A

DISSERTATION REPORT

ON

MODELING AND SIMULATION OF HYDRODYNAMICS OF A TRICKLE BED REACTOR

In partial fulfilment for the award of degree

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ABSTRACT

Trickle bed reactors are widely employed in petroleum industry to carry out variety of operations such as hydrogenation, hydrocracking, hydrotreating etc. Over the last two decades, many models have been proposed to account for complex interfacial momentum interactions between different phases, but still no consensus is developed on a model to describe different hydrodynamic parameters under different flow conditions with acceptable accuracy. In this study three widely used models for defining the variation of porosity in packed bed of spherical catalyst particles in cylindrical reactors are compared with experimental data. The radial porosity model that best corresponds to the experimental data is further used for carrying out hydrodynamic simulation of Trickle bed reactor.

For determining the hydrodynamic parameters, two hydrodynamic models were considered. These models differ in their models for defining momentum interactions between phases. These models are compared based on their predictions of hydrodynamic parameters viz. pressure drop and liquid holdup. The predictions are also compared with experimental values of these parameters. Models compared in this study include- Saez and Carbonell (1985), a pseudo two phase model based on relative permeability concept, and Attou and Ferschneider (1999), a three phase model based on Ergun momentum exchange model.

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NOMENCLATURE

Symbol	Description
E_1,E_2	Constants of Ergun equation
d_p	Diameter of Catalyst particle
D	Reactor diameter
Re_q	Reynolds number of phase q.
F_q	Force per unit volume exerted by phase q
k_q	Relative permeability of phase q
Ga_q	Galileo number of phase q
d_e	Equivalent particle diameter
V_p	Volume of particle
A_p	Total surface area of particle
S_g	Saturation of gas-phase in bed
a,b	Constants determined by reactor diameter to particle diameter ratio in Mueller(1991) correlations
A,B	Constants in Bazmi(2012) correlation.
r^*	Dimensionless distance from wall
t	Time
v_q	Velocity of phase q
P	Pressure
g	Gravitational acceleration

K_{pq}	Inter-phase momentum exchange coefficient between phase p and phase q.

Greek symbols-

Symbol	**Description**
μ_q	Viscosity of phase q
ε	Bed porosity
$\varepsilon_l^{\,o}$	Static liquid holdup
ε_B	Bulk porosity of the bed
δ_l	Reduced liquid saturation
ρ_l	Density of liquid phase
ρ_{lo}	Density of liquid at Normal temperature and pressure
$\Delta\rho_{lp}$	Change in density due to change in pressure
$\Delta\rho_{lT}$	Change in density due to change in Temperature

Subscripts-

Symbol	**Description**
S	Solid phase
L	Liquid phase
G	Gas phase

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CHAPTER-1
INTRODUCTION

1.1 Trickle bed reactor (TBR)

Trickle bed reactor (TBR) can be described as a packed bed of catalyst particles with co-current or counter-current flow of gas and liquid phase reactants to produce gas and liquid phase products. In a trickle bed reactor, the liquid trickles over the catalyst particles, down the column, and hence it is called a trickle bed reactor. Trickle bed reactors are widely employed in petroleum and petrochemical units to carry out a variety of operations such as hydrogenation, hydrocracking, hydrotreating, etc. Trickle bed reactors (TBRs) also find application in the treatment of VOC compounds in air pollution control and of organics in wastewater.

A TBR can be operated in three different modes: co-current (both fluids enter from the top of the reactor), counter-current (liquid enters from the top while the gas from the bottom of the reactor), and co-current up-flow (both fluids enter from the bottom of the reactor). Fig. 1.1 shows the different modes of operation of TBRs. In most industrial operations, top to bottom co-current mode of gas-liquid phase is commonly practiced.

TBRs are preferred because of their modest design, low pressure drop (compared to liquid full operation), good heat and mass transfer efficiency, high reaction rate and convenience of using inter-stage quenching to control temperature in case of exothermic reactions. The trickle flow operation is known to be advantageous in many chemical processes to achieve high conversion efficiency in the production of chemicals or the removal of pollutants from gas or liquid feeds as the flow profile in these reactors corresponds to that of a plug flow reactor. However, TBRs also have some shortcomings. Liquid mal-distribution in a TBR may lead to a decrease in the expected conversion. Hotspots may be encountered in the case of exothermic reactions. The complex hydrodynamics of multiphase flow in these reactors also pose a formidable challenge in understanding and estimating the interaction among different phases in the reactor. The prediction of hydrodynamic parameters are essential and integral in designing these reactors as these affect the overall conversion and yield obtained in these reactors.

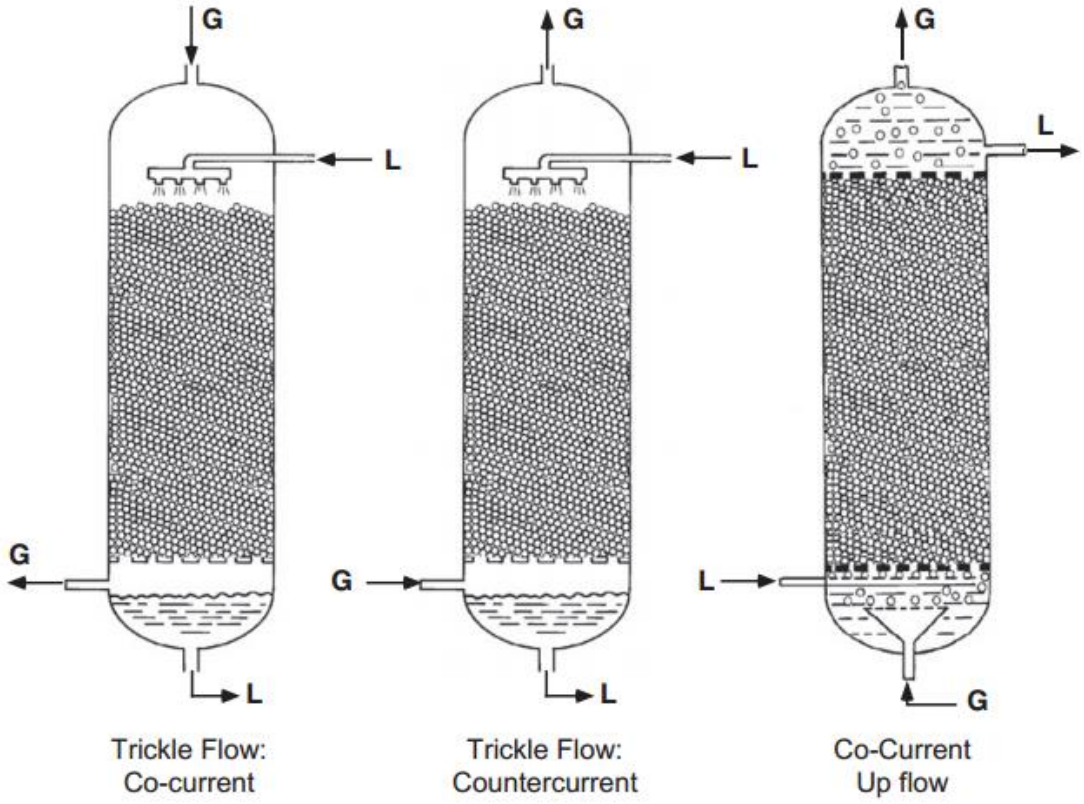


Fig. 1.1: *Operating modes of a Trickle bed reactors*

(Source: Ramachandran and Chaudhari, 1983)

1.2 Flow regimes of a Trickle bed reactor.

Four distinct flow regimes are generally observed in a TBR. These are given as follows:

- Trickling flow regime.
- Pulsing flow regime.
- Spray flow regime.
- Bubble flow regime.

1. *Trickling flow regime*: In this regime the liquid flows down the column over the surface of packed catalyst particles whereas the gas travels as a single continuous phase in the remaining void space. Trickling flow regime is most frequently used in industrial operations. Trickling flow regime can further be subdivided into two regimes based on the catalyst particle wetting characteristics:
    - *Partial wetting trickling regime*: This is characterised by low gas and liquid flow-rates. The efficacy of this flow regime is characterised by the wetting efficiency

i.e. the fraction of the catalyst bed wetted by the liquid. The liquid trickles down in laminar flow regime. Wetting efficiency can be improved by increasing the gas and liquid flow-rates.

- *Complete wetting trickling regime*: This regime is characterised by high gas and liquid flow-rates ensuring complete wetting of catalyst bed by the trickling liquid.

2. *Pulsing flow regime:* This regime is characterized by the liquid and gas slugs moving alternately through the column. In this flow regime, the channels between the particles are clogged by the liquid which forms slug. The liquid slug is immediately followed by blowing off by the gas slug. The liquid pulse is not completely free of gas bubbles, especially at the beginning of liquid pulse. Also the gas pulse is not free from liquid entrainment and that there is always a thin layer of liquid phase present over the catalyst bed.

3. *Spray flow regime*: This regime encounters high gas flow rate and low liquid flow rate. The gas forms a continuous phase and the liquid is entrained in gaseous phase. This flow regime is least favourable as it invariably results in low mass transfer and heat transfer rates.

4. *Bubble flow regime*: This regime is characterised by high liquid flow rate and low gas flow rate. The liquid phase is continuous carrying gas bubbles. Thus, the gas phase is dispersed.

A schematic representation of different flow regimes observed in a TBR is depicted in Fig.1.2.

1.3 Wetting efficiency in a Trickle bed reactor

Wetting efficiency can be defined as the fraction of the catalyst surface area which is covered by the flowing liquid film. Wetting efficiency, in general, refers to external catalyst wetting efficiency as internal catalyst wetting efficiency is generally taken as unity because of capillary effects ensuring complete wetting of the internal pore surface. Partial wetting of the catalyst surface is attributed to lower liquid flow rates. With an increase in the liquid flow rate, the wetting efficiency also increases. In order to determine the catalyst utilization in a trickle bed reactor, the determination of the wetting efficiency is very important. Several

correlations are available for the determination of the wetting efficiency which is found to be a function of the liquid Reynolds number, liquid Galileo number and dimensionless pressure drop.

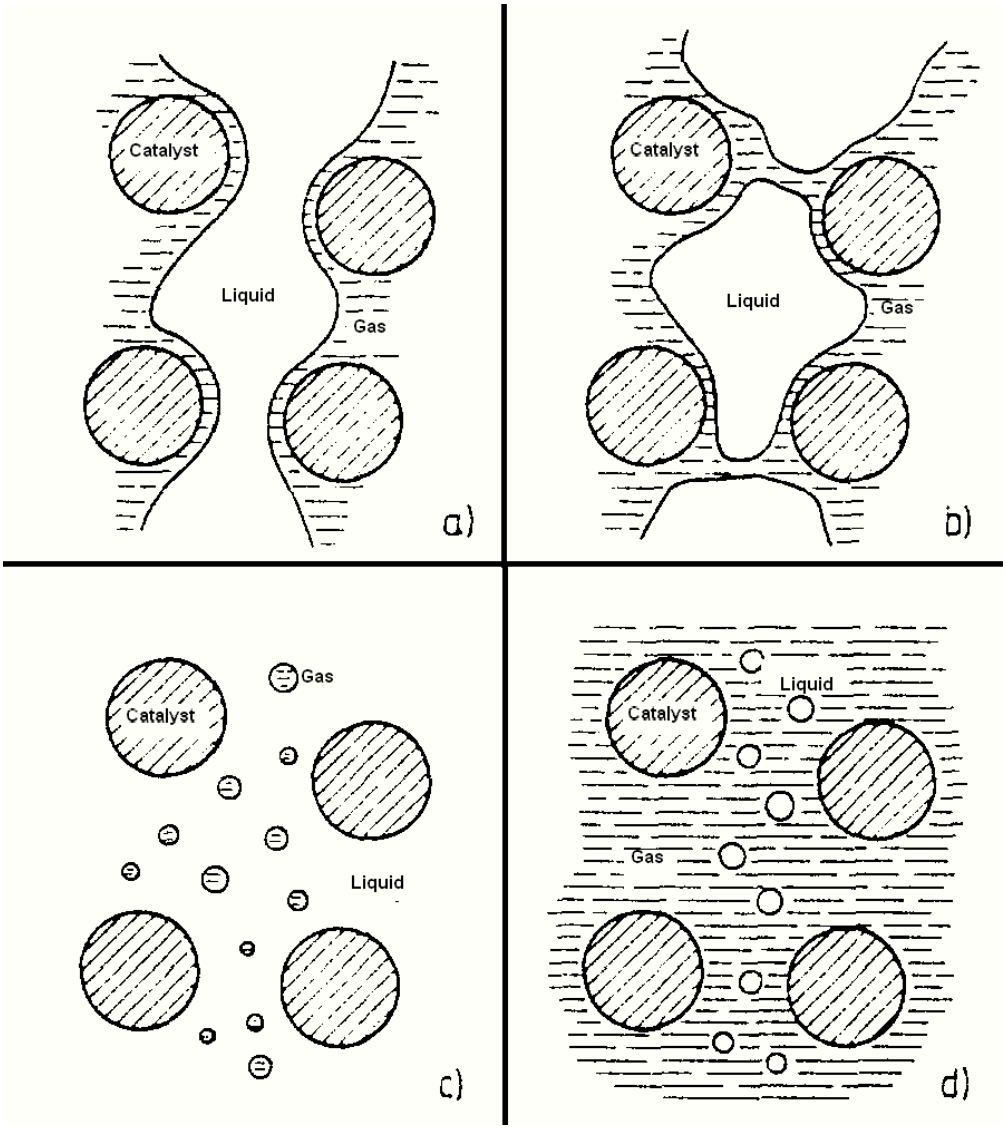


Fig. 1.2: *A schematic representation of the flow regimes encountered in a trickle bed reactor: a) Trickle flow, b) Pulse flow, c) Spray flow, and d) Bubble flow (Reinecke and Mewes, 1996)*

The rate of reaction in a trickle bed reactor also depends upon its wetting efficiency. However, the rate of reaction can be higher or lower in partial wetted regime when compared with the completely wetted flow regime, depending upon the properties of the reactants. If the liquid reactant is non-volatile, and the reaction is liquid-limited, an increase in wetting efficiency increases the rate of reaction as is the case of hydrogenation reactions. The increase in the rate of reaction can be explained by an increase in the contact area between the catalyst and the liquid phase in which the reaction takes place. In case of a volatile liquid

phase, an increase in the wetting may result in the lowering of the rate of reaction as reaction can take place in any phase- liquid or gas.

In partial wetting trickling flow regime, the flow of liquid over the catalyst surface results in the formation of different patterns. These patterns include:

- Films – A thin, laminar liquid stream that partially covers a particle.
- Rivulets – A continuous stream of liquid over the surface of a particle.
- Filaments – A liquid stream that flows down the bed in the form of a film
- Rivulet flow - connecting liquid pockets

Fig. 1.3 shows different flow patterns observed in partial wetting trickle flow regime in a TBR.

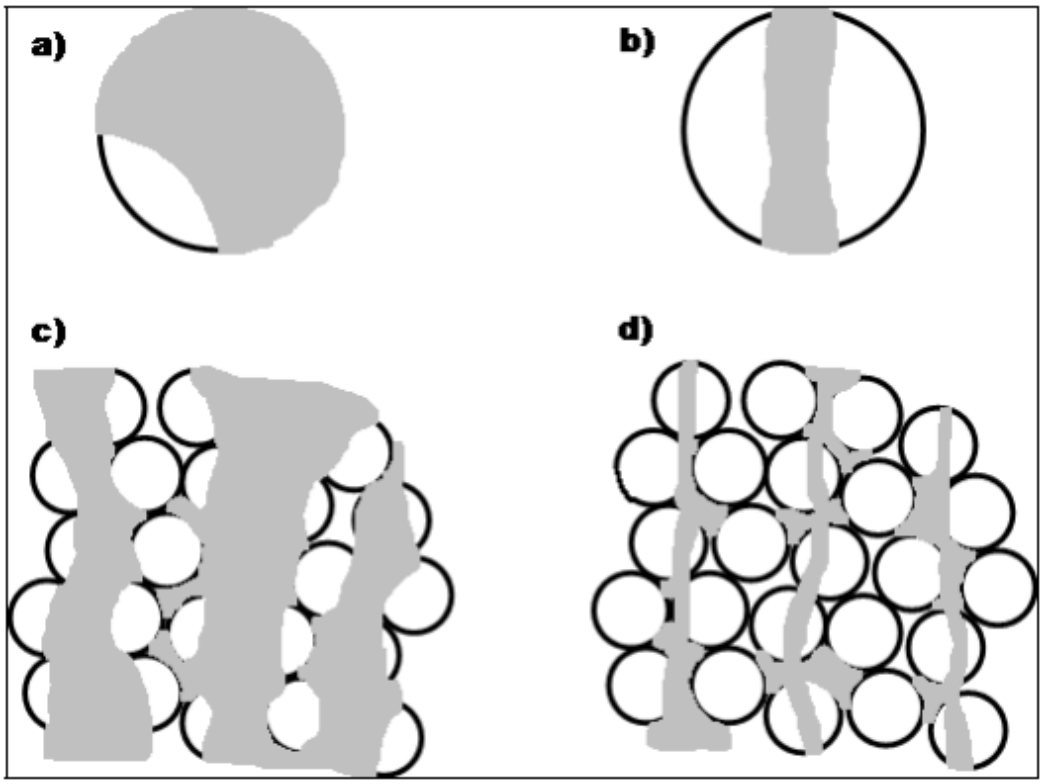


Fig.-1.3: *Schematics of flow patterns: a) Particle-scale film flow b) Particle-scale rivulet flow c) Bed-scale film flow d) Bed-scale rivulet flow (Mederos et al., 2009)*

The relative amount of these patterns may vary with inlet distribution of gas and liquid, flow rates of gas and liquid phases, wetting properties of the catalyst particle, and the shape and size of the catalyst particles.

1.4 Hysteresis in a Trickle bed reactor

Multiplicity of hydrodynamic states in a trickle bed reactor due to flow history of the trickle bed reactor is termed as hysteresis in TBR. Hysteresis is observed for the pressure drop, liquid holdup, and wetting efficiency. Effect of hysteresis on pressure drop can be as high as 100% and for liquid holdup up to 30% (Maiti et al. (2006)). Factors that affect hysteresis in a TBR are given below:

- *Porosity of Particles:* The type of catalyst particles (porous or non-porous) has pronounced effect on extent of hysteresis nature observed for a TBR. It is higher for porous particle reactors when compared with non-porous ones.
- *Start-up procedure*: In the case of start-up procedure of wetted bed, the extent of hysteresis observed has been found to be much smaller than that of the dry bed start-up procedures.
- *Fluid Flow rates*: It is observed that the hysteresis in constant gas flow condition is much higher than that of the constant liquid flow conditions.
- *Particle size*: The effect of hysteresis is more pronounced for smaller particles than for larger particles.
- *Inlet liquid distribution:* The extent of hysteresis can be significantly controlled by ensuring nearly uniform distribution of liquid at the inlet of the reactor.

1.5 Challenges in the operation of TBRs

TBRs have many advantages like modest design and higher reactant conversion efficiency. The higher conversion efficiency can be attributed to plug flow like flow field in the trickle bed reactor. However, there are a few operational difficulties associated with TBRs which are discussed in the following section-

- Scale-up – The hydrodynamics of TBR is complex and highly sensitive to the scale of the reactor. Conventional models are not able to account for these hydrodynamic complexities viz. variation in porosity in the bed, momentum transfer between phases, distribution of phases in the reactor. These parameters also affect the conversion in the reactor. This problem has been overcome to a certain extent with the advances in Computational Fluid Dynamics (CFD). The CFD studies have helped in a more realistic modelling of the hydrodynamics of a TBR

- *Liquid mal-distribution:* Liquid mal-distribution significantly reduces the conversion efficiency of a TBR. It also leads to the formation of hot spots in case of exothermic reactions. Liquid mal-distribution generally occurs at low liquid velocities. It can be reduced by ensuring uniform distribution of liquid at the inlet of the reactor and maintaining a moderate superficial velocity of the liquid phase.

1.6 Brief history of Trickle bed Reactors

Trickle bed reactors were first used to remove organic matter from wastewater stream, using aerobic/facultative microbial activity (Satterfield, 1975). Air and water were passed over a stone bed on which aerobic/ facultative microbes were allowed to grow, thereby removing organic compounds from the wastewater. Although TBRs have since been used in many chemical processing plants, most of the available literature hovers around their use in hydro treating petroleum products.

Commercial development of TBRs for hydrodesulphurization, hydrotreating and hydro-cracking, as described by some studies (Le Nobel and Choufoer, 1959; van Deemter, 1964), were carried out by British Petroleum (BP) and Shell during 1950s. The historical update of the development of hydrodesulphurization and hydrotreating by other companies (Exxon, Union oil, Gulf) can be made from the proceedings of the World Petroleum Congress.

1.7 Research overview of hydrodynamics of TBR

The study of hydrodynamics of TBRs, because of its complexity and wide usage, has been a subject of immense interest for scientific community. The earliest documented study in the field of hydrodynamics of TBR dates as back as 1950s. The prospect of completely understanding the interactions in complex liquid-gas-solid flow fields with development of CFD models proved helpful to revive interest in this field of study. The widespread use of TBR in industries and ever increasing stringency in the environmental regulations

concerning auto- emissions and thereby in upgrading the fuel characteristics have generated renewed research interest in this field. A brief research overview of publications and citations in this field as generated from Web of Science, an online academic citation index by Thomson Reuters is given below.

Literature as shown by Web of Science-

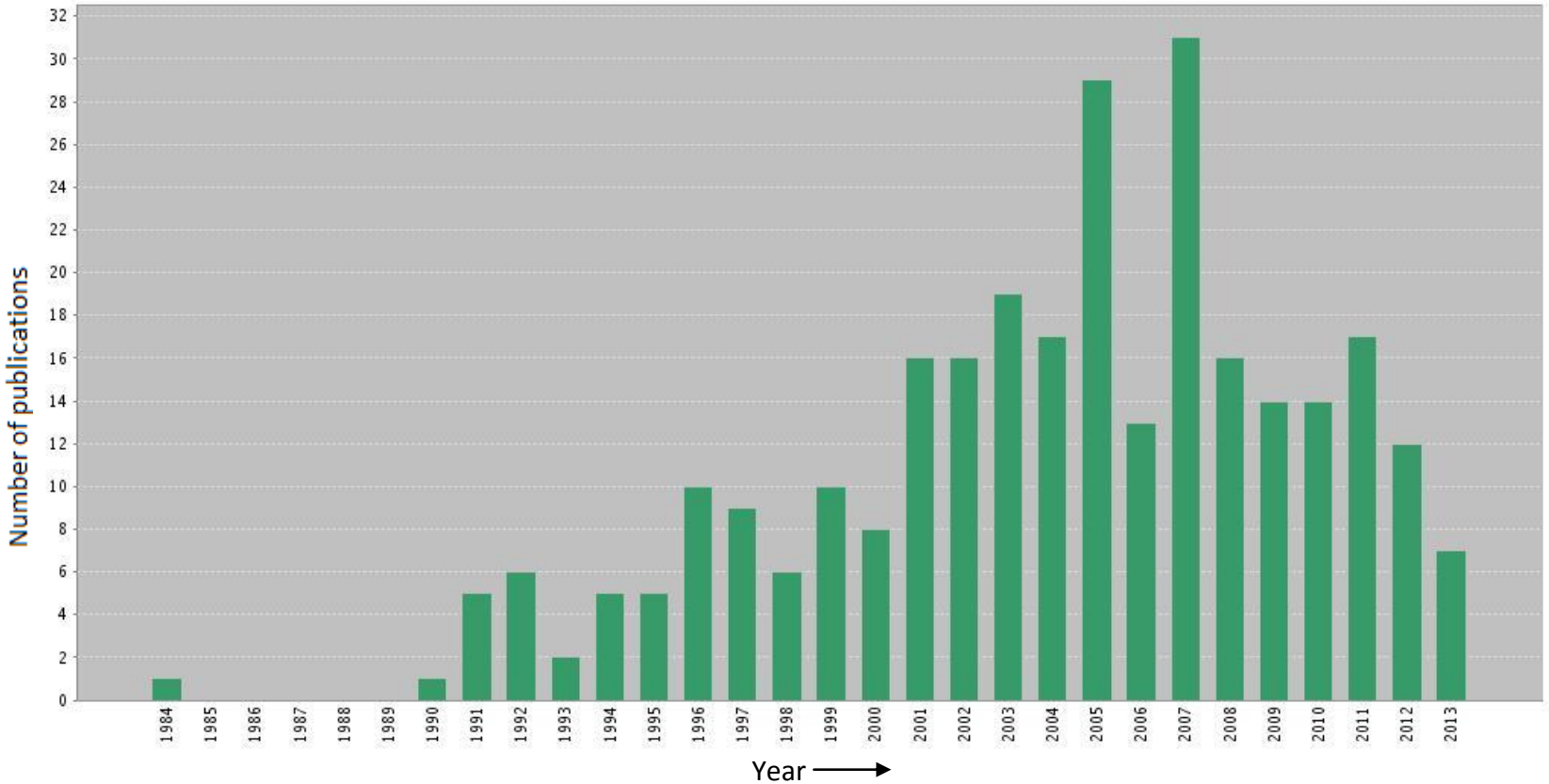


Fig. 1.4: *Number of publications in each year.(Downloaded from Web of Science as on 24th May 2013).*

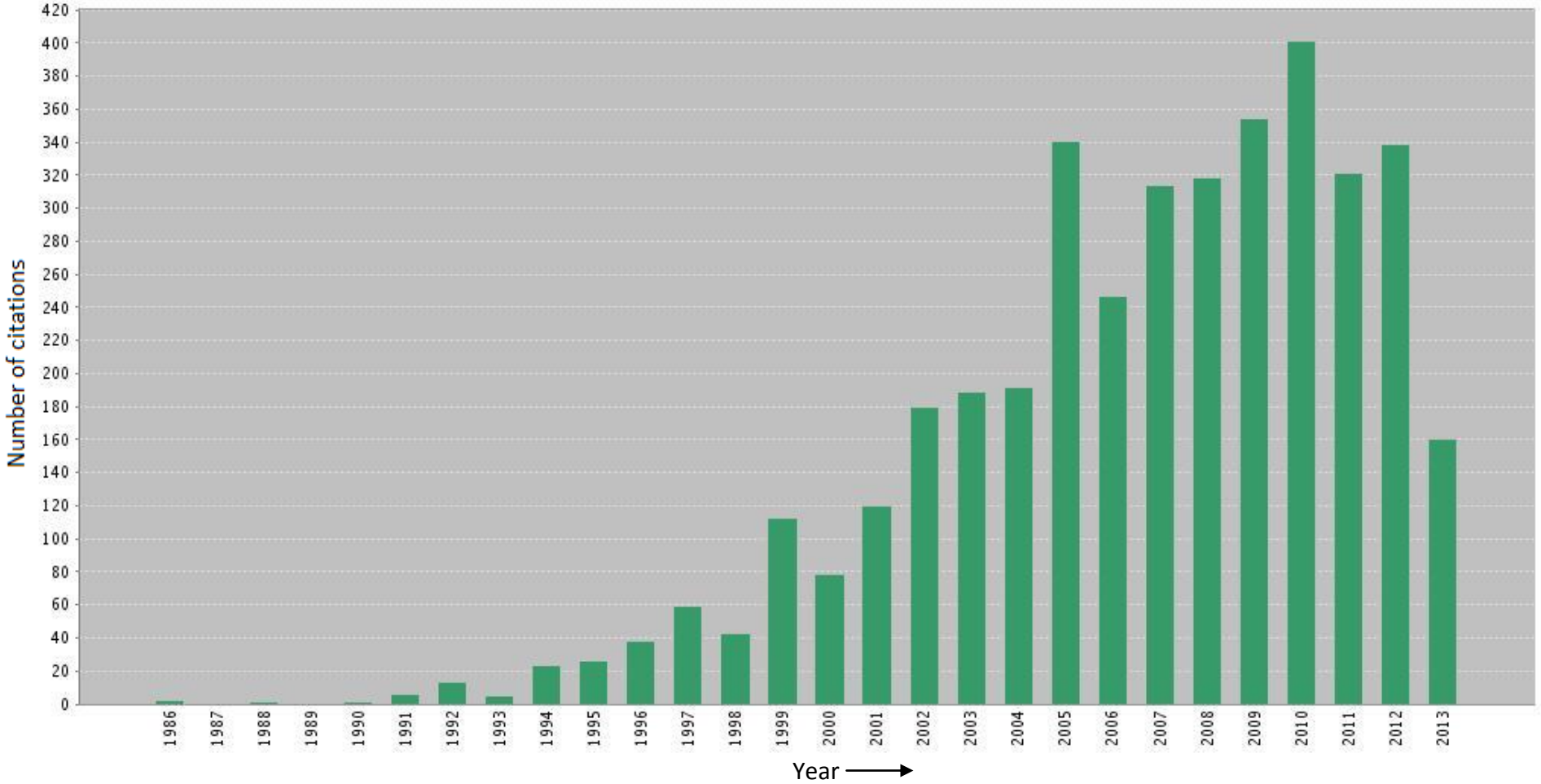


Fig. 1.5: *Number of citations each year.(Downloaded from Web of Science as on 24th May 2013)*

Fig. 1.4 shows the bar graph for the number of publications in the field of "Hydrodynamics of Trickle bed reactors" from 1996 to 24th May, 2013. Fig. 1.5 shows the bar graph for the number of citations of research publications in the field of "Hydrodynamics of Trickle bed reactor" from 1996 to 24th May, 2013. A brief summary of total publications, citations, etc. in this field is given in Table 2.2.

Table 1.1 : Number of publications reviewedfrom 1996 to May,2013(downloaded from Web of Science)

Results found	289
Sum of the Times Cited	3886
Sum of Times Cited without self-citations	2619
Citing Articles	1779
Citing Articles without self-citations	1536
Average Citations per Item	13.45
h-index	31

The bar graph as prepared by the Web of Science clearly demonstrates that up till 1990s, the publications on trickle bed reactors seemed to be very few. The reason for this is that the search sites like Web of Knowledge do not report correctly all the papers and citations prior to 1995.

In recent years, the number of researches in this area has gradually increased owing to enhanced interest in middle distillate production and scarcity of low sulfur crude. Also the advances in CFD and the increasing computational power have made the area of hydrodynamics of trickle bed reactor very fascinating for research. The number of research papers increased and more than 16 research papers appeared from the year 2001 onwards. Similarly the numbers of citations of papers also increased with more than 260 citations from the year 2005 onwards.

Citation report for 'CFD study of Hydrodynamics of Trickle bed reactor' downloaded from the Web of Science is given in following section.

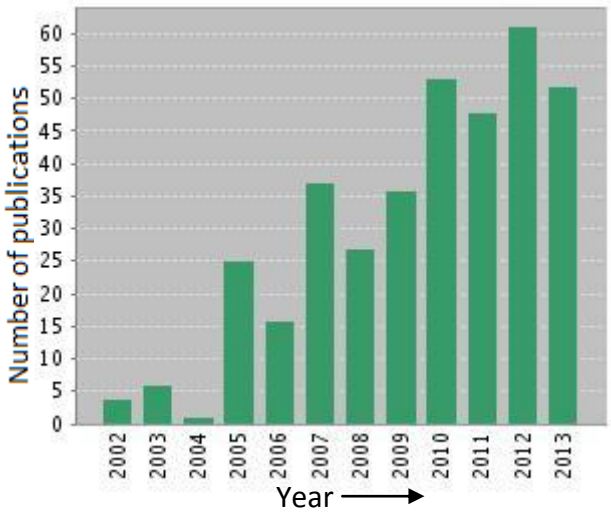


Fig. 1.6: *Number of publications in each year (Downloaded from Web of Science on 24th May, 2013).*

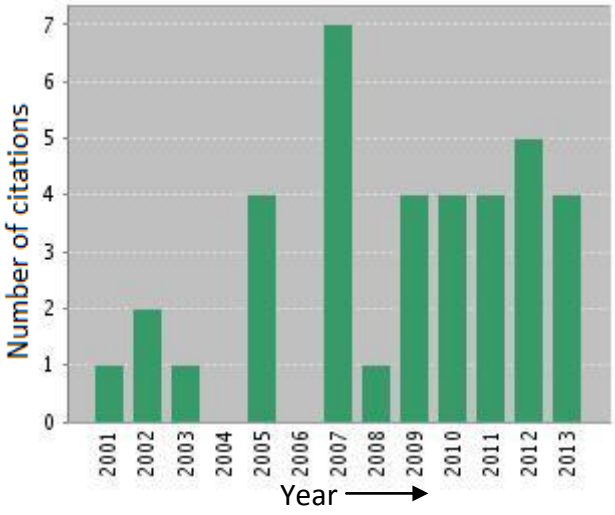


Fig. 1.7: *Number of citations each year.(Downloaded from Web of Science on 24thMay, 2013*

Table 1.2 : Number of publications reviewed since 2000 (downloaded from the Web of Science)

Results found	37
Sum of the Times Cited	366
Sum of Times Cited without self-citations	239
Citing Articles	184
Citing Articles without self-citations	152
Average Citations per Item	9.89
h-index	11

1.8 Motivation

With the shortage in supply of sweet crude and ever- increasing oil prices, it is imperative to optimize the hydro processing operations as far as possible. In most of the industrial processes, TBRs are used for the hydro-processing of heavy crudes. The efficiency of a TBR is dependent upon its hydrodynamic parameters which include variables like catalyst pre-wetting, liquid hold-up, catalyst size and pressure drop. The importance of understanding hydrodynamics of trickle bed reactor cannot be overstated.

Although TBRs find use in several areas other than hydro-processing in hydrocarbon industry and have been subjected to intensive investigation, the current understanding of these reactors is still not adequate. To measure and describe complex multiphase interactions in the trickle bed reactors is a formidable challenge. It is also very difficult to understand the effect of parameters like shape and size of catalyst particles, and the method used for packing the particles that constitute the bed on flow field in trickle bed reactors. Many models have been proposed for describing the hydrodynamics in a trickle bed reactor but none of these hydrodynamic models has been able to predict the hydrodynamic parameters for all flow regimes in trickle bed reactor with satisfactory accuracy. Recently, Eulerian multiphase models with CFD approach have shown a lot of promise in predicting the flow dynamics in a TBR.

In view of the above, it was decided to work on the modeling and simulation of the hydrodynamics of TBRs.

1.9 Problem description and the work to be done

Hydrodynamics of flow through a trickle bed reactor was studied for laboratory scale reactors with due emphasis on variation of porosity due to wall effects. The understanding of hydrodynamics plays a crucial role in scale up operations for multiphase flow systems.

In this study, two models based on Eulerian approach of multiphase modelling have been compared. The two models are given by Saez and Carbonell (1985) and Attou and Ferschneider (1999). These models differ in their approach to model the force/ momentum transfer between different phases.

The data required for simulation a TBR include bed properties, shape and size of catalyst particles, reactor dimensions-diameter and length, density and viscosity of both the phases, viz. the liquid and gas phase, surface tension of the liquid phase, liquid and gas flow rates, operating conditions-temperature and pressure, Ergun constants for two phase flow, and the bed bulk porosity.

For simulating the three phase model as proposed by Attou and Ferschneider (1999), the reactor dimension of 0.5m x 0.019m was taken from the experimental study of Chowdhury et al. (2002). In this study, diesel oil (specifications given in Table 4.6) was used as the liquid phase and hydrogen was used as the gas phase. Catalyst particles were spherical in shape and were 2 mm in diameter. Bulk porosity of the bed was taken as 0.5. Ergun constants for fluid pair at operating conditions were taken as 263 and 4.99, as given by Gunjal and Ranade (2007). Density and viscosity of diesel oil were calculated using equations 3.35-3.39. The liquid to gas flow rate ratio was maintained at 200 m^3/m^3. The liquid hourly space velocity was varied from 1 to 8 h^{-1}. Pressure was taken as 24 bar and the temperature was taken as 633 K. Hydrogen properties were taken from ASPEN data bank. The model was validated by comparing the simulation results with the results reported by Gunjal and Ranade (2007).

For simulating pseudo-two phase model as proposed by Saez and Carbonell (1985), the reactor dimensions of 0.5715 m x 0.0219 m were used as were given in the experimental study of Al-Dahhan and Dudukovic (1994). In this study, hexane and water were used as the liquid phase and helium and nitrogen were used as the gas phase. Catalyst particles were considered to be spherical (diameter 1.14 mm) and porous extrudate (equivalent diameter 1.99 mm). Bulk porosity of the bed was taken to be equal to 0.392 for spherical particles and

0.355 for porous extrudate as given by Al-Dahhan and Dudukovic (1994). Ergun constants for fluid pairs were taken as 334.1 and 3.23. Density and viscosity data for both the phases were extracted from ASPEN database. Gas superficial velocity varied from 0.01-0.117 ms^{-1} and liquid superficial velocity varied from 2.39-14.82 ms^{-1} in the experimental study. Pressure was varied from 0.31 to 5 MPa and the temperature was reported to be 298 K. Further, the three phase model of Attou and Ferschneider (1999) was also simulated for the aforementioned flow conditions. The predictions by both the models were compared with the experimental data given by Al-Dahhan and Dudukovic (1994).

1.10 Objectives

- To collate all the information available in the literature on the modeling of hydrodynamics of a trickle bed reactor.
- To compare the radial porosity distribution correlations for TBRs with spherical catalyst particles available in literature and compare these with experimental data in order to find the best correlation. To use the best-fit correlation as a User Defined Function (UDF) and hook it to hydrodynamic simulation of a TBR.
- To simulate a comprehensive model for the determination of hydrodynamics of a TBR, taking into consideration the radial porosity variation and inter-phase momentum exchange between different phases
- To compare the results obtained with the predictions by different models as well as with the experimental data available in literature in order to validate the simulation.
- To compare the predictions of the three phase model based on phase momentum interaction and a two phase porous media model based on relative permeability, with the experimental data.
- To study the variation of hydrodynamic parameters with variation in flow rates of the two interacting phases.

CHAPTER-2
LITERATURE REVIEW

Several excellent reviews on trickle bed reactors were published over the years. Some of these reviews are discussed here.

A masterpiece review was given by **Satterfield (1975)** that beautifully collated and updated all the available information on trickle bed reactors into one document. Many hydrodynamic aspects like liquid holdup, flow patterns, pressure drop, and mass transfer coefficients and their correlations available in literature were discussed. Satterfield also carried out detailed comparison of different models and their applicability. Each aspect of mass transfer viz. pore diffusion limitation, gas to liquid mass transfer, and liquid to solid mass transfer were separately dealt with. The experimental data and models on wetting efficiency were discussed in great detail.

Herkowitz and Smith (1983) reviewed the experimental data and methods for estimating overall effectiveness factor for TBRs. The effectiveness factor was found to depend upon wetting efficiency, intra-particle diffusion, intrinsic kinetics and interphase mass transfer. Also equilibrium liquid distribution and the length required to attain this equilibrium distribution was also reviewed. Effect of surface tension and temperature profiles in case of non-isothermal reactor was also discussed.

An incisive review was given by **Maiti et al. (2004)** on distribution of liquid phase and flow field in co-current trickle bed reactors. Many factors were pointed out in this study that affected the liquid flow distribution in TBRs. Among these factors, distribution of liquid at inlet, shape and size of catalyst particles used for packing, method of packing used, and operating flow rates of the two phases were discussed in detail. Many other factors were also found to be influencing the flow texture in TBRs. These factors include procedures used for start-up, wetting efficiency of the operation, and changes in flow rates (also known as flow history).

Different methods of measuring and characterizing the liquid distribution and flow texture in TBRs were discussed in this study. These methods included methods like liquid collection, pressure drop measurement, residence time distribution (RTD), different types of tomography, magnetic resonance imaging (MRI), colorimetric techniques and conductometric probes. The effect of wall flow on hydrodynamic parameters in a TBR was

also studied. It was observed that due to more structured packing of catalyst particles; the porosity distribution near the wall was much more fluctuating. Because of this fluctuation in porosity near the wall, channelling takes place and significant wall flow is observed in laboratory scale reactors. This study suggested that the reactor to particle diameter to be kept greater than 25 in order to reduce the wall flow effects arising due to porosity variation along radial direction. It was observed that an increase in the liquid flux improved the wall flow. Gas flux was found to improve wall flow only up to a certain flow rate.

TBRs encounter hysteresis during their operation. **Maiti et al. (2006)** presented an incisive review on hysteresis in trickle bed reactors. Many factors were identified on which the extent of hysteresis depend on. These factors include the shape and size of catalyst particles, the porosity of catalyst particles, the flow history of catalyst bed used to study the extent of hysteresis, the liquid distributor used at the inlet of the reactor. The extent of hysteresis was also shown to be dependent on the start-up conditions of the trickle bed reactor.

Mederos (2009) gave an assessment on conditions to ensure ideal behaviour of trickle bed reactor. They observed that the influence of three factors, namely plug flow deviation, external wetting efficiency, and the reactor wall effect needed to be minimised in oder to operate the reactor ideally. Laboratory trickle bed reactor can be used to account for the catalytic reaction kinetics as long as the three factors discussed earlier are kept under control. Mederos stressed that the ideal flow pattern (plug flow or perfectly mixed) and isothermal conditions were required for producing reliable experimental data regarding trickle bed reactors for their scale-up.

Recently a state of the art review on all available CFD models for modeling and simulation of hydrodynamics of trickle bed reactors was given by **Wang et al. (2013).** The study discussed the recent advances in the field of CFD simulation of TBRs. All the available CFD models and closure equations for modeling interpenetrating phase interactions, porosity variation within the bed along radial as well as axial direction were beautifully collated and discussed. Different available methods for modeling mal-distribution and wetting efficiency in trickle bed reactors were also discussed. The study also laid great emphasis on the formulation of new models for defining interfacial phase interactions which they considered to be the building blocks for more robust and accurate hydrodynamic model for a trickle bed reactor.

2.1 Review of experimental studies

A brief review of experimental studies to determine the gas-liquid distribution in down flow trickle bed reactors is given in table 2.1.

Table 2.1: A review of experimental studies on hydrodynamics of trickle bed reactor.

Author	Bed properties	System	Method of study	Flow rates	Comments
Herkowitz and Smith (1978)	Column diameter (mm) : 40.8, 114. Height (mm) : 260-700 Packing Diameter (mm) Granular : 2.52 - 11.1 Spherical : 3.0 - 9.5 Cylindrical : 3.8 - 8.9	Air-water	Annular collector: 3,4 or 5 annular point source, uniform distributor	L=1-5 G=0.0014-0.07	Provided a useful method for determining bed length required for attaining equilibrium distribution.
Toye et al. (1996)	Column diameter : 600mm Height: 2000mm Packing diameter- 5mm	Air-water	X-ray tomography	L=0-1	Observed the increase in rivulet number to be proportional to liquid flowrate
Reinecke et al. (1996)	Column diameter: 120mm Height: 2000mm Packing diameter: 3mm, 10.5mm Ceramic spheres.	Air-water	Capacitance tomography	Pulse flow	Visualization of three dimensional shapes of gas and liquid rich zones

Ravindra et al. (1997)	Rectangular (60mm*80mm) Height: 200mm Packing diameter (mm): 1.6-6.3 Glass beads and alumina particles.	Air-water	Dye adsorption method and collector (16 zones).	L=1-8 G=0.005	Required catalyst particles to be washed after each run.
Saroha et al (1998)	Column diameter:152mm Height:550mm Packing diameter (mm): 1.5 Cylindrical extrudates.	Air-water	Annular collector (6 annular)	L=0.7-5 G=0-0.027	Studied effect of gas flowrates and liquid flowrates on liquid radial distribution.
Jiang et al. (1999)	2D trickle bed (72mm*90mm) Height: 288mm Packing Diameter(mm): 3-20 Glass beads	Air-coloured water	Video imaging method	L=1.48-3.52 G=0.059	Effect of liquid distributor and particle prewetting discussed in detail.
Kundu et al. (2001)	Column diameter: 152mm Height:620mm Packing diameter (mm): 3-7.3 Sphere,extrudates,tablets,holed tablets	Air-Water surfactants Air-kerosene Air-ethylene glycol.	Annular collector (6 annular)	L=0.69-7.31 G=0-0.043	Discussed the effect of different shapes of catalyst particles on radial liquid distribution.

Sederman and Gladden (2001)	Column diameter: 40mm Particle diameter: 5mm	Water-dry air	Magnetic Resonance Imaging (MRI)	U_G= 66-356mm/s U_L= 0.5-5.8mm/s	Wide range of flow rates used for both fluids. Studied effect of prewetting on liquid distribution.
Boyer and Fanget (2002)	Column porosity: 0.36 Column diameter: 60mm Height:300mm Particle diameter:1.66mm	Heptane-dry alr	Gamma ray tomography.	U_L=1-17mm/s Gas fraction 0-1.	Developed computed gamma ray tomography.
Tsochatzidis et al. (2002)	Column diameter:140mm Height: 1240mm Particle diameter: 1.6mm Spherical packing	Air-Water	Conductance probe	L=1.36-20.34 G=0.136-0.366	Tested three different liquid distribution devices viz. Uniform, Half-blocked, quarter-blocked.
Gunjal et al. (2003)	Column diameter: 100mm Height:1000mm Spherical	Air-Water	Conductivity probe.	G=0-0.0043 L=1.5-11	Triangular pitch distributors were used. Radial distribution of

					porosity model used for CFD analysis.
Borremans et al. (2004)	Column diameter: 300mm Height: 1300mm Particle diameter (mm): 3mm spherical.	Air-Water	9 zone collector	-	Liquid flow maldistribution attains a minimal value at 0.006ms^{-1} liquid superficial velocity.
Llmas et al. (2008)	Column diameter: 300mm Height:1300mm; Cylindrical particles;Diameter=1.2mm, Length=4.3mm	Air-Water	Wire mesh	L=0-0.41 G=1.6-8.2	Introduced wire mesh tomography for maldistribution measurement.
Bazmi et al.(2012)	Column diameter:140mm Height: 100-1000mm Trilobe particles	Nitrogen-water	X-ray tomography	L=0-5.4 G=0-0.12	Liquid Maldistribution also measured. Gave a correlation to describe porosity distribution for trilobe particles.

2.2 Review of modeling and simulation studies

Modeling and simulation studies have been quite useful for scale-up and optimization of operating conditions of Trickle bed reactors. The other techniques used for scale-up are analysis of dimensionless groups and pilot plants. Pilot plants are, in general, very time consuming and expensive and dimensionless group analysis has poor accuracy because of complex hydrodynamics of these reactors. Hence, both these techniques have proved to be of limited use which provided impetus to developing models for hydrodynamics of trickle bed reactors.

There are three modeling approaches reported in literature in order to model multiphase flow systems. These include-

1. *Euler–Langrange approach*: In this approach, the primary fluid phase is treated as a continuum and the conservation equations are solved treating it a single phase system. The secondary phase is assumed to be a dispersed phase having low mass velocity and occupying very little volume in the reactor compared to primary phase. The dispersed or secondary phase is solved for by tracking the number of bubbles or droplets using equations of motion throughout the reactor. Applicability of this approach is limited by the assumption of low volume fraction for the dispersed phase.

2. *Euler–Euler approach*: Each phase is considered to be in continuum in this approach and a set of conservation equations for momentum and continuity is solved for each phase. Pressure is taken to be common for all the phases in the system and the inter-phase momentum exchange terms were used for drag force exerted by different phases. This is most commonly used approach for modeling multiphase flow phenomenon in a TBR.

3. *Volume of Fluid (VOF) approach*: The VOF model also known as surface-tracking technique is applied to a fixed Eulerian mesh. The VOF model is generally used for modelling of system with two or more immiscible fluids. Since it is a surface tracking technique the interface between the fluids is given great importance. In the VOF model, all the fluids share a single set of momentum equations. The volume fraction of all the fluids is kept under track for all computational cells.

A review of the works carried out by various investigators on hydrodynamics of trickle bed reactors with special emphasis on modeling and simulation aspect has been detailed and discussed in the following section of report.

With a view to compare the different correlations given by **Satterfield(1975), Charpentier and Favier (1975)** presented experimental data of twenty gas-hydrocarbon systems. It was shown that the predicting correlations with respect to water were flawed when used for hydrocarbons. Flow patterns in foaming liquids were also studied and four distinct patterns, namely foaming flow, foaming pulsing flow, pulsing flow and spray flow were observed.

A procedure for finding effectiveness factor for non-uniform boundary conditions which exist when some part of catalyst is covered by gas was given by **Herkowitz et al. (1979).** The rate of hydrogenation reaction was measured in a recycle trickle bed reactor using Pd/Al catalyst. The reaction rate was found to drop significantly with decreasing liquid flow, thereby emphasising the effect of wetting efficiency on the rate of reaction. The global rate was found to increase for effectiveness factor less than unity for same hydrogen concentration. This effect has been attributed to be the higher contribution from gas covered surface as compared to that covered by the liquid.

A correlation for determining variation in porosity for cylindrical beds packed with solid non-porous catalyst particles was given by **Mueller (1991).** Catalyst particle diameter and reactor diameter were used to determine radial distribution of porosity in a packed bed of spherical catalyst particles. The correlation was found to be satisfactorily accurate when compared with the experimental data for porosity variation.

Attou and Ferschneider (1999) developed interphase momentum interaction closure equations to model the physical momentum exchange between interacting phases. The model equations were developed assuming the TBR to be operating under trickling flow regime. The model also took into account the presence of liquid films and gas liquid slip motion and was based on Kozeny-Carman equation.

A new mechanistic film model was developed by **Iliuta et al. (2002)** based on slit models for describing the hydrodynamic parameters in TBRs. A novel approach based on falling film model was used for modelling the packed bed reactors. Also the interaction between different phases was defined using an interaction factor for fluid pairs. The accuracy of prediction of

proposed model was checked by comparing the results of simulation against a huge database that composed of about five thousand experimental studies on hydrodynamics of TBRs.

A steady state non-isothermal model for simulating the reactor performance for hydrogenation reaction was developed by **Dietz et al. (2003).** The model was used to simulate consecutive hydrogenation of 1,5,9-cyclododecatriene on a Pd/Al_2O_3 catalyst in trickle bed reactor. The model was also compared with experimental results obtained from literature. The heterogeneous model proposed takes into account the resistances to heat and mass transfer at all phase interfaces viz. gas–liquid, liquid–solid and solid–gas interfaces as well as the partial wetting of the catalyst particles. The model the catalyst particles to be divides into two zones that is wetted and dry catalyst surface and material transfer between these two zones was described by simplified diffusion mechanism. The model gave improved prediction of outlet concentration of products hydrogenation reaction as compared to other models prior to it.

Bhaskar et al. (2004) developed a three phase, non-isothermal, heterogeneous model based on two film theory in order to simulate the hydrodynamics and reaction yield of a TBR. The model incorporates mass transfer phenomenon at gas-liquid and liquid-solid interphases. The three phase model was solved to find the kinetic parameters for various hydrotreating reactions. A partial wetting model was also proposed in this study in order to account for incomplete wetting in the bed. The model predictions were found to be in good agreement with extensive experimental data available in literature over the range of operating conditions. Using the kinetic parameters from the pilot plant study, the model was applied to an industrial reactor assuming complete wetting, and was found to simulate the reactor adequately. The model was further used for studying the effect of feed rate and reactor temperature on product specifications.

The spread of liquid flow in a trickle bed reactor was studied by **Boyer et al. (2005)**. Gamma-ray tomography and a liquid collector was used to study the spread of liquid along the reactor from a single point source in a trickle bed reactor. Further, a two dimensional computational fluid model was simulated and validated with the experimental data obtained in this study.

Jiang et al. (2002) used a k-fluid Eulerian model to simulate the flow in packed beds. The porosity within the trickle bed was considered to be normally distributed. Phase interactions between different phases were considered to be governed by model proposed by Attou et al.

(1999). The predicted results of the modelled were compared with the experimental data in the literature. The influence of liquid and gas flow rates and the impact of prewetting condition on liquid distribution on hydrodynamic parameters was also discussed in this study.

A two phase single lump mathematical model of trickle bed reactor was developed by **Murli et al. (2006)** to simulate commercial hydrotreating reactors. This model accounted for main hydrotreating reactions which include hydrodesulfurization, hydrodearomatization and olefin saturations. The model was validated by plant performance data for ultra-low sulfur levels. The model also took into account feed vaporization in energy balance equations. The model predictions also closely resembled the product quality, hydrogen consumption and temperature profile of the catalyst bed.

In order to describe liquid-gas non-uniform distribution in a packed bed **Alopaeous et al. (2006)** developed a cellular automata model. The model is inspired by visual observations of rivulet flow under influence of gravity, wavy surface of liquid film flowing on inclined plates, and interpretations from transparent wall trickle bed apparatuses. The study investigated many factors that may lead to non-uniform distribution of liquid phase in a trickle bed reactor. These factors include the inlet liquid distributor, the radial distribution of porosity due to wall effects, wetting efficiency of the operation and surface tension of the liquid phase. Axial and radial dispersion of the liquid flow are inherently included in the model, since the fundamental model probability parameters are directly related to the dispersion coefficients. This model was found to be very robust and fast and also used parallel computations to speed up convergence of the solution. Because of its parallel approach the number of calculations required to carry out this approach was a fraction of what other algorithms required. The model predictions were evaluated for three different examples.

Gunjal and Ranade (2007) developed a CFD model based on Euler-Euler approach to simulate the flow and reaction kinetics in a TBR. The same model was used in order to simulate flow in a laboratory scale reactor as well as a commercial scale reactor. The variation in porosity within the reactor was modelled using Mueller correlation for radial variation in porosity of spherical catalyst particles in a cylindrical packed column (**Mueller, 1991**). The interphase momentum interaction between different phases was modelled using **Attou and Ferschneider (1999)** studied the hydrodynamics and also simulated the reaction performance of hydrotreating TBRs.

Atta et al. (2007) used the concept of relative permeability in describing the drag forces between two phases. The predictions by the model were compared with experimental data available in literature. The model laid emphasis on uniformity in distribution of liquid phase and also includes factors to account for non-uniform distribution. In order to determine better alternatives for determining the distribution of liquid phase, sensitivity analysis of hydrodynamic parameters with respect to liquid distribution was carried out. The model was found to be less demanding in terms of computational power and was found to predict the hydrodynamic parameters for large scale and industrial scale plants with good accuracy.

Lopes et al. (2009) modelled multiphase flow in a trickle bed reactor. In this study, a three dimensional Eulerian-Eulerian multiphase model for predicting hydrodynamic parameters was proposed. The model was only applicable for trickling flow regime and used a three dimensional grid to simulate the reactor. The predictions of the model were compared with the experimental data for pressure drop and liquid holdup in trickling flow regime available in the literature. The model also led to the study of flow development and liquid mal-distribution with three types of liquid distributors on top of the packed bed. The study also inquired into changes in the hydrodynamics with changing liquid and gas flow rates. It was observed that the liquid flow rate had pronounced effect on radial pressure drop profiles for high interaction regimes whereas gas flow has prominent effect at low interaction regimes. It was evident from this study that the main reason for non-optimum use of catalyst and thermal instability was liquid mal-distribution.

Atta et al. (2009) presented the initial development of a comprehensive CFD based model in order to predict hydrodynamic parameters like pressure drop and liquid saturation in TBRs under high pressure. A two-phase hydrodynamic Eulerian-Eulerian CFD model foreseeing the flow domain as porous region for assessing these hydrodynamic parameters even for high pressure operations has been proposed. Evaluation of model estimates have been carried out with reported experimental data, collected under diverse set of operating conditions.

CFD based model was used to find wetting efficiency and catalyst efficiency by **Augier et al. (2010)**. In this study, volume of fluid (VOF) model was used to describe hydrodynamics which led to realistic and promising results for surface wetted ratio. It was also suggested in this study to include tortuosity as a parameter along with equivalent diameter and porosity to completely account for the geometry of the particle and its packing characteristics in a trickle bed reactor.

Bazmi et al. (2012) developed a numerical model for determination of liquid mal-distribution in randomly packed trickle bed reactor. A three phase CFD model based on the Eulerian-Eulerian approach is used and a two-fluid model is used to describe the interphase momentum exchange between different phases. Also porosity was considered to vary along the radial direction in order to account for the wall effects. Two types of liquid distributors (mono and multi orifice distributor) at the inlet were used in order to study the effect of liquid distribution on hydrodynamic parameter prediction by the model. In order to validate the CFD model, the predictions by the model are compared with the experimental data from the literature and also with predictions from the porous media concept which use the relative permeability model to describe the inter-phase momentum exchange between different phases. The experimental results to check the validity of model were obtained using a pilot scale reactor set-up using trilobe catalyst operating under trickling regime. Along with the experimental data the model is also validated by the results obtained by porous media concept. This model was a definite improvement over other CFD models in terms of accuracy of the predictions.

CHAPTER-3
MODEL DESCRIPTION

Modeling of flow in multiphase system is commonly considered to be a formidable challenge because it involves modeling and description of interaction forces/momentum transfer between different phases. The Eulerian-Eulerian model is widely used to model hydrodynamics of the trickle bed reactors. The accuracy of prediction of a CFD Eulerian hydrodynamic model is highly dependent upon how accurately it describes the interphase momentum exchange. Two models based on Eulerian approach that differ in their description of momentum interaction between phases are discussed in the following section.

The following assumptions are considered for the Eulerian model:

1. The pressure inside the reactor is considered to be uniform i.e. pressure drop is insignificant as compared with the operating pressure.
2. The liquid phase is non-volatile.
3. The catalyst particles are completely wetted i.e. wetting efficiency of catalyst particles in trickle bed is unity.
4. The capillary pressure is negligible as the bed is taken to be completely wetted.
5. The bed is considered to be isothermal.
6. An ideal liquid and gas distribution is assumed at inlet. This means that the velocity profile is assumed to be flat at the inlet boundary of the reactor

3.1 Three phase two dimensional Euler-Euler model.

The three phase model was proposed by Attou and Ferschneider (1999). This model considers the solid phase as a separate phase and the velocity of the solid phase in both the dimensions is considered to be zero. The momentum exchange equations are based on phase interaction momentum transfer between all the three phases.

Continuity equation:

The continuity equation for phase q (q is G for gas phase, S for solid phase and L for liquid phase) is given as

$$\frac{\partial(\rho_q\,\varepsilon_q)}{\partial t} + \nabla\,.\left(\rho_q\,\varepsilon_q\overrightarrow{v_q}\right) = 0 \qquad (3.1)$$

Where, ε_q is the volume fraction of phase q, v is the velocity vector, and ρ is the density with the constraint:

$$\Sigma\varepsilon_q = 1 \qquad (3.2)$$

$$\overrightarrow{v_S} = 0 \qquad (3.3)$$

The velocity of the catalyst solid particles is considered to be fixed and equal to zero. Volume fraction of solid phase can easily be calculated as

$$\varepsilon_S = 1 - \varepsilon \qquad (3.4)$$

Where, ε is the porosity of the bed and is calculated by correlation for radial porosity distribution, as discussed later on.

Momentum conservation equation:

$$\frac{\partial(\rho_q\,\varepsilon_q\overrightarrow{v_q})}{\partial t} + \nabla\,.\left(\,\rho_q\,\varepsilon_q\overrightarrow{v_q}\overrightarrow{v_q}\right) = \,-\varepsilon_q\nabla\,P + \nabla.\left(\varepsilon_q\mu\nabla v_q\right) + \rho_q\,\varepsilon_q\vec{g} + \sum \mathrm{K_{pq}}\left(\overrightarrow{v_q} - \overrightarrow{v_p}\right) \qquad (3.5)$$

where, P is the pressure shared by all the phases in the system, μ is the viscosity of the phase considered, and K_{pq} is the inter-phase momentum exchange coefficient between phase p and phase q.

For defining interphase momentum exchange coefficient, a model proposed by Attou and Ferschneider (1999) and which is based on Ergun equation is used.

Interphase momentum exchange coefficients (Attou and Ferschneider (1999)):

Gas-Liquid momentum exchange coefficient is given as

$$K_{GL} = \varepsilon_G\left(\frac{E_1\mu_G(1-\varepsilon_G)^2}{\varepsilon_G^2 d_p^2}\left[\frac{\varepsilon_S}{1-\varepsilon_G}\right]^{0.667} + \frac{E_2\rho_G(U_G-U_L)(1-\varepsilon_G)}{\varepsilon_G d_p}\left[\frac{\varepsilon_S}{1-\varepsilon_G}\right]^{0.333}\right) \qquad (3.6)$$

Gas-solid momentum exchange coefficient is given as

$$K_{GS} = \varepsilon_G \left(\frac{E_1 \mu_G (1-\varepsilon_G)^2}{\varepsilon_G^2 d_p^2} \left[\frac{\varepsilon_S}{1-\varepsilon_G} \right]^{0.667} + \frac{E_2 \rho_G U_G (1-\varepsilon_G)}{\varepsilon_G d_p} \left[\frac{\varepsilon_S}{1-\varepsilon_G} \right]^{0.333} \right) \quad (3.7)$$

And the liquid-solid momentum exchange coefficient is given as

$$K_{LS} = \varepsilon_L \left(\frac{E_1 \mu_L \varepsilon_S^2}{\varepsilon_L^2 d_p^2} + \frac{E_2 \rho_L U_G \varepsilon_S}{\varepsilon_L d_p} \right) \quad (3.8)$$

where, E_1 and E_2 are Ergun constants (Attou and Ferschneider, 1999) . The values of constants E_1 and E_2 can be obtained either from experiments or from numerical simulations. The value of these constants cannot be taken the same as that for a single phase system.

The model described above was used to simulate trickle bed of dimension 0.5m x 0.019m as used by Chowdhury et al. (2002) for their experimental studies. The catalyst particle is considered to be spherical in shape and 2 mm in diameter. Variation of radial porosity is considered using porosity distribution models discussed later on. The model results are then validated with simulation results reported by Gunjal and Ranade (2007) as the experimental results (Choudhury et al., 2002) were available only for conversion and kinetic parameters.

The different particle shape and dimensions as used in the simulation along with Ergun constants are taken from the work of Gunjal and Ranade (2007). The values of Ergun constants given are considered to be applicable for liquid velocity in the range of 0.07-0.5 mm/s and gas velocity in the range of 0.7-6 mm/s. These values are given in Table 3.1

Table 3.1: The shape and size of the particles and the values of E_1 and E_2 (Gunjal and Ranade 2007).

Shape	Size(mm)	E_1	E_2
Sphere	2.5	215	1.8
Sphere	2	263	4.99
Trilobe	2	263	4.99

Simulation setup and evaluation of properties of liquid and gas phase at operating conditions are discussed in the next chapter.

3.2 Two phase two dimensional Euler-Euler model in porous media.

Pseudo-two phase model which is based on porous media concept was proposed by Saez and Carbonell (1985). The momentum exchange equations used in this model are based on relative permeability of flowing phases and the flow field is considered as a porous medium.

Continuity equation:

The volume averaged continuity equation for phase q (q is taken as G for gas phase and L for liquid phase) is given as

$$\frac{\partial(\rho_q\,\varepsilon_q)}{\partial t} + \nabla\,.\left(\rho_q\,\varepsilon_q\overrightarrow{v_q}\right) = 0 \qquad (3.9)$$

where, ε is the volume fraction of each phases, v is the velocity vector, and ρ is the density, for phase q with the constraint that

$$\Sigma\varepsilon_q = 1 \qquad (3.10)$$

The flow field is considered to be a porous medium with porosity variation described by Mueller (1991) correlation.

$$\frac{\partial(\rho_q\,\varepsilon_q\overrightarrow{v_q})}{\partial t} + \nabla\,.\left(\,\rho_q\,\varepsilon_q\overrightarrow{v_q}\overrightarrow{v_q}\right) = \,-\varepsilon_q\nabla\,P + \nabla.\left(\varepsilon_q\mu\nabla v_q\right) + \rho_q\,\varepsilon_q\vec{g} + \overrightarrow{F_q} \qquad (3.11)$$

where, P is the pressure shared by all the phases in the system. F_q is the drag force per unit volume of the bed exerted by phase q (liquid or gas).

For defining the drag force experienced by fluid phases, a model based on relative permeability concept and as proposed by Saez and Carbonell (1985) is used. This is mathematically represented as

$$\frac{F_q}{\varepsilon_q} = \frac{1}{k_q}\left[E_1\,\frac{Re_q}{Ga_q} + E_2\,\frac{Re_q^2}{Ga_q}\right]\rho_q g \qquad (3.12)$$

$$Re_q = \frac{\rho_q v_q d_e}{\mu_q(1-\varepsilon)} \qquad (3.13)$$

$$Ga_q = \frac{\rho_q^2 g d_e^3 \varepsilon^3}{\mu_q^2(1-\varepsilon)^3} \qquad (3.14)$$

$$d_e = \frac{6V_p}{A_p} \quad (3.15)$$

The direction of drag force is opposite direction to the velocity of fluid in every cell.

The relative permeability of the liquid and gas phase was calculated by using the correlations proposed by Saez and Carbonell (1985):

$$k_l = \delta_l^{2.43} \quad (3.16)$$

$$k_g = S_g^{4.8} \quad (3.17)$$

where, δ_l is the reduced saturation and S_g is Saturation of gas phase in the bed.

δ_l is related to liquid holdup as follows:

$$\delta_l = \frac{\varepsilon_l - \varepsilon_l^o}{\varepsilon - \varepsilon_l^o} \quad (3.18)$$

where, ε_l = Dynamic liquid holdup

ε_l^0 = Static liquid holdup

ε = Bed porosity

The static liquid holdup is defined as the volume fraction of liquid in trickle bed reactor that remains in the bed after draining and is given as

$$\varepsilon_l^o = \frac{1}{20 + 0.9E_o^*} \quad (3.19)$$

where, $E_o^* = \frac{\rho_l g d_p^2 \varepsilon^2}{\sigma_l (1-\varepsilon)^2}$ (3.20)

The model described above was used to simulate trickle bed of dimension 0.5715m x 0.0219m as used by Al-Dahhan and Dudukovic (1994) for their experimental studies. The catalyst particle is considered to be spherical (diameter 1.14mm) and porous extrudate (equivalent diameter 1.99mm). A detailed account of bed properties and Ergun constants used for simulation is given in Table: 3.3. Variation of radial porosity is considered using porosity distribution models discussed later on. The radial porosity distribution for porous extrudate catalyst particles was considered to be similar to that of spherical particles, and the same

correlation was used to determine it. The physical properties of both the liquid and gas phases were used from ASPEN database, and are being given in Table: 3.4

The model results are then validated with the experimental results given by Al-Dahhan and Dudukovic (1994). The three phase model discussed earlier is also simulated for this reactor and the predictions of the two models are then compared.

The trickle bed reactor is considered to have radial distribution of porosity. Several researchers, notably Mueller (1991, 1992), and De Klerk (2003) have given correlations for radial variation of porosity in trickle bed reactors for spherical catalyst particles. The radial porosity distribution is dependent upon the shape and size of the particle, and the diameter of the reactor. For describing the porosity variation of trilobe shaped particle, a correlation which was recently proposed by Bazmi(2011) has been used. These correlations are discussed in detail in the following section.

3.3 Radial porosity distribution model

Radial porosity distribution in a trickle bed reactor plays an important role for cases in which the wall effects dominate. This is generally true for laboratory scale trickle bed reactors. For industrial scale reactor the porosity variation is generally neglected as the reactor diameter is much larger than that of the catalyst particle diameter, and the variation of porosity can be neglected at a distance of approximately ten particle diameters from the reactor wall.

The radial porosity distribution in a cylindrical trickle bed reactor using the bed of spherical particles with different bed to particle diameter ratios has been proposed by Mueller (1991) as follows:

$$\varepsilon(r) = \varepsilon_B + (1 - \varepsilon_B) J_0(ar^*) e^{-br^*} \qquad (3.21)$$

$$a = 8.243 - \frac{12.98}{(D/d_p - 3.156)} \qquad \text{(for } 2.61 < D/d_p < 13\text{)} \qquad (3.22)$$

$$a = 7.383 - \frac{2.932}{(D/d_p - 9.864)} \qquad \text{(for r } D/d_p > 13\text{)} \qquad (3.23)$$

$$b = 0.304 - \frac{0.724}{D/d_p} \qquad (3.24)$$

$$r^* = r/D \qquad (3.25)$$

where,

ε_B = bulk porosity of the bed.

r= distance from the reactor wall.

r*= dimensionless distance from the wall.

D= reactor diameter.

d_p= particle diameter.

$J_0(x)$= zeroth order Bessel function, given as.

$$J_0(x) = 1 - \frac{\left(\frac{x}{2}\right)^2}{(1!)^2} + \frac{\left(\frac{x}{2}\right)^4}{(2!)^2} - \frac{\left(\frac{x}{2}\right)^6}{(3!)^2} + \frac{\left(\frac{x}{2}\right)^8}{(4!)^2} \quad (3.26)$$

Mueller (1992) modified the constants of the above model to incorporate the effect of bed diameter to particle size ratio up to 2.

He proposed that the constants may be calculated as

$$a = 7.45 - \frac{3.15}{(D/d_p)} \quad \text{(for } 2.02 < D/d_p < 13) \quad (3.27)$$

$$a = 7.45 - \frac{11.25}{(D/d_p)} \quad \text{(for } D/d_p > 13) \quad (3.28)$$

$$b = 0.304 - \frac{0.724}{D/d_p} \quad (3.29)$$

De Klerk (2003) proposed the following correlation for radial porosity distribution:

$$\varepsilon(r) = 2.14r^{*2} - 2.53r^* + 1 \quad \text{for } r^* < 0.63 \quad (3.30)$$

$$\varepsilon(r) = \varepsilon_B + 0.29\exp(-0.6r^*)\cos\left(2.3\pi(r^* - 0.16)\right) + 0.15\exp(-0.9r^*) \quad \text{for } r^* > 0.63 \quad (3.31)$$

For trilobe catalyst particles in cylindrical trickle bed reactor, the radial porosity distribution is given by Bazni(2011). His correlation is given as

$$\varepsilon = (\varepsilon_b + 0.045) + (1 - (\varepsilon_b + 0.045))\left[\left(e^{-0.1252\frac{x}{d_p}}\right)^2 + M\right] \quad (3.32)$$

Where,

$$M = \sum_{i=1}^{3} \left(\frac{A_i \left(\frac{x}{d_p}\right)^2}{\frac{x}{d_p}^{(3+2(i-1))} + B_i} \right) \quad (3.33)$$

x= distance from the wall of the reactor (m).

d_p= equivalent Sauter mean diameter (m) $= \frac{6V_p}{S_p}$ (3.34)

V_p= volume of the catalyst particle (m^3).

S_p= surface area of the catalyst particle (m^2).

The values of constants A_i and B_i for different values of i (i=1,2,3) are given in Table 3.2

Table 3.2: Values of the constants for radial porosity correlation given by Bazmi et al. (2011)

i	A_i	B_i
1	-1.8	0.048
2	1.18	0.357
3	0.026	0.002

3.4 Experimental data and properties used for simulation

For simulating the hydrodynamics of TBRs, two experimental studies have been considered: those given by Al-Dahhan and Dudukovic (1994) and Chowdhury et al. (2002). The above mentioned models are simulated for these reactors. The catalyst bed properties used in the simulation studies are given in Table 3.3.

Table3.3: Description of bed porosity and catalyst particle shape and size used in simulations.

Experimental study	Bed-dimensions, m	Catalyst particle shape	Catalyst Particle size, m	Bulk porosity	E_1	E_2
Al-Dahhan and Dudukovic (1994)	L=0.5715 D=0.0219	Spherical/ Porous extrudate	0.00114/ 0.00199	0.392/ 0.355	334.1	3.23
Chowdhury et al.(2002)	L=0.500 D=0.019	spherical	0.0025	0.5	263	4.99

Properties of components described in Al-Dahhan and Dudukovic (1994) at different operating conditions are taken from ASPEN database. These properties are given in Table 3.4.

Table 3.4: Properties of the gas and liquid phase components at operating conditions used for simulations.

Investigators	Gas/ liquid phase component	Pressure, Mpa	Temperature, K	Density, Kg/m^3	Viscosity, Pa.s	Surface tension, N/m
Al-Dahhan and Dudukovic (1994)	Hexane	0.31	298	656.16	0.0002938	0.017928
		2.13	298	656.16	0.0002938	0.017928
		3.55	298	656.16	0.0002938	0.017928
	nitrogen	0.31	298	3.504977	1.77E-05	-
		0.5	298	5.65319	1.77E-05	-
		2.1	298	23.7434	1.77E-05	-
		3.55	298	40.13765	1.77E-05	-
	Helium	2.13	298	3.440949	1.99E-05	-
	water	0.5	298	994.7491	0.0009155	0.0728436
		2.1	298	994.7491	0.0009155	0.0728436

The correlation given by Standing-Katz correlation and as used by Gunjal and Ranade (2007) was used for calculating the variation of oil density with pressure and temperature:

$$\rho_l(P.T) = \rho_{l0} + \Delta\rho_{lP} + \Delta\rho_{lT} \quad (3.35)$$

$$\Delta\rho_{lP} = [0.167 + 16.181 * 10^{-0.0425\rho_{l0}}] * \left[\frac{P}{1000}\right] - 0.01 * [0.299 + 263 * 10^{-0.0603\rho_{l0}}] * \left[\frac{P}{1000}\right]^2 \quad (3.36)$$

$$\Delta\rho_{lT} = [0.0133 + 152.4(\rho_{l0} + \Delta\rho_{lP})^{-2.45}][T - 520] - \left[8.1 * 10^{-6} - 0.0622 * 10^{-0.764(\rho_{l0}+\Delta\rho_{lP})}\right] * [T - 520]^2 \quad (3.37)$$

where,

ρ_l = Oil density, lb/ft^3

ρ_{l0} = Oil density at normal temperature and pressure (15.6°C, 101.3 kpa), lb/ft^3.

$\Delta\rho_{lP}$ = Change in density of oil with change in pressure, lb/ft^3.

$\Delta\rho_{lT}$ = Change in oil density with temperature lb/ft^3.

P= Pressure, psia.

T= Temperature, R.

For calculating the oil viscosity, the following correlation was used which was given by Glasso and published in Ahmed (1989).

$$\mu = 3.141 * 10^{10} * (T - 460)^{-3.444} * [log_{10}(API)]^a \quad (3.38)$$

$$a = 10.313 * [log_{10}(T - 460)] - 36.447 \quad (3.39)$$

where, μ is in mPa.s and T is in °R.

CHAPTER-4
GRID AND SIMULATION SET-UP

4.1 Three phase model (Attou and Ferschneider (1999)).

ANSYS Gambit 2.3.16 is used in creating a trickle bed reactor of dimensions 0.5 m long and 0.019 m wide. The reactor size is taken from the experimental study conducted by Chowdhury et al. (2002). The grid was then meshed and exported to simulation software ANSYS FLUENT 6.3.26. The results of the simulations were then compared with those given by Gunjal and Ranade (2007).

Given below is the grid used for simulations (Fig. 4.1)

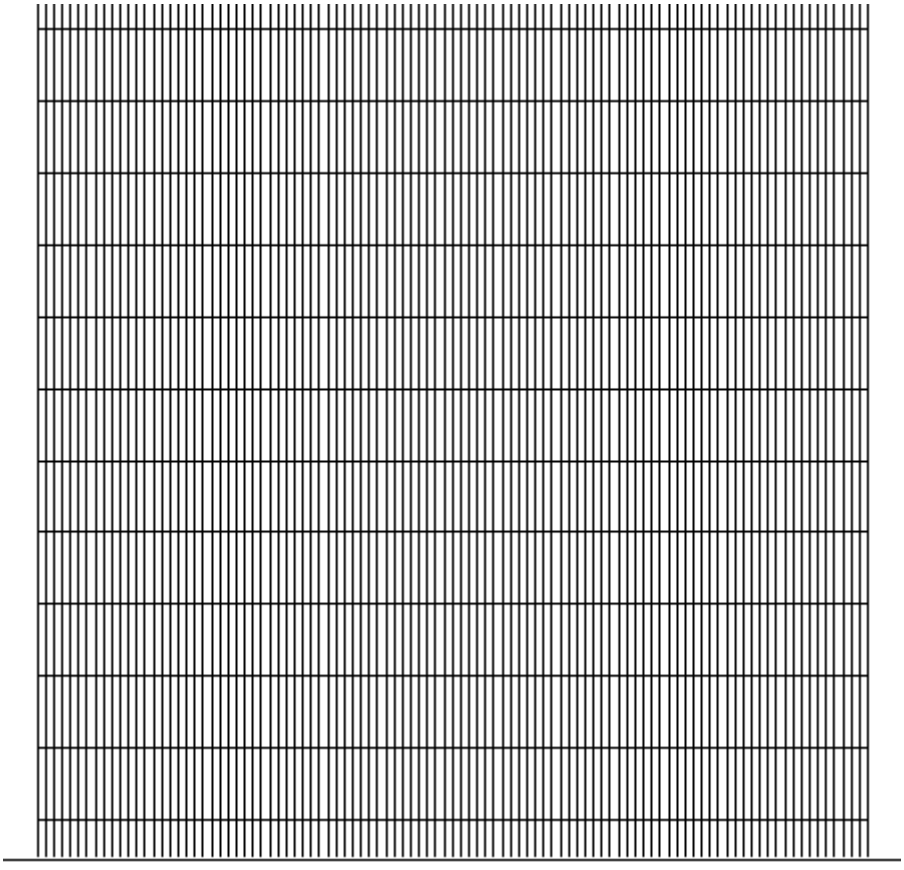


Fig. 4.1: Section of grid used for simulation.

Table: 4.1-4.8 describes the settings used for simulation in ANSYS FLUENT 6.3.26.

Table 4.1: Geometry description

Height(m)	0.5
Width(m)	0.019
No. of cells	5000
No. of faces	10150
No. of nodes	5151

Table 4.2: Boundary Conditions

Inlet boundary condition	Velocity inlet
Outlet boundary condition	Pressure outlet (24Mpa)
Wall boundary condition	No slip

Table 4.3: Model description

Model	Settings
Space	2D
Time	Unsteady, 1^{st}-Order Implicit
Viscous	Reynolds stress model
Wall	No-slip, stationary
Multiphase RSM model	Mixture RSM

Table 4.4: Operating Conditions

Pressure (Mpa)	24
Temperature (K)	633
Gravitational acceleration(m/s^2)	x-direction:0 y-direction:-9.81

Table 4.5: Gas phase-Hydrogen (Properties of pure hydrogen taken from ASPEN database)

Component	Hydrogen
Density (kg/m^3)	0.96863258
Viscosity(kg/m-s)	0.00001492
GHSV(h^{-1})	200, 400, 600, 1000, 1600

Table 4.6: Liquid phase-Diesel oil.

Components (Chowdhury et al. 2002)	Total Aromatics: 33.50% Mono-aromatics: 17.96% Di-aromatics: 8.77% Tri-aromatics: 1.64% Tetra-aromatics: 0.953% Unidentified: 4.19% Naphthenes: 19.25% S: 16 ppm N: 218 ppm
Density (kg/m^3)	1043.2
Viscosity (kg/m-s)	0.00028529
LHSV (h^{-1})	1,2,3,5,8.

Table 4.7: Solid phase-Aluminium

Diameter	2mm,2.5mm
Shape	Sphere, Trilobe
Bulk Porosity	0.5
Fixed value (zero velocity)	$u_s=0$ $v_s=0$

Table 4.8: Solution controls

Time step size	0.001s
Convergence criteria	10^{-4}
Discretization method	First order upwind

4.2 Two phase model with porous media concept (Saez and Carbonell (1985))

ANSYS Gambit 2.3.16 is used in creating a trickle bed reactor of dimensions 0.5715 m long and 0.0219 m wide. The reactor size is taken from the experimental study conducted by Al-Dahhan and Dudukovic (1994). The grid was then mashed and exported to simulation software ANSYS FLUENT 6.3.26. The results of simulations were then compared to those given by Gunjal and Ranade (2007)

Given below is the grid used for simulations (Fig. 4.2).

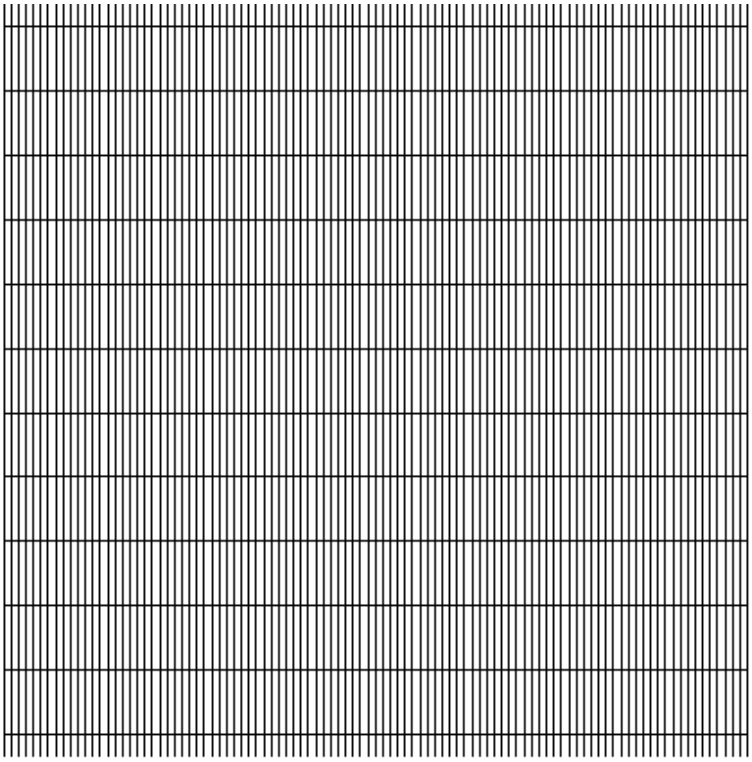


Fig. 4.2: Section of the grid used for simulation.

Table 4.9: Geometry description

Height(m)	0.5715
Width(m)	0.0219
No. of cells	5000
No. of faces	10150
No. of nodes	5151

Table 4.10: Boundary Conditions

Inlet boundary condition	Velocity inlet
Outlet boundary condition	Pressure outlet
Wall boundary condition	No slip

Table 4.11: Model description

Model	Settings
Space	2D
Time	Unsteady, 1^{st}-Order Implicit
Viscous	Reynolds stress model
Wall	No-slip, stationary
Multiphase RSM model	Mixture RSM

Table 4.12: Operating Conditions

Pressure (Mpa)	Variable (given in model description)
Temperature(K)	298
Gravitational acceleration(m/s^2)	x-direction:0 y-direction:-9.81

Table 4.13: Solution controls

Time step size	0.001s
Convergence criteria	10^{-4}
Discretization method	First order upwind

Properties of gases and liquids used in the simulation set up are given in Table 3.4.

CHAPTER-5
RESULTS AND DISCUSSIONS

5.1 Comparison of radial porosity models

The correlations given by Mueller (1991) (Eq. 3.21-3.26), Mueller (1992) (Eq. 3.21-3.29) and De Klerk (2002) (Eq. 3.30-3.32) were used to determine radial porosity variation which was plotted with experimental data from Benanti and Brosilov (1962) on MATLAB R2010a. The plot is given in Fig. 5.1.

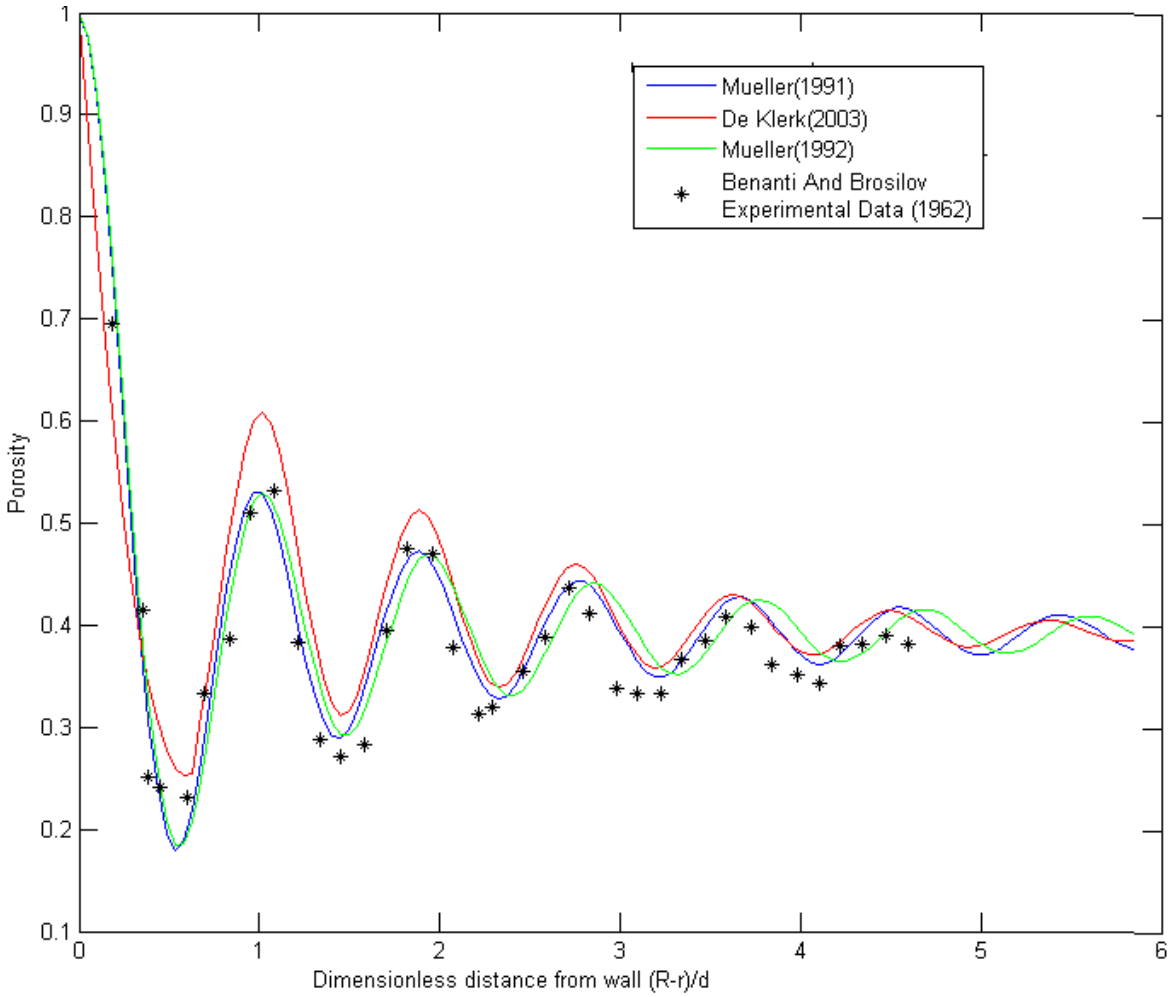


Fig. 5.1: Variation of radial porosity with respect to dimensionless distance from reactor wall.

Table 5.1: Error analysis of porosity variation models.

Models considered	Mueller(1991)	De Klerk(2003)	Mueller(1992)
Average Relative error	7.39%	11.56%	9.17%

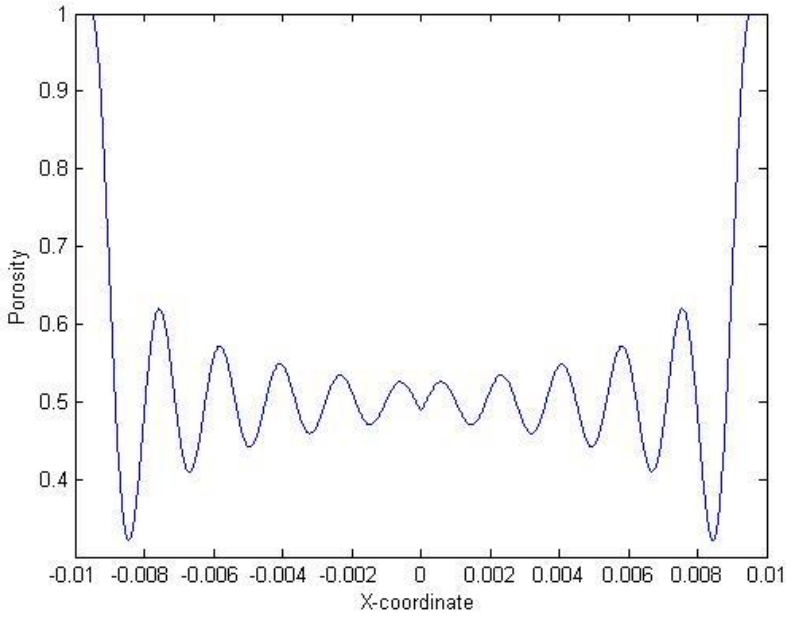
Average relative percentage error for each of the correlation with respect to experimental data is calculated and error analysis is given in Table: 5.1. Mueller (1991) was found to have lowest average relative error and hence is used for determining the porosity variation in hydrodynamic simulations.

5.2 Effect of reactor diameter to particle diameter ratio (D/dp) on porosity distribution

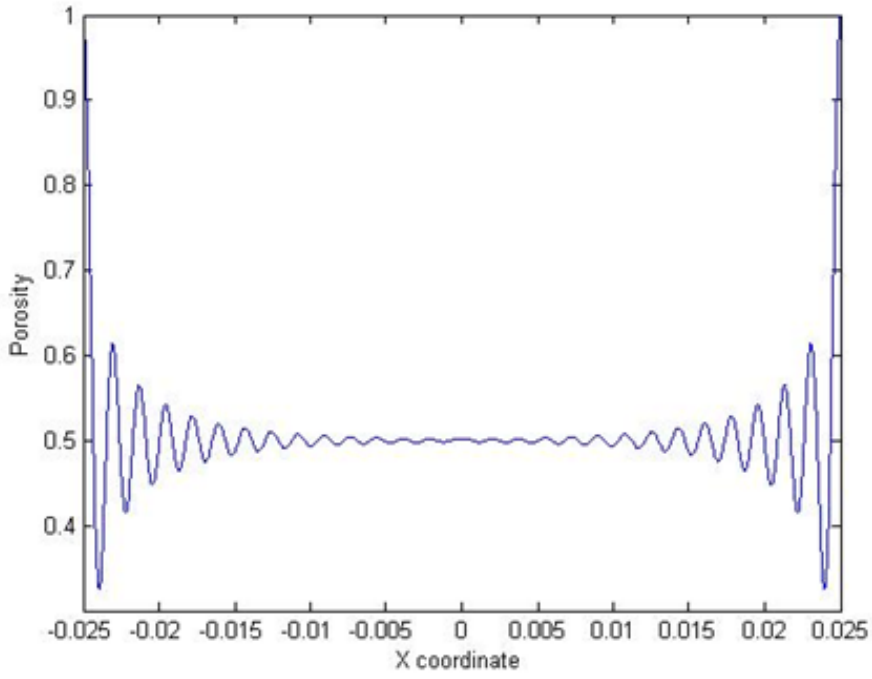
The porosity distribution as predicted by Mueller (1991) correlation (Eq. 3.21-3.25) was calculated for the reactor of dimensions used by Choudhury et al. (2002). In order to determine the effect of reactor diameter on porosity distribution, the reactor diameter was increased to 0.05m. The variation of porosity for both the cases is given in Fig. 5.2

High fluctuations in bed porosity can be observed from graphical representation of the porosity distribution (Fig. 5.2) near the wall. This can be attributed to more structured packing near the wall. As one moved away from the wall, the packing structure gets randomised and beyond a distance of 10 particle diameters, the porosity can be considered to be constant equal to bulk porosity of the bed. Therefore, in case of industrial reactors, where the diameter of the reactors is much larger than that of the catalyst particle diameter, the porosity fluctuations along the radial direction in bed can be neglected and porosity can be considered to be equal to bulk porosity. However, these fluctuations become important when predicting the outlet concentrations or hydrodynamics in case of laboratory scale reactors which are frequently used for scale-up of operations.

Radial porosity variation was calculated using a computer code written in MATLAB R2012a. The porosity, whence calculated, was exported as a matrix to C program thereby eliminating the need to calculate porosity for simulation iteration and to make the simulation faster. This C program was used as User Defined Function (UDF) to implement the radial distribution of porosity in ANSYS FLUENT 6.3.26. The C program used is provided in the Appendix to the dissertation text.



(a)



(b)

Fig. 5.2: Porosity variation for particle diameter of 2 mm and reactor diameter (a) 0.019 m (Choudhury et al. (2002)), and (b) 0.05 m as predicted by Muller(1991) correlation

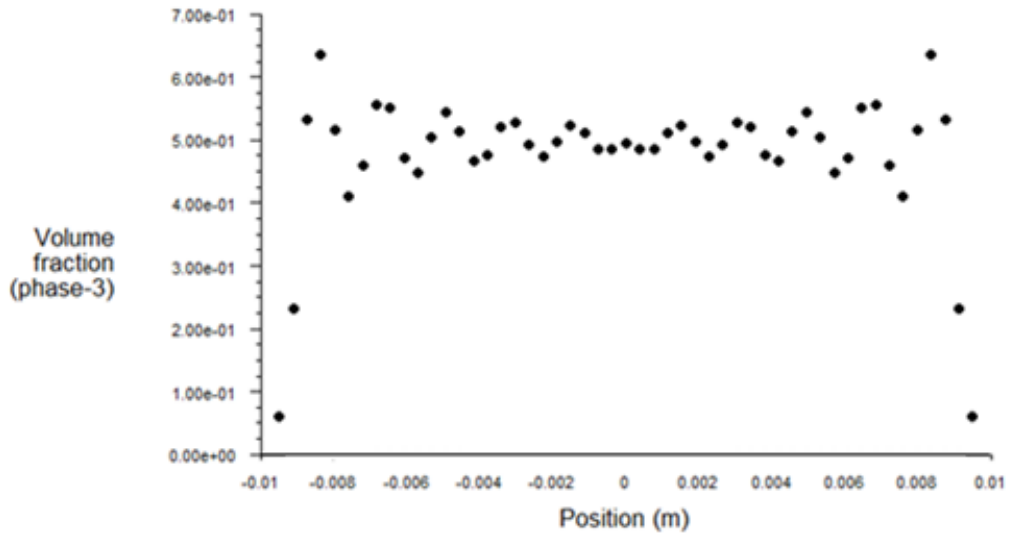


Fig. 5.3: Graphical representation of radial distribution of Solid phase volume fraction as implemented in ANSYS FLUENT 6.3.26.

5.3 Validation of three phase model

The three phase hydrodynamic model, Attou and Ferschneider(1999) was simulated using Mueller (1991) as model for radial porosity distribution. The simulation was done on ANSYS FLUENT 6.3.26. The reactor dimension of 0.5mx0.019m was used and was taken from experimental study of Chowdhury et al. (2002). Diesel oil (specifications given in Table 4.6) was used as liquid phase and hydrogen was used as gas phase. Catalyst particle was spherical and 2mm in diameter. Bulk porosity of bed was 0.5. Ergun constants for fluid pair at operating conditions were taken as 263 and 4.99, as given by Gunjal and Ranade (2007). Density and viscosity of diesel oil were calculated using equations 3.35-3.39. The liquid to gas flow rate ratio was maintained at $200m^3/m^3$. The liquid hourly space velocity was varied from 1-8 h^{-1}. Pressure was taken as 24 bar and temperature 633 K was taken. Hydrogen properties were taken from ASPEN data bank. The model was validated by comparing simulation results with results reported by Gunjal and Ranade (2007).

The result of simulation and comparison with simulated results of Gunjal and Ranade (2007) is given in following section.

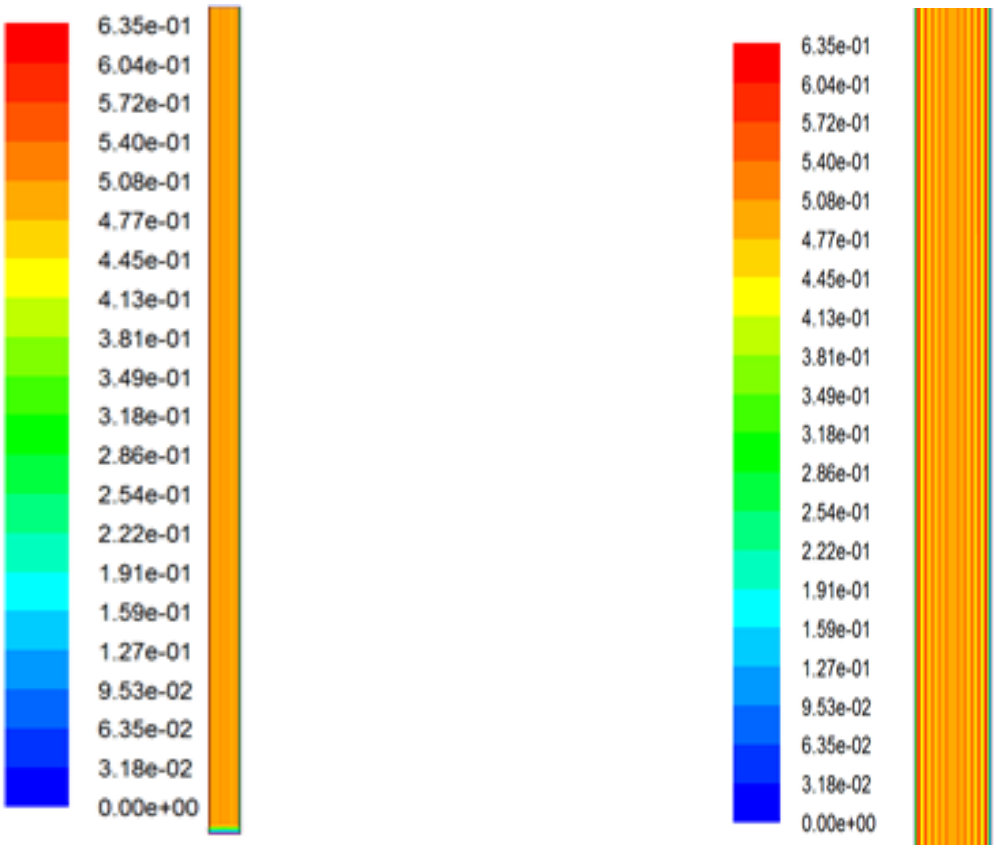


Fig. 5.4: Contours of volume fraction of solid phase for 2mm particle diameter and reactor diameter of 0.019m.

The contours of solid volume fraction clearly demonstrates the variation of porosity in the reactor beds filled with solid spherical catalyst particles, based on correlation suggested by Muller (1991). There have been some suggestions in literature for implementation of axial porosity variation based on statistical normal distribution function, but the extent of standard deviation to be considered, though small, is highly controversial and disputed. Hence, in this study only radial variation of porosity is considered.

Contours of liquid volume fraction generated after simulation is depicted in Fig. 5.5.

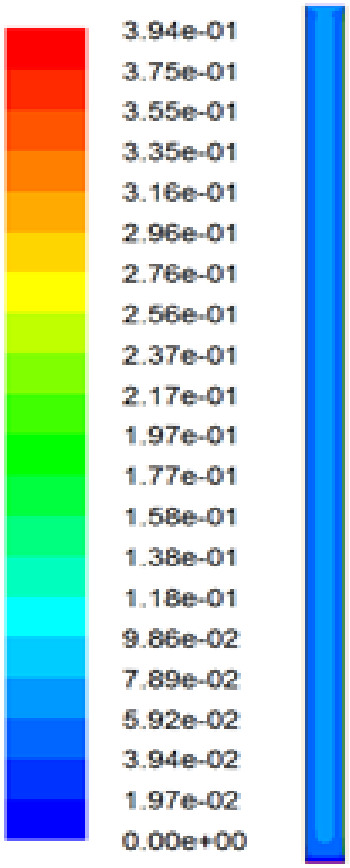
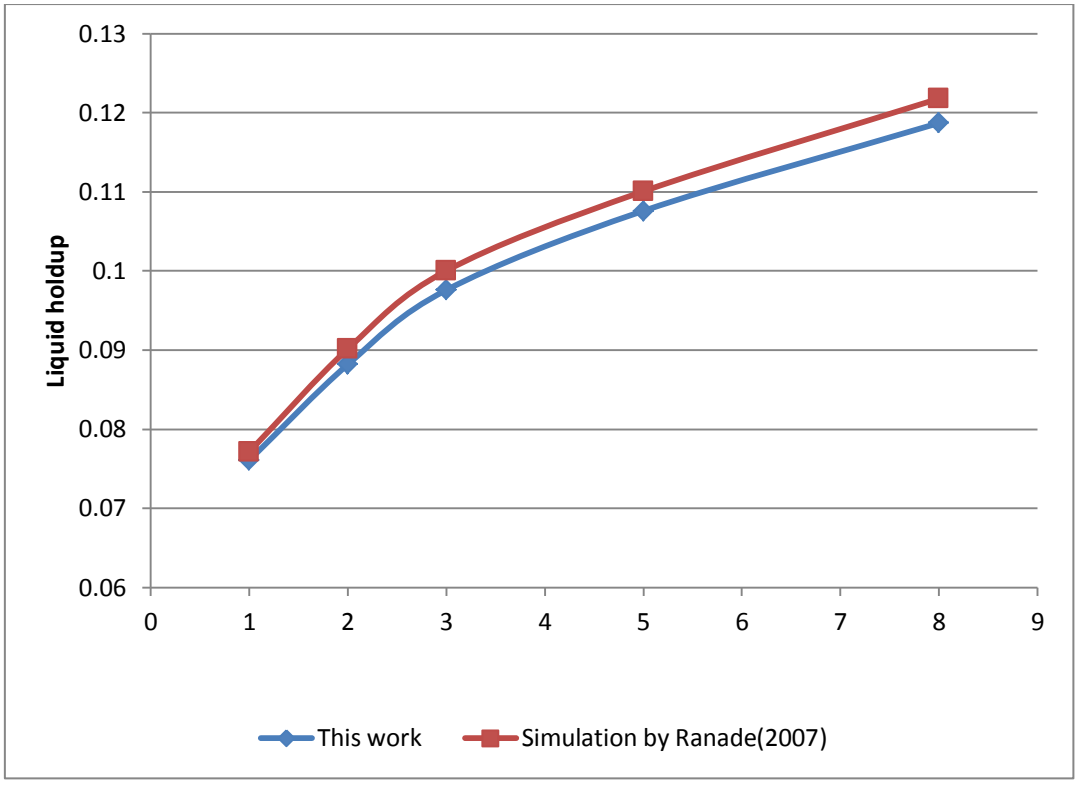


Fig. 5.5: Contours of volume fraction of solid phase for 2 mm particle diameter and reactor diameter of 0.019 m.

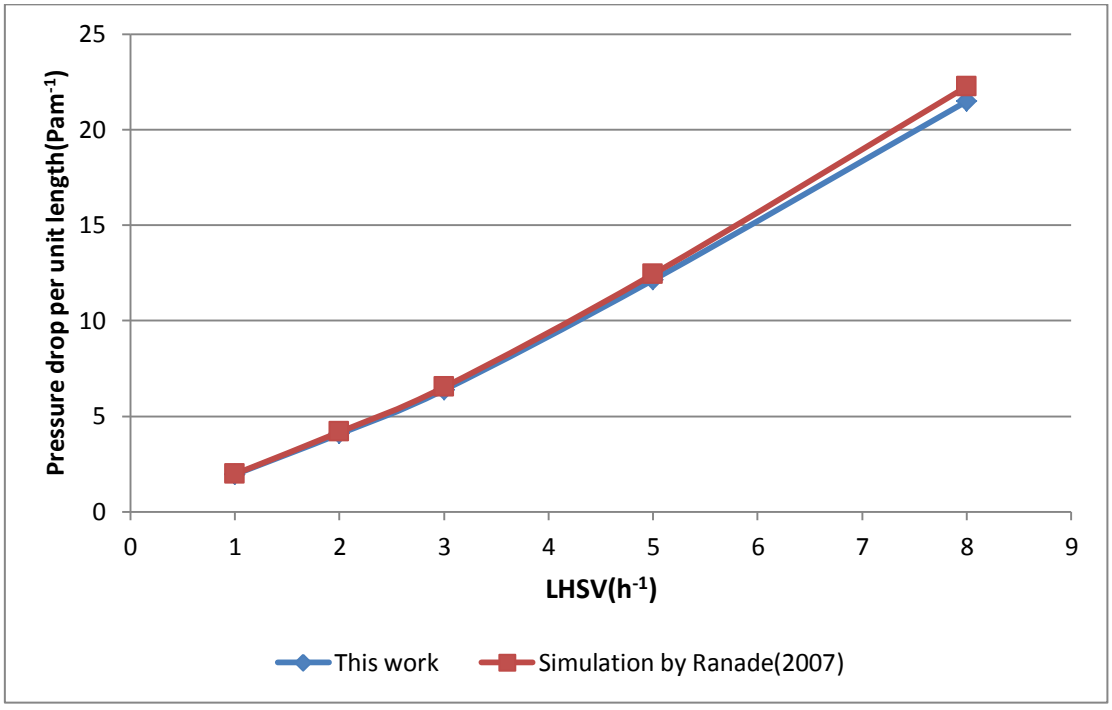
It can be observed that volume fraction of liquid fluctuates near the wall in a manner similar to the porosity of the bed. The average volume fraction of liquid in the bed in this case was found to be 0.076, which agrees with that predicted by Gunjal and Ranade (2007).

Comparison between prediction of liquid holdup by this study with simulation study by Gunjal and Ranade (2007) is given in Fig: 5.6 (a). The Liquid hold up calculated was found within error of 5% from the graph given by Gunjal and Ranade (2007).

Prediction of pressure drop by this study is compared with simulation study by Gunjal and Ranade (2007) is given in Fig: 5.6 (b). The pressure drop predicted by simulation was found within 5% error from the graph given by Gunjal and Ranade (2007).



(a)



(b)

Fig. 5.6: Simulated results for (a) liquid holdup (b) pressure drop for varying LHSV for operating conditions described in Gunjal and Ranade (2007).

5.4 Comparative study of three phase Attou and Ferschneider (1999) model and pseudo two phase Saez and Carbonell (1985) model

For comparing the two models, Saez and Carbonell (1985) and Attou and Ferschneider (1999), the reactor dimension of 0.5715mx0.0219m was used and was taken from experimental study of Al-Dahhan and Dudukovic (1994). In this study, hexane and water were used as liquid phase and helium and nitrogen were used as gas phase. Catalyst particles were considered to be spherical (diameter 1.14 mm) and porous extrudate (equivalent diameter 1.99 mm). Bulk porosity of the bed was taken to be equal to 0.392 for spherical particles and 0.355 for porous extrudate as given by Al-Dahhan and Dudukovic (1994). The results of comparative study are given in following section.

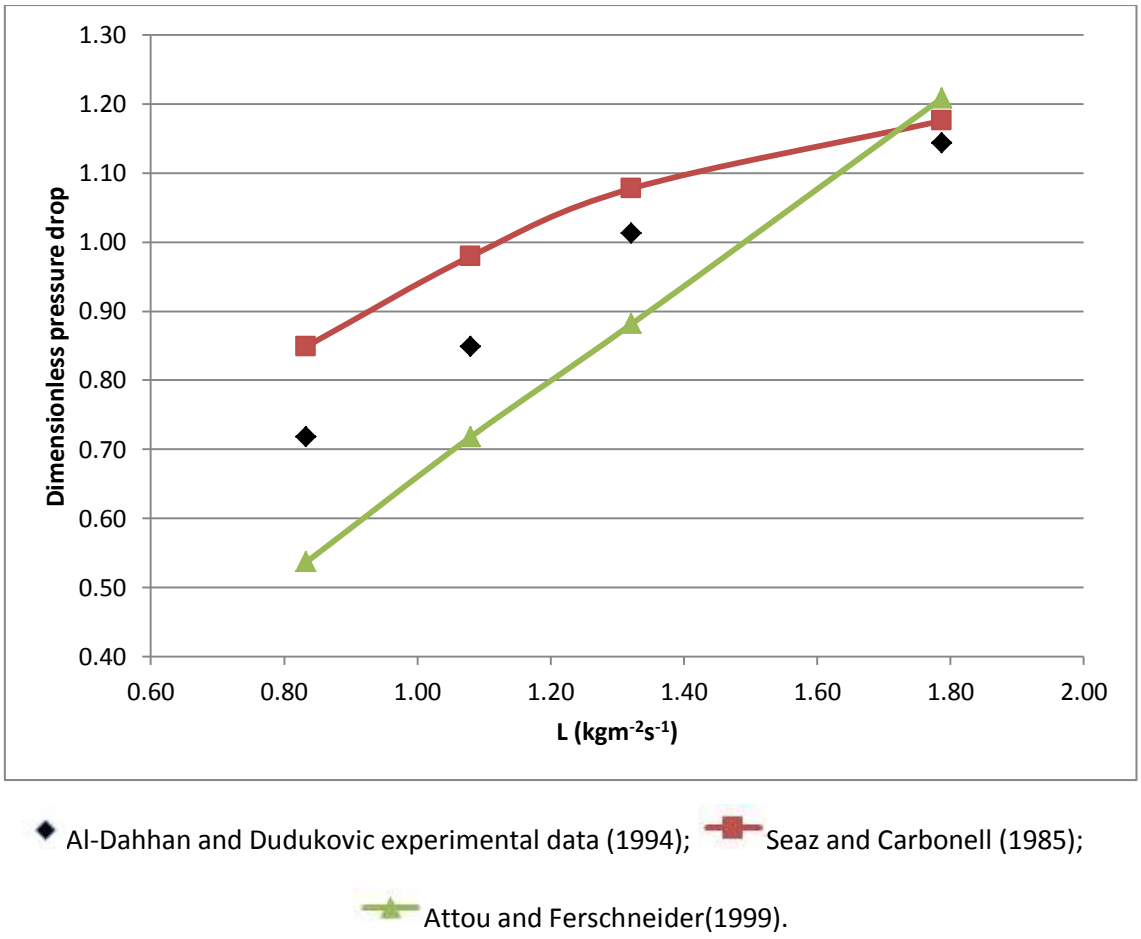


Fig. 5.7: Comparison of simulated pressure drop with experimental data.
System: hexane–nitrogen; porous extrudate of 0.5% Pd on alumina;
Operating conditions: Pressure=0.31MPa and u_g=0.0873 ms^{-1}

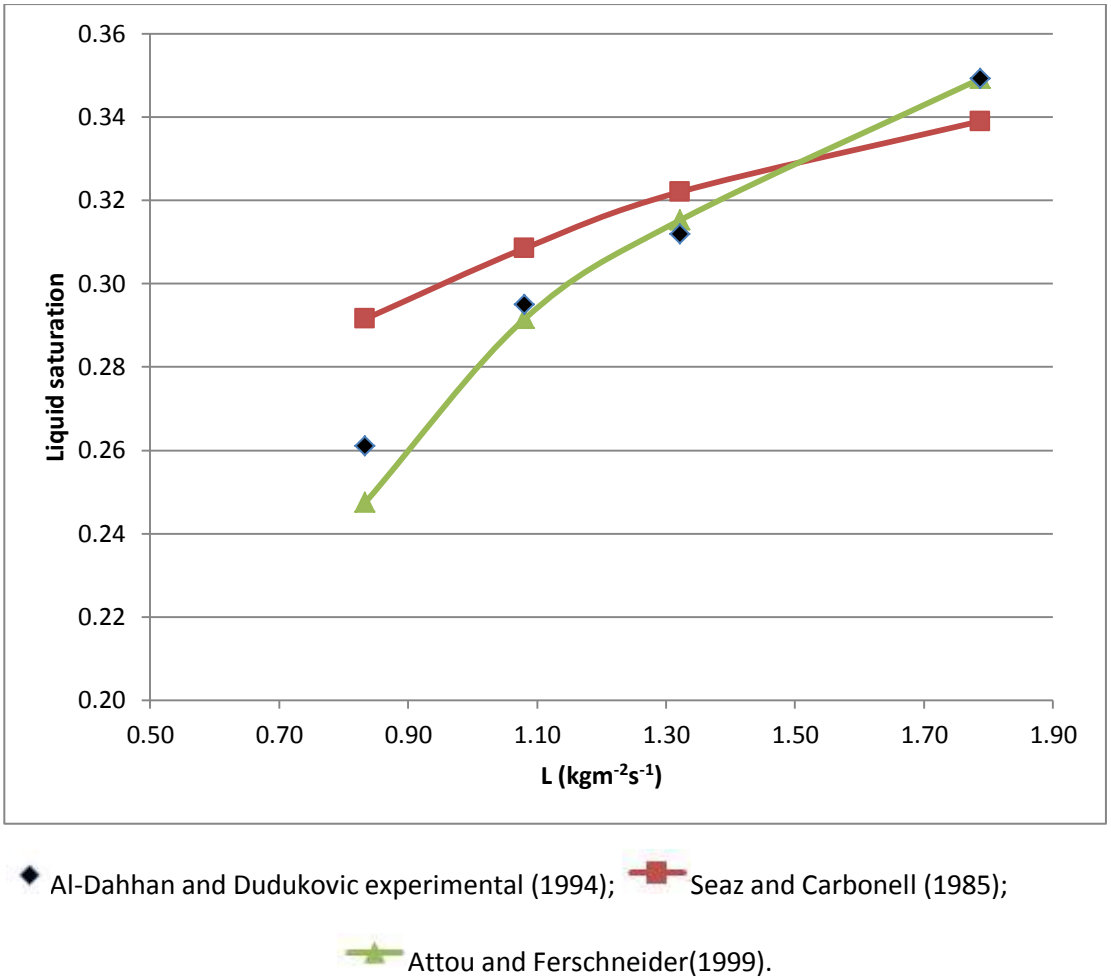


Fig. 5.8: Comparison of simulated liquid holdup with experimental data.
System: hexane–nitrogen; porous extrudate of 0.5% Pd on alumina;
Operating conditions: Pressure=0.31MPa and u_g=0.0873 ms^{-1}

From the above figures, it can be observed that the three phase model is better suited for the given operating conditions. For liquid holdup, it is observed that maximum relative error for three phase model is less than 5%. However, it is to be noted that both the models yield more than 10% average relative error when compared with the experimental data for pressure drop.

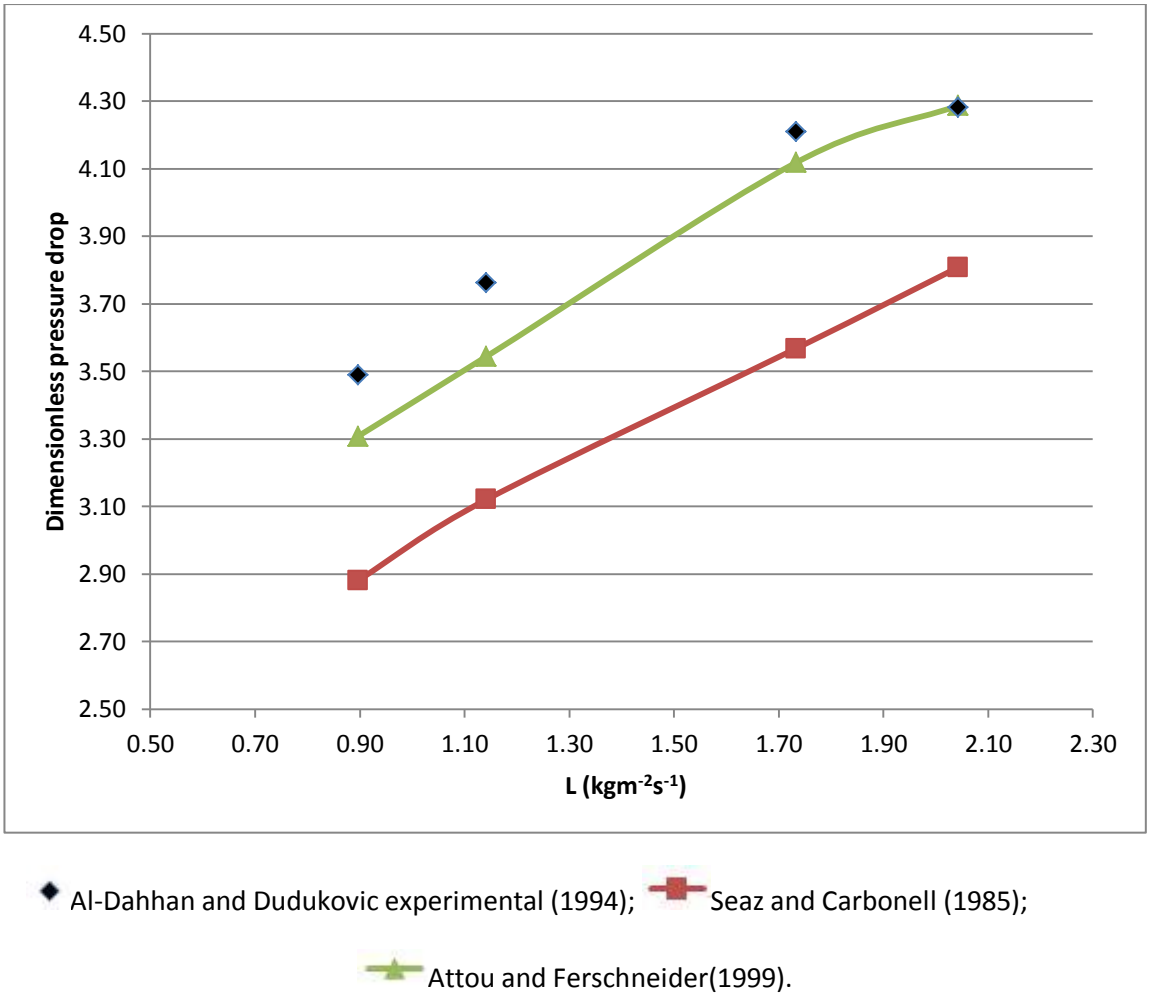


Fig. 5.9: Comparison of simulated pressure drop with experimental data.
System: hexane–nitrogen; porous extrudate of 0.5% Pd on alumina;
Operating conditions: Pressure=3.55MPa and u_g=0.0873 ms^{-1}

It can be observed from the Figure 5.9 that on increasing the pressure, the predictions by three phase model improved in terms of relative error when compared to experimental data. Maximum relative error for three phase model was found to be less than 6%. It is observed that the two phase porous media based model has deviated further away from experimental data and average relative error for this model was found to be 15%. Higher pressure drop was observed on increasing the operating pressure which can be explained by an increase in gas density with pressure.

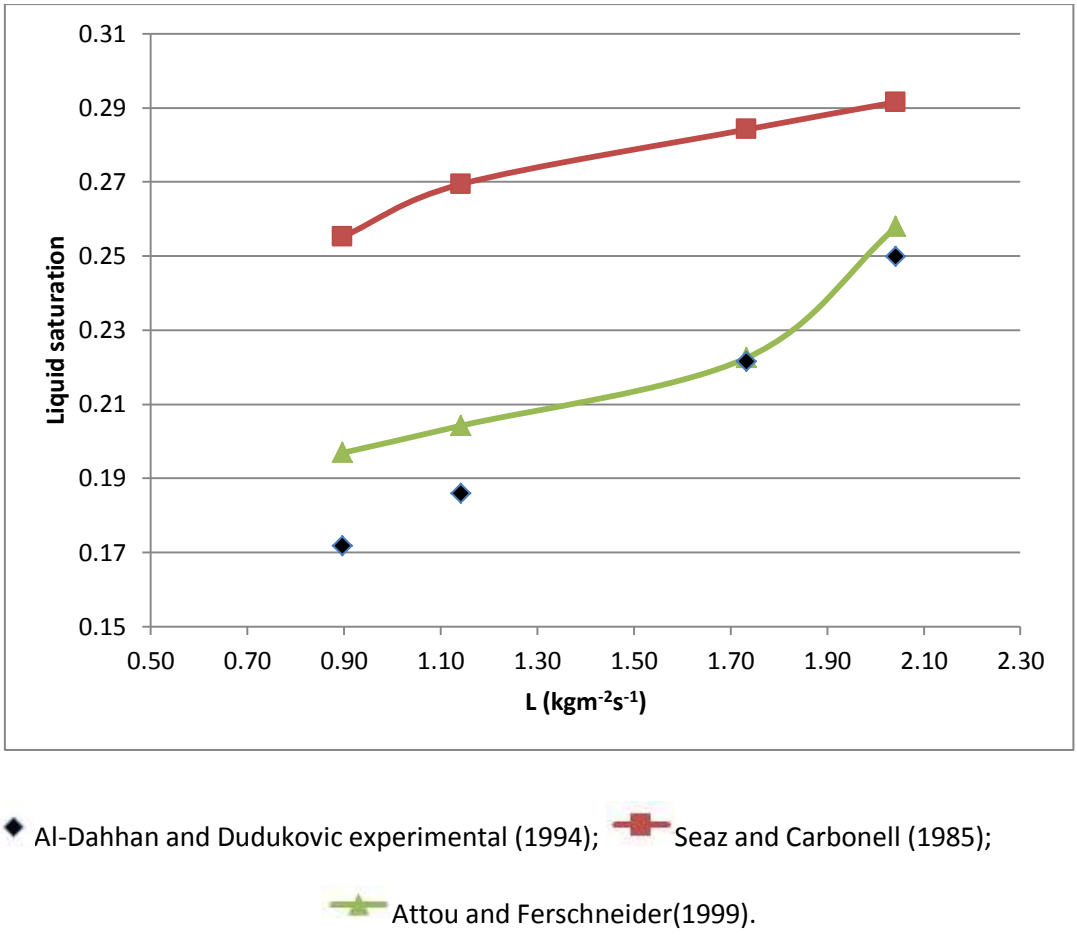


Fig. 5.10: Comparison of simulated liquid holdup with experimental data.
System: hexane–nitrogen; porous extrudate of 0.5% Pd on alumina;
Operating conditions: Pressure=3.55MPa and u_g=0.0873 ms^{-1}

It can be observed from the comparison of the Fig. 5.10 with Fig. 5.6 that on increasing the pressure the liquid saturation of the bed decreases. The predictions of the three phase model are better for the operating conditions. Maximum relative error was found to be 14.6%. However, these predictions seem to be reasonably accurate when compared with the two phase porous media model which yielded a minimum relative error of 16%.

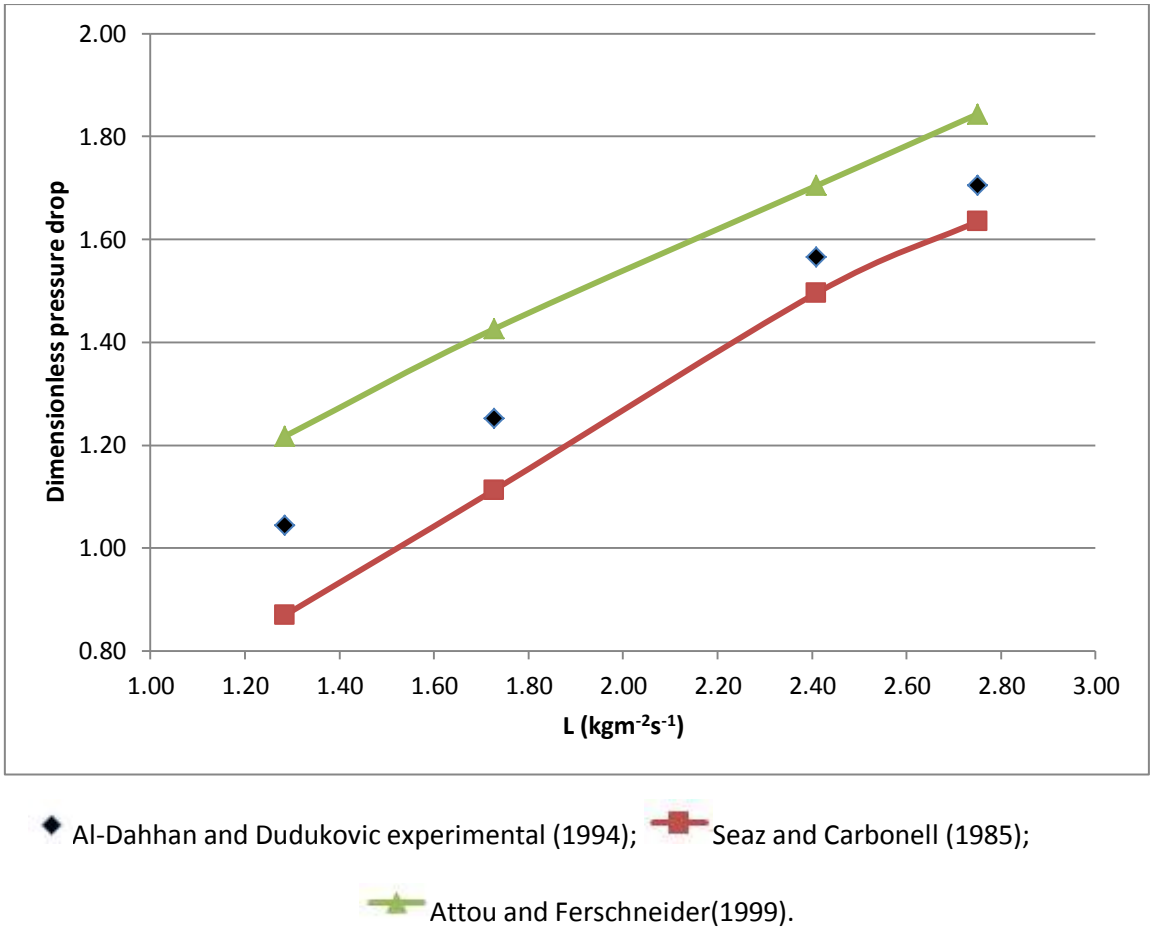


Fig. 5.11: Comparison of simulated pressure drop with experimental data.
System: hexane–nitrogen; non porous glass bead;

Operating conditions: Pressure=0.31MPa and u_g=0.042 ms^{-1}

Further simulations were carried out using non-porous glass beads as catalyst particles. Both the models appear to predict the pressure drop for low pressure and low gas velocity with reasonable accuracy of around 10% relative error with respect to experimental data. Though the two phase relative permeability based model by Seaz and Carbonell (1985) was found to be marginally better at predicting pressure drop for this case, its predictions for liquid saturation (Fig. 5.11) were more erroneous when compared with the three phase model.

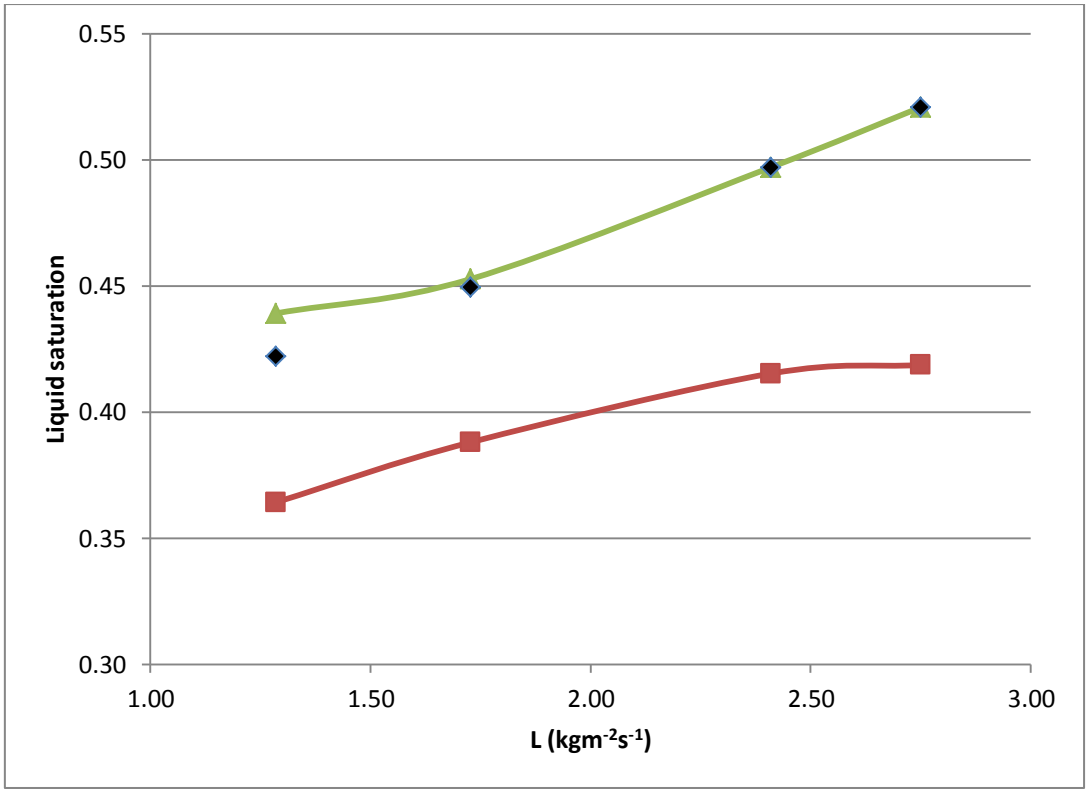


Fig. 5.12: Comparison of simulated liquid holdup with experimental data.
System: hexane–nitrogen; non porous glass bead;
Operating conditions: Pressure=0.31MPa and u_g=0.042 ms^{-1}

It can be observed that the three phase model predicts the liquid saturation very well, with a maximum relative error of 4%, while for the same case pressure drop was over predicted by it. In the case of two phase model, prediction of liquid saturation was found to be significantly lower when compared with the experimental values. Hence, for the predictions of hydrodynamic parameters at moderate pressure and low gas flow conditions, the three phase model is preferred.

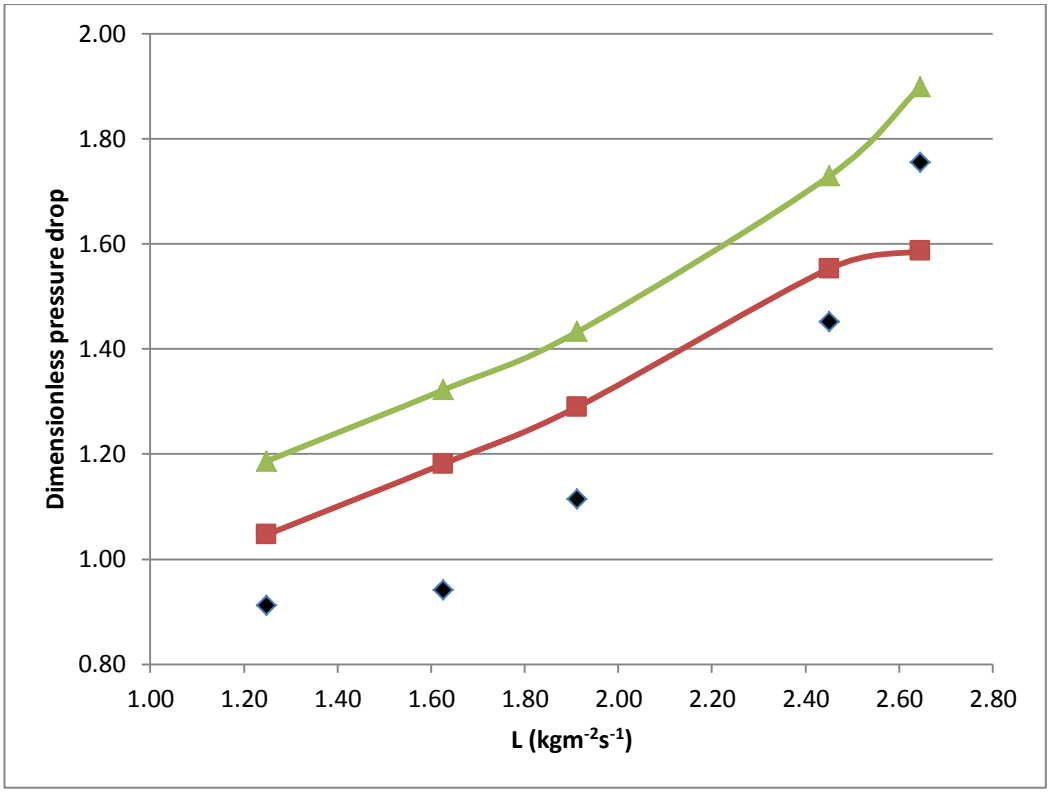


Fig. 5.13: Comparison of simulated pressure drop with experimental data.
System: hexane–helium; non porous glass bead;
Operating conditions: Pressure=2.31MPa and u_g=0.0415 ms^{-1}

The behaviour of hydrodynamic parameters in this case is shown to be similar to Hexane-Nitrogen system at 0.31 Mpa. This is due to the fact that a change in pressure has pronounced effect only on density of gas, and helium at 2.31 Mpa has almost equal density to that of nitrogen at 0.31 Mpa. Pressure drop is observed to be higher than that in Fig. 5.10, owing to slightly higher gas viscosity of helium compared to that of nitrogen. From Fig. 5.13, it can be observed that the two phase model is much more sensitive to gas viscosity when compared with the experimental data.

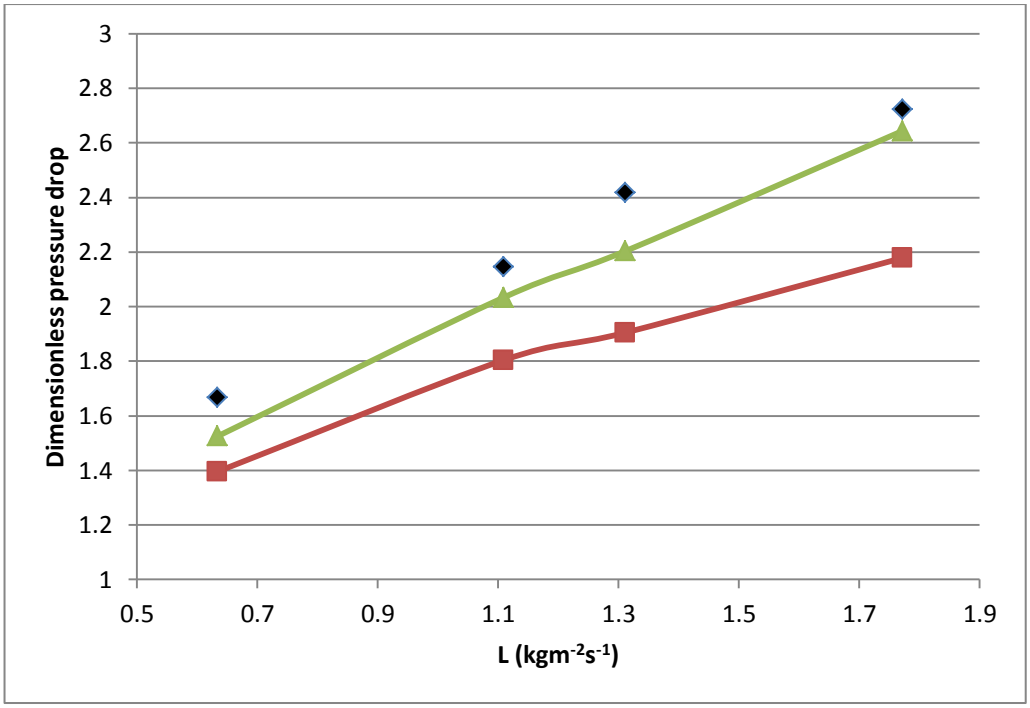


Fig. 5.14: Comparison of simulated pressure drop with experimental data.
System: hexane–nitrogen; non porous glass bead;
Operating conditions: Pressure=0.31MPa and u_g=0.0875 ms^{-1}

The effect of an increase in gas flow rate on the predictions by both the models can now be discussed. In this case, the three phase model was found to be under-predicting the pressure drop marginally. The two phase model also under-predicted the liquid saturation but its deviation from the experimental values was much higher as compared with that predicted by the three phase model.

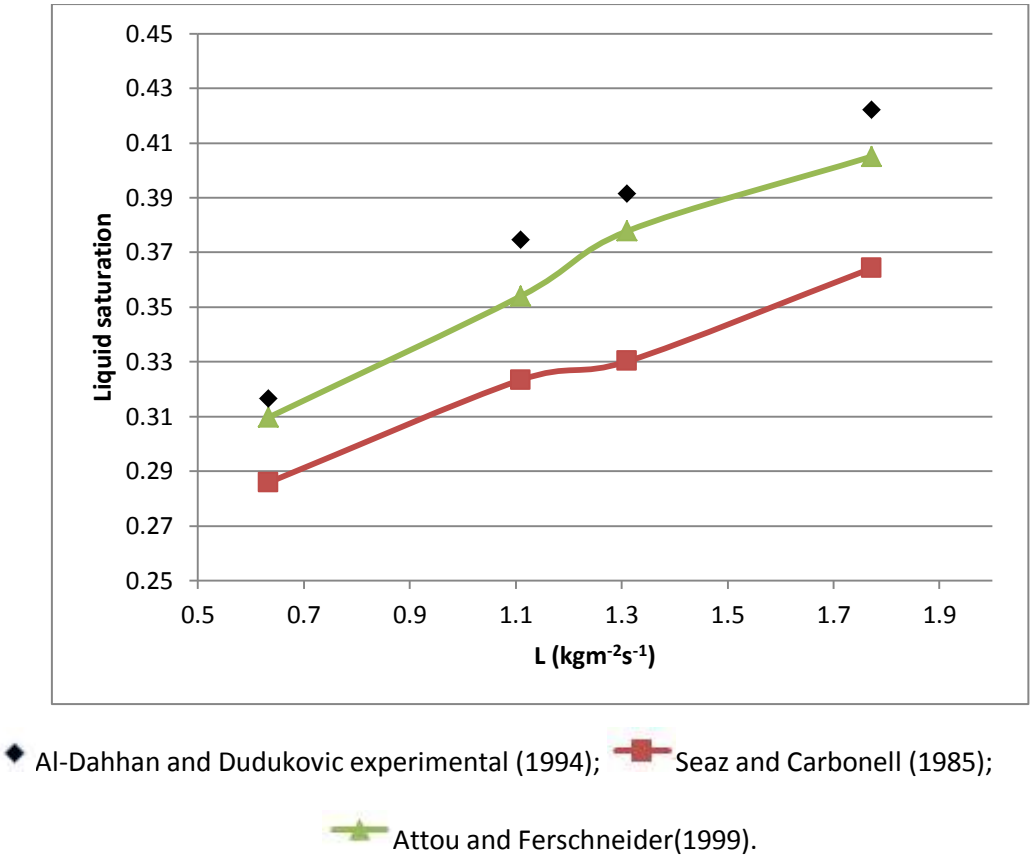


Fig. 5.15: Comparison of simulated liquid holdup with experimental data.
System: hexane–nitrogen; non porous glass bead;
Operating conditions: Pressure=0.31MPa and u_g=0.0875 ms^{-1}

It can be observed that liquid saturation for this case is under predicted by both the models. Predictions by the three phase model were found to be much better as compared to that obtained by using its pseudo two phase counterpart. Maximum relative error for three phase model was found to be about 5% whereas it was found to be about 15% for the two phase model.

A comparative summary of the two models based on the aforementioned simulation studies is given in Table 5.2. For this comparison, the average relative error of both the models with the experimental data is used. It is observed that the average relative error for the three phase model was about 9% as compared to 16% obtained for the two phase porous media model.

Table 5.2: Comparison between pseudo two phase and three phase models.

Model	Attou and Ferschneider (1999)	Saez and Carbonell (1985)
Average Relative error	8.67%	15.71%

CHAPTER-6
CONCLUSIONS AND RECOMMENDATIONS

6.1 Conclusions

A comparative study of two CFD based models using Euler-Euler approach has been presented and the results are compared with the experimental data. The two models differ in their treatment of solid phase and also in momentum exchange between the phases. The two models are

- Pseudo two phase model based on porous media concept as proposed by Saez and Carbonell (1985). The momentum exchange equations used in this model are based on relative permeability of flowing phases and the flow field was considered as a porous medium.
- Three phase model proposed by Attou and Ferschneider (1999). In this model the solid phase was considered as a separate phase and the velocity of solid phase in both dimensions was considered to be zero. The momentum exchange equations were based on phase interaction momentum transfer between all three phases.

Both the models were validated with simulated results presented in the literature and predictions by these are compared at different operating conditions. From the results, the following can be inferred:

1. Predictions of three phase model based on Ergun equation were found to be, in general, closer to experimental data when compared with the predictions of the two phase model based on phase permeability.
2. Porosity variation models were compared with the experimental data and the predictions of Mueller (1991) model were found to be closest to experimental data.
3. The pressure drop estimation at lower pressure (0.31Mpa for Hexane-Nitrogen system) using the two phase model was found to be marginally better as compared to that predicted by the three phase model.
4. A general trend in hydrodynamic parameters was observed:
    a. Pressure - With an increase in pressure, the pressure drop across the bed increases and the liquid hold up decreases.

b. Liquid flow-rate – With an increase in liquid flow rate, the pressure drop across the bed increases and the liquid holdup also increases.
c. Gas flow-rate – With an increase in gas flow rate, the pressure drop across the bed increases and the liquid holdup decreases.

6.2 Recommendations

Though the recent advances in the field of computational fluid dynamics along with an increase in computational power has greatly assisted in the hydrodynamic study of trickle bed reactors, yet there are areas which need to be studied in the future.

1. Development of phase momentum exchange models – Although formidable amount of research literature is available on hydrodynamics of trickle bed reactors, yet there is no consensus in scientific community on the approach to be taken to model phase interactions in the trickle bed reactors
2. Development of parallel algorithms: The present practice of simulations involving unsteady Navier Stokes equations require high computational power and is also time consuming. More efficient and robust algorithms for simulating unsteady state flow problems must be developed.
3. Experimental data at high pressure – Only a few studies have reported high pressure experimental data on hydrodynamics of trickle bed reactors. Carefully designed experiments need to be carried out for developing effective and more realistic mathematical models.