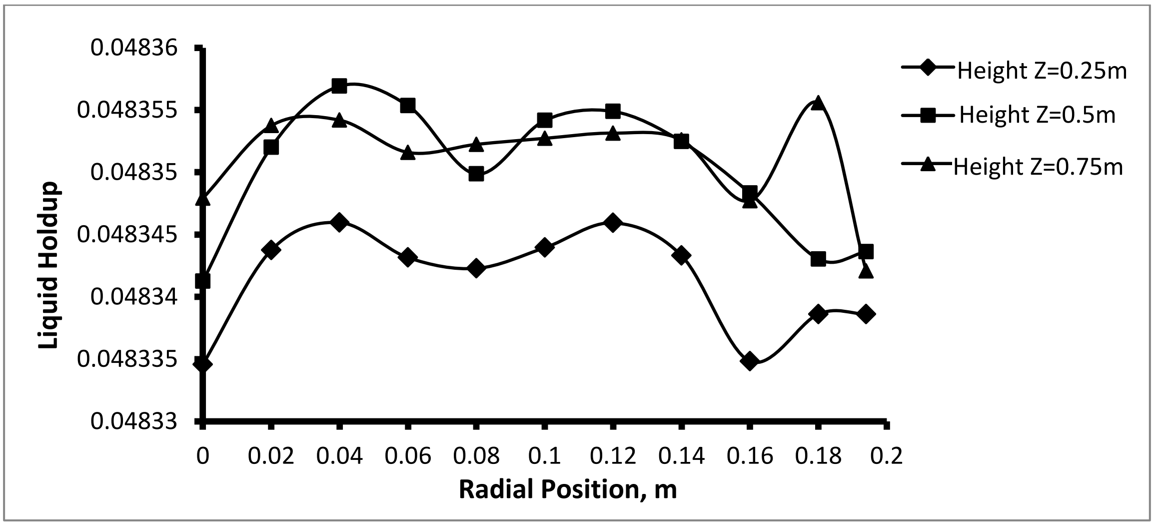


Figure 5.8 (a) Radial Averaged Liquid Holdup variation along the diameter of the column at different height at gas velocity of 0.11m/s and liquid velocity 0.009 m/s

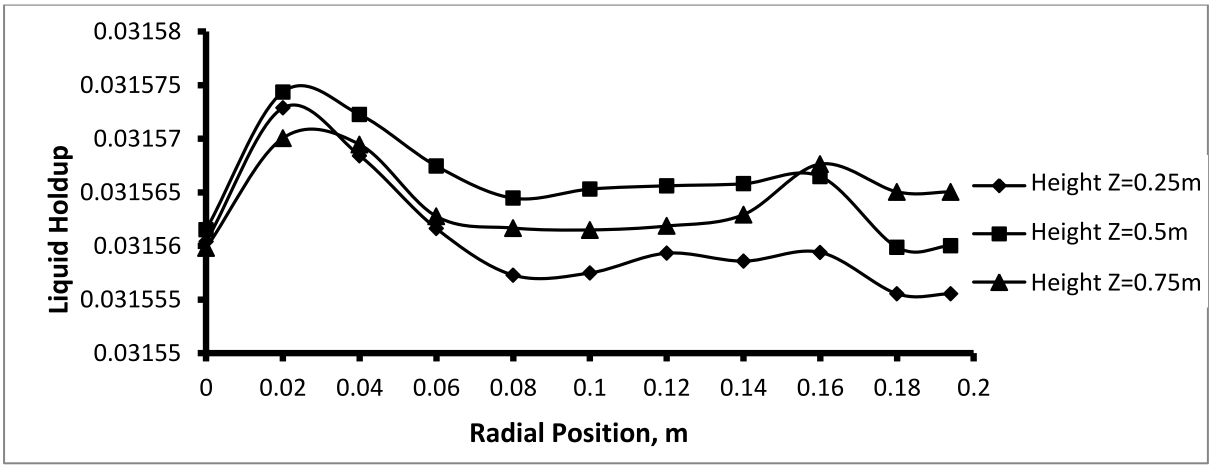


Figure 5.8(b) Radial Averaged Liquid Holdup variation along the diameter of the column at different height at gas velocity of 0.20m/s and liquid velocity 0.009 m/s.

5.1.2 Gas Holdup

Gas holdup is obtained as mean area-weight average of volume fraction of the gas phase at sufficient number of axial positions in the Trickle bed reactor. The variation of gas holdup with superficial liquid velocity obtained from CFD simulation is shown in figure 5.9. The Graph shows a decrease in gas holdup with liquid velocity. The experimental data form Gunjal et al (2005) and other workers also shows the similar tendency of the gas holdup in literature

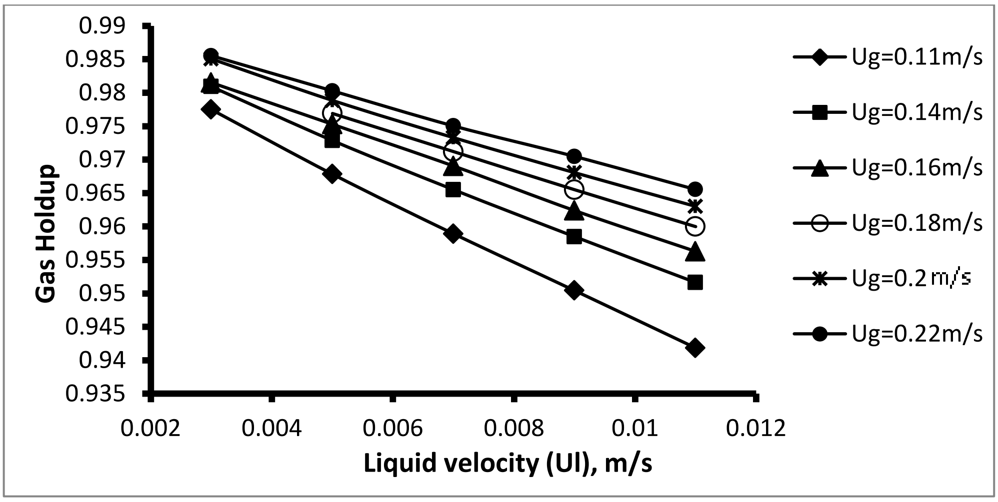


Figure 5.9: Gas holdup for different liquid velocity

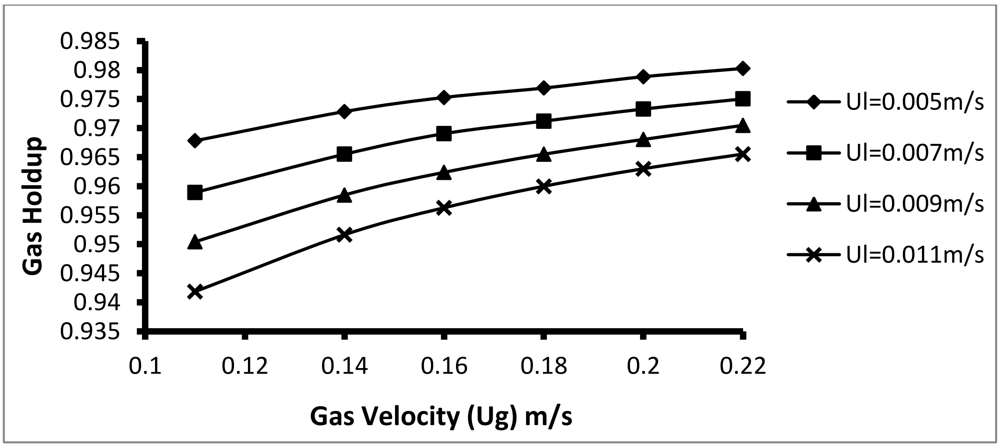


Figure 5.9: Gas holdup for different gas velocity

When gas velocity is increased the gas holdup in the trickle bed reactor increases. This tendency is shown in figure 5.9; it may be because more amount of volumetric gas is flowing when gas velocity is increased. Since the flow domain has a constant porosity, the phase holdup of gas and solid are inter-dependent.

The gas holdup behavior along the height of the column for two different liquid velocities was shown in the figure 5.10. In both cases the liquid holdup is more at the bottom part of the column. The gradient is more prominent for lower liquid flow rate and almost equal distribution is observed at higher liquid flow rate. The possible reason may be because gas has a resistance to flow downward in comparison to liquid, because of its low density.

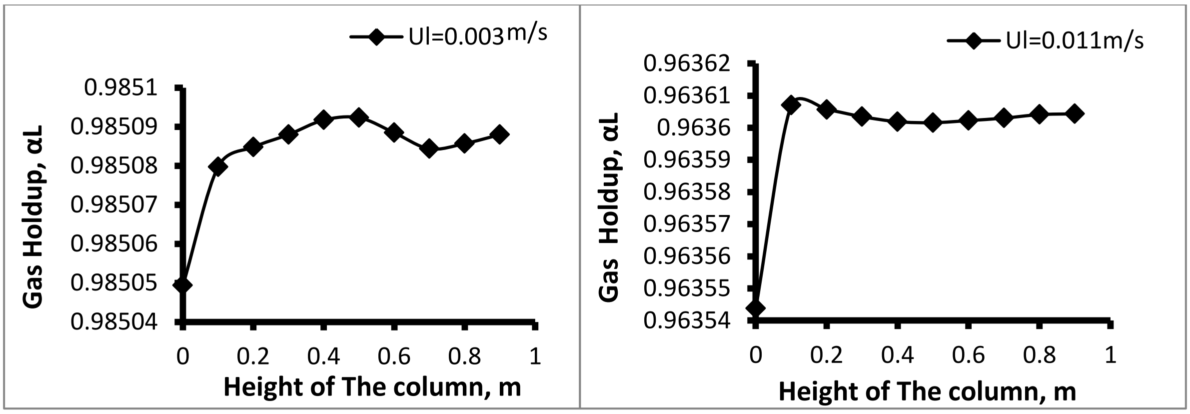


Figure 5.10: Gas Holdup variation with Height of the column at liquid velocity of 0.003m/s and 0.011m/s. (gas velocity= 0.2m/s)

Figures 5.11(a) and (b) show the radial variation of gas holdup at different hights of the column at two different liquid velocities. At low liquid velocity the variation of gas holdup is more prominent than the corresponding high liquid velocity

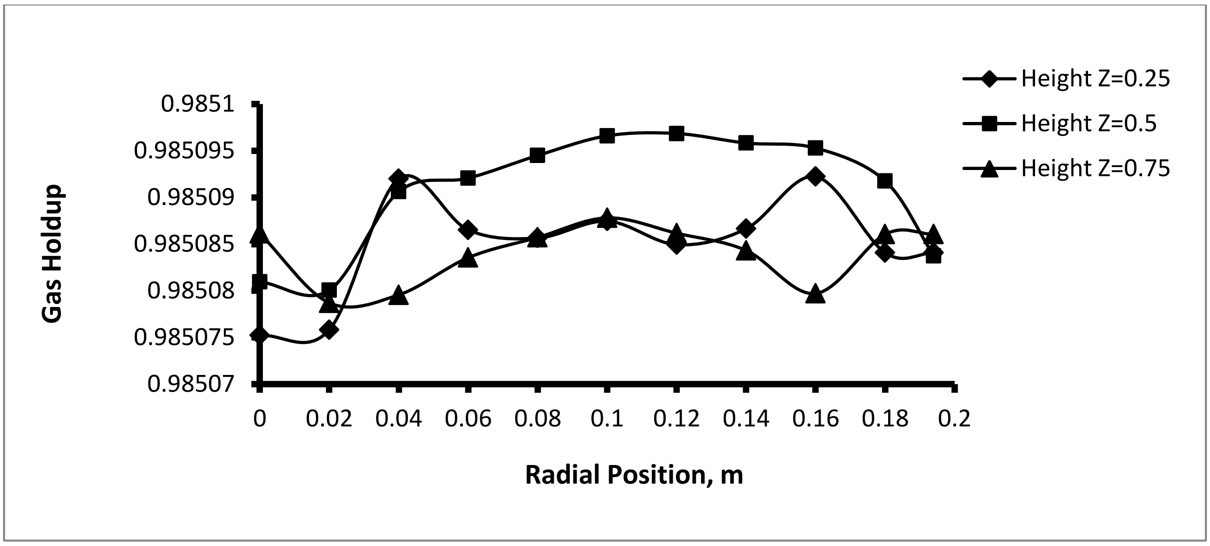


Figure 5.11(a) Gas Holdup variation along the diameter of the column at different height at gas velocity of 0.20m/s and liquid velocity 0.003 m/s

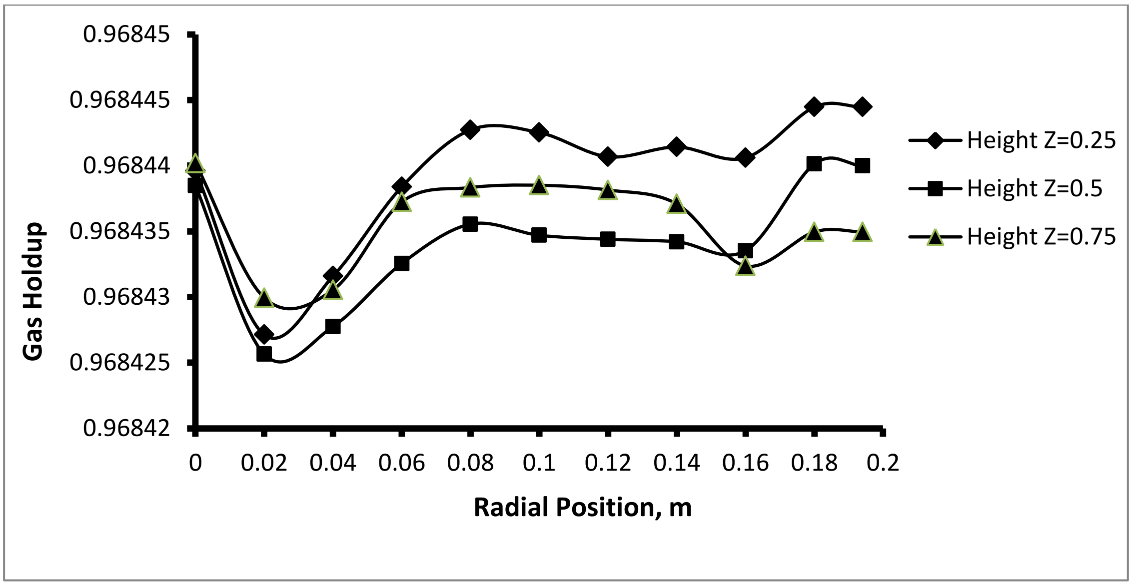


Figure 5.11(b) Gas Holdup variation along the diameter of the column at different height at gas velocity of 0.20m/s and liquid velocity 0.009 m/s

But in both the cases it is observed that the gas tend to accumulate at the center as well as near to the wall leaving a annular region for liquid. This kind of liquid-gas mal-distribution is a problem in industrial Trickle bed reactor, which reduces the efficiency of the reactor.

5.1.3 Pressure Drop:

Pressure drop is another important hydrodynamics property of a trickle bed-reactor. Pressure drop in the bed were predicted by taking different flow conditions and have been represented graphically in the following figures.

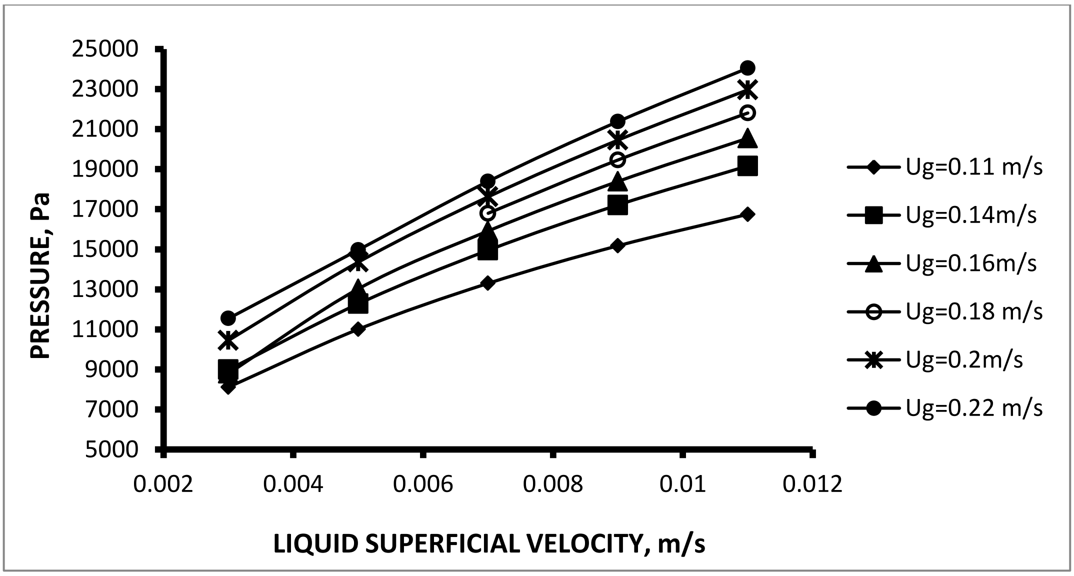


Figure 5.12: Variation of Pressure drop per unit length with liquid velocity at different superficial gas velocities.

Pressure drop in a trickle bed will be different in pre-wetted and non-pre-wetted bed condition. For an ideal assumption pre-wetted bed condition is assumed where capillary force is neglected.

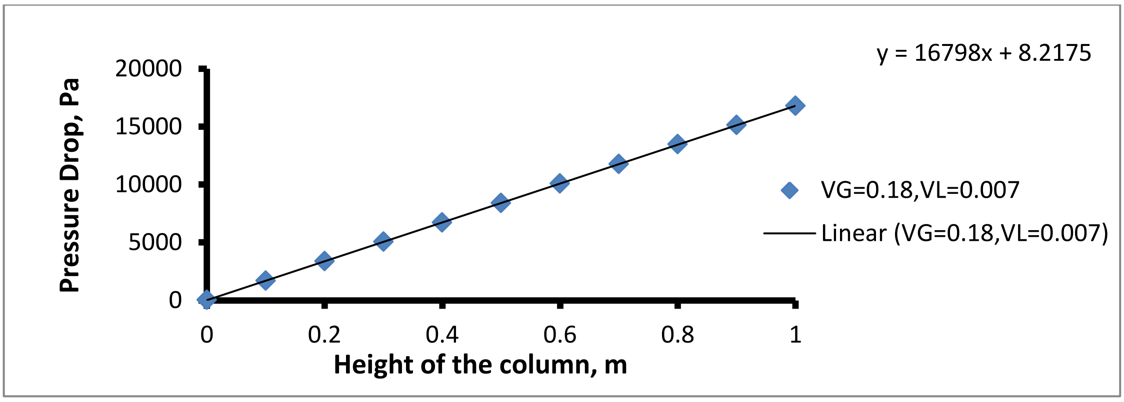


Figure 5.13: Graph showing Pressure drop along axial length of the bed.

Figure 5.10 shows the pressure gradient across the bed. Radial averaged pressure drop were predicted at different places in the column and plotted against height. The slope of the linear variation can be represented as pressure drop per unit length. Similarly pressure drop for all the flow conditions in the experiment were predicted and they were plotted in figure 5.9. Sauadnia et al (2001) also predicted the axial pressure drop variation for gas and found the same profile at different liquid and gas flow velocities.

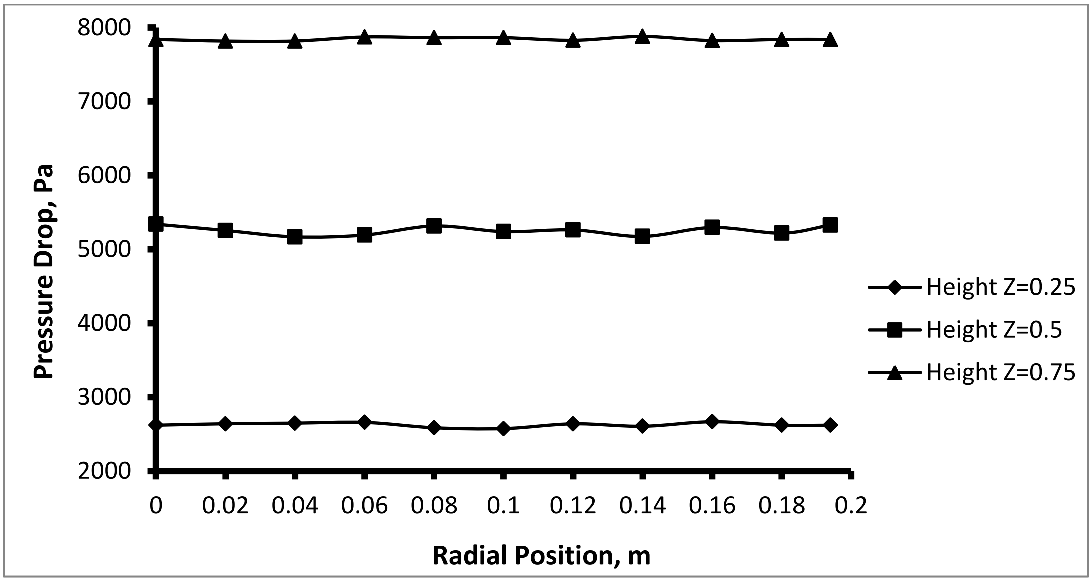


Figure 5.14: Radial-Averaged Pressure drop along the diameter of the column at different height at gas velocity of 0.2m/s and liquid velocity 0.003 m/s

The Figure 5.11 shows the radial pressure drop variation at three different heights. The radial pressure variation is not of much concern until the operating condition of the reactor is not at the boiling condition of the fluid. Such an oscillating profile for pressure drop along the radial direction was also predicted by Rodrigo et al (2009).

5.2 Comparison with the literature data:

Many scholars have studied trickle bed under different operating conditions. The present work is compared with the work of Sunderesan et al (1991), Gunjal et al (2005) and Atta et al (2007).

Table 5.1 The different experimental setup for the data compared.

Source	Bed Diameter	Bed Length, m	Particle Diameter, Dp	D/Dp ratio	Bed porosity	Gas velocity, m/s	Liquid velocity, m/s
Sunderesan et al, 1991	0.1650	1.49	0.003	55	0.37	0.22	0.002 - 0.008
Gunjal et al 2005	0.114	1	0.006	19	0.37	0.22	0.0017-0.0092
Atta et al, 2007	0.2	1	--------	------	0.37	0.22	0-0.008,,
Present work	0.194	1	0.006	32.33	0.37	0.22	0.003-0.011

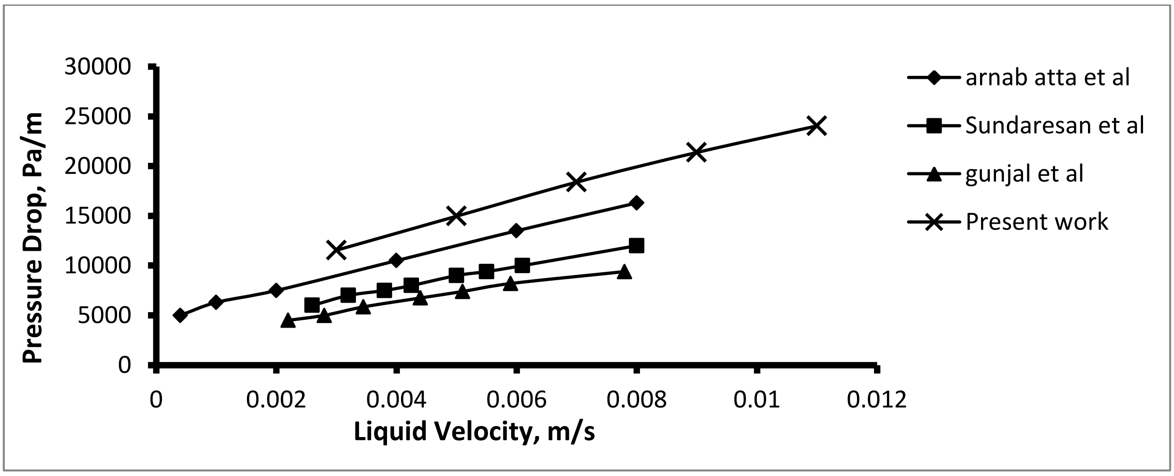


Figure 5.15: The Pressure drop Comparison with Previous works

Gunjal et al (2005) obtained the drag exchange coefficients from the interfacial force model developed by Attou et al (1999). Atta et al (2007) obtained the drag exchange coefficients from relative permeability concept developed by Saez and Carbonell (1985). In the present work Multiphase granular flow model has been adopted and the corresponding drag force model has been mentioned in table 4.2.

The results have a fair agreement with the work of Arnab Atta et al (2007). The deviation occurs because of idealistic assumption and negligence of capillary force and porosity distribution. Equations for capillary force can be modeled and implemented for greater accuracy.

The liquid holdup at different radial positions at gas velocity 0.11m/s and liquid velocity 0.003m/s has been compared with that of Jiang et al (2001) at same gas velocity and liquid velocity 0.001m/s and found to be agreeing well. variation of liquid holdup in radial direction is more in Jiang et al, because of his defined radial porosity profile.

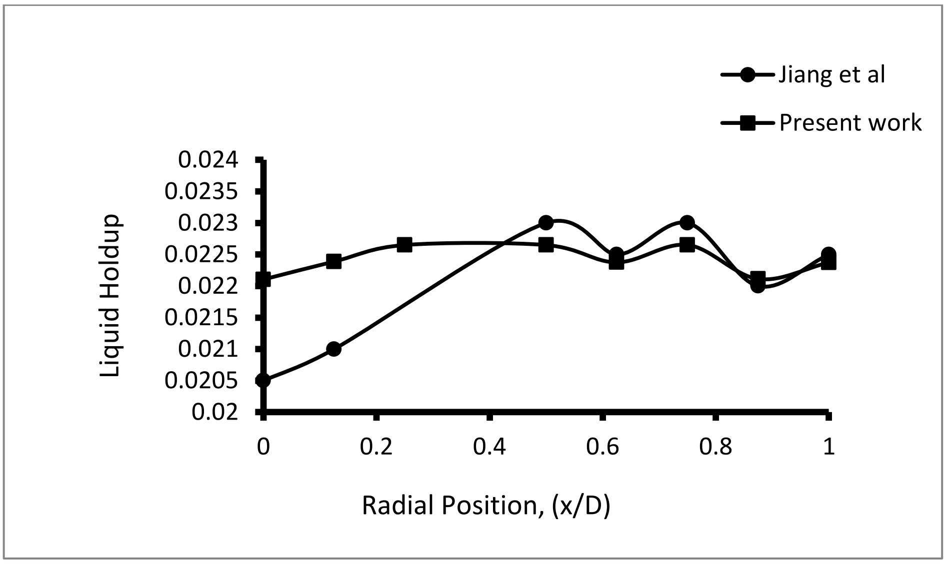


Figure 5.16: comparison of liquid holdup of along the diameter of the column at a height 0.879 Z at gas velocity of 0.11m/s with previous work

CHAPTER 6

CONCLUSIONS

CFD simulations of three phase trickle-bed reactor were carried out by employing Eulerian-Eularian approach for different operating conditions and flow conditions (Gas velocity 0.11m/s to 0.22m/s and liquid velocity of 0.003m/s to 0.011m/s). Liquid holdups, Gas holdups and Pressure drop which are important hydrodynamics parameter were studied. The results have been represented in graphical form and analysed.

The main conclusions that can be drawn are:

- Liquid holdup increases with increase in liquid velocity and decrease with gas velocity. When liquid velocity was increased from 0.003 to 0.011 m/s the liquid holdup increased from 0.021 to 0.006 for gas velocity 0.11m/s. But on increasing the gas velocity from 0.11m/s to 0.22m/s liquid holdup decreased from 0.06 to 0.03.
- Gas holdup increases with increase in gas superficial velocity and decreases with increase in liquid superficial velocity. On increasing the gas velocity from 0.11m/s to 0.2 m/s gas holdup increased from 0.94 to 0.96 at liquid velocity of 0.011m/s. when liquid velocity is increased from 0.003m/s to0.011m/s gas holdup decreased to 0.94 from 0.978 at gas velocity of 0.11m/s.
- Radial distribution of liquid is found to be better at higher gas velocity in compared to lower gas velocity. At higher gas velocity of 0.2m/s the radial variation of liquid holdup is nearly flat, but at lower gas velocity of 0.11m/s the radial liquid holdup variation is almost hyperbolic.

- The liquid saturation is not uniform throughout the length of the column. The saturation is more at the bottom of the column. However the gradient of saturation of liquid along the height decreases with increase in liquid velocity. A reverse behaviour is observed in case of Gas holdup.
- Pressure drop across the bed increases with increase in both gas and liquid velocities. Increase in liquid velocity from 0.003m/s to 0.011m/s increases pressure drop from 7 KPa to 15 KPa at gas velocity of 0.11m/s. Similarly when gas velocity is increases from 0.11m/s to 0.22m/s pressure increases from 15KPa to 25KPa at liquid velocity of 0.011m/s. Increase in gas velocity has a greater impact on pressure drop.
- The pressure gradient along the bed height is almost linear. At gas velocity of 0.18m/s and liquid velocity of 0.007 m/s the pressure gradient along the axial direction of bed was determined to be linear with 16798 Pa/m. Radial pressure variation is not prominent.
- The results have been compared with the work of Atta et al and Jiang et al and found to be agreed well.

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