B. Tech Thesis on

CFD Simulation of Pressure Drop and Liquid Holdup in a Trickle Bed Reactor

For partial fulfilment of the requirement for the degree of

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In

Chemical Engineering

Submitted by: Antariksha Pattnaik

Roll No. 111CH0600

Under the supervision of:

Prof (Dr.) H. M. Jena

Department of Chemical Engineering,

National Institute of Technology, Rourkela

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CERTIFICATE

This is to certify that the thesis entitled "**CFD Simulation of Pressure drop and liquid holdup in a Trickle Bed Reactor**" submitted by Antariksha Pattnaik, Roll No.-111CH0600, in partial fulfilment of the requirement for the award of degree of Bachelor of Technology in Chemical Engineering at National Institute of Technology Rourkela, is an authentic work carried out by him under my supervision and guidance.

Date:

Place: Rourkela

Prof. (Dr.) H. M. Jena

Department of Chemical Engineering

National Institute of Technology, Rourkela-769008

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Antariksha Pattnaik

Roll No-111CH0600

Department of Chemical Engineering

NIT Rourkela.

ABSTRACT

Trickle Bed Reactors have etched a ubiquitous presence in chemical processing sector. From petroleum and petrochemical products, fine chemicals to biochemical, wastewater treatment, they are almost everywhere. Products worth of 300 billion US $ are processed by these reactors on an annual average. A complete understanding of hydrodynamics, fluid phase mixing, interphase and interparticle heat and mass transfer and reaction kinetics of TBR can help us to extract the full potential of TBR. Studying the variation of pressure drop and liquid holdup is crucial for evaluation of performance of trickle bed reactors and can help in further optimizing their performance.

This project focuses on the effect of gas and liquid velocities on the pressure drop and liquid holdup in a trickle-Bed reactor operating at ambient temperature and atmospheric pressure. Pressure drop and liquid holdup are two critical hydrodynamics parameters that influence other parameters directly and indirectly and hence, these two parameters are preferred for hydrodynamic study of TBR. Their variation along longitudinal and transverse direction is the focus of this project. A comparison of results from different simulation scenarios (using different pressure values as patching values) made in this project helps in understanding how different initial guess can affect the final solution in simulating real-life TBR operation. It is found that pressure ranging up to 10000 Pa as patching pressure value can lead to a converging solution. Afterwards, solution instability creeps in leading to impractically higher values of pressure and liquid holdup and sometimes ending up with divergence. Even the effect of gas and liquid velocity is studied on the two parameters. The variation of the two hydrodynamic parameters with changing liquid velocities and gas velocities are also studied.

Keywords: TBR, Hydrodynamics, Pressure drop, Liquid holdup

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LIST OF SYMBOLS USED

α	permeability of porous media, m^2
α_k	volume fraction of k phase
C_0, C_1	user-defined empirical constants for power law form of Darcy's Law
C_2	internal resistance factor, 1/m
$\nabla.$	divergence (gradient operator with dot product)
d_p	effective particle diameter, m
ε	turbulence dissipation rate, J/kg; bed voidage
E_k	energy for phase k, J
F	body force, N
g	acceleration due to gravity, m/s^2
h_k	sensible enthalpy for phase k, J/mole
k	kinetic energy, J
k_{eff}	effective thermal conductivity, W/(m.K)
k_t	turbulent conductivity, W/(m.K)
μ_k	viscosity of k phase, kg/(m.s)
μ_m	viscosity of mixture, kg/(m.s)
P	pressure, Pa
ρ_k	density of phase k, kg/m^3
ρ_m	mixture density, kg/m^3
S_E	any other volumetric heat source, W/m^2
S_i	momentum source term, kg m/s
T	temperature, K
t	time, s
$v_{dr,k}$	the drift velocity for k phase, m/s
v_i	x-component of velocity, m/s
v_k	velocity of k phase, m/s
v_{pq}	relative slip velocity of phase p and q, m/s

ABBREVIATIONS

1-D	One dimensional
2-D	Two dimensional
CFD	Computational Fluid Dynamics
CT	Computed Tomography
DES	Detached Eddy Simulation
DNS	Direct Numerical Simulation
EVM	Eddy Viscosity Model
LES	Large Eddy Simulation
MRI	Magnetic Rsonance Imaging
RANS	Reynolds Average Naviers Stokes
RNG	Renormalized Group
TBR	Trickle Bed Reactor
U_g	Superficial gas velocity
U_l	Superficial liquid velocity
VOC	Volatile Organic Chemicals
VOF	Volume of Fluid

CHAPTER 1

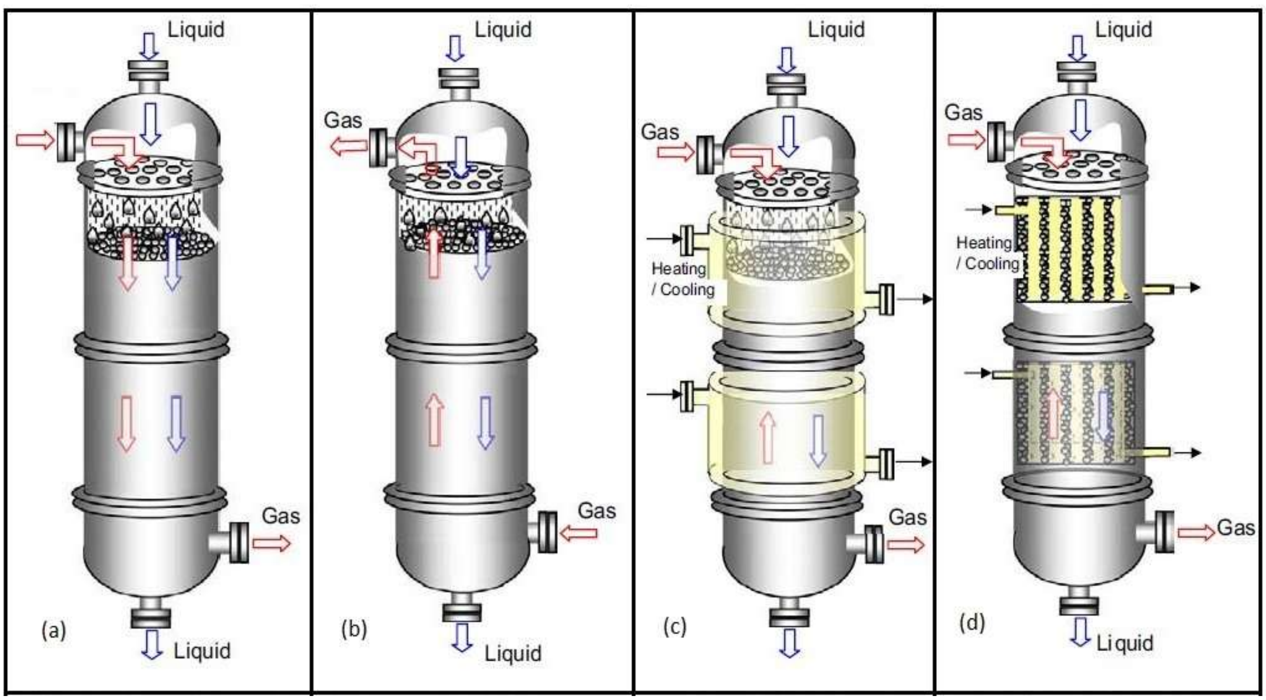
INTRODUCTION

1.1Definition

The term trickle bed refers to Gas-liquid contacting equipment with concurrent downward flow through stationary solid catalyst packing (Satterfield,1975). There exists a wide variety of reactor designs with the concurrent gas-liquid flow across a fixed catalyst bed remaining its intrinsic feature. The term “trickle” literally refers to characteristic intermittent liquid flow within voids of catalyst packing forming films or rivulets or droplets present in such reactors.

To appreciate the complexity of hydrodynamics of Trickle Bed Reactor, a peek into different multiphase flow regimes (especially gas-liquid even though it is a three-phase flow) is necessary.

1.2 Configurations of Trickle Bed Reactors



(a) Concurrent Trickle Bed Reactor, (b) Counter current Trickle Bed Reactor,(c) Jacketed Trickle Bed Reactor, (d) Internally cooled Trickle Bed Reactor

Figure 1.1: Various configurations of Trickle Bed Reactors (Ranade et al., 2011)

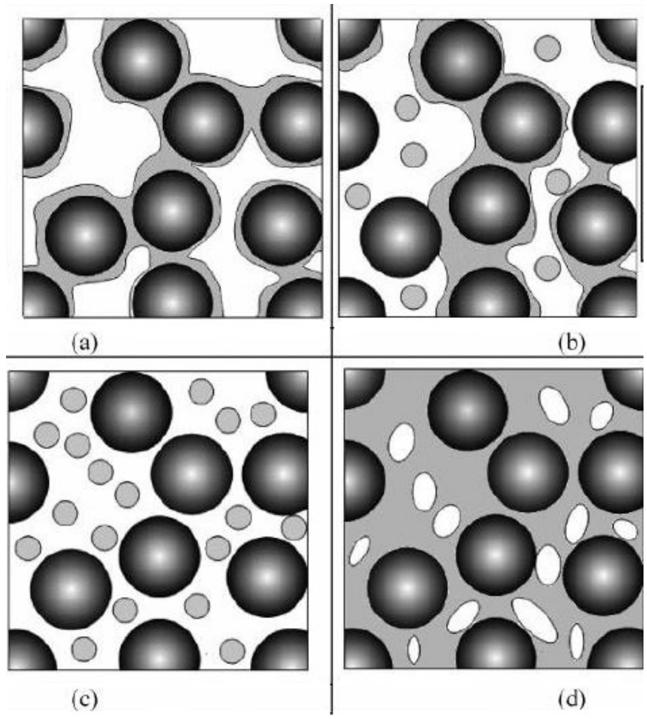
Trickle bed reactors are generally used in four different configuration setups based upon packing structure (Ranade et al., 2011):

a. Concurrent Trickle Bed Reactor
b. Counter current Trickle Bed Reactor
c. Jacketed Trickle Bed Reactor
d. Internally cooled Trickle Bed Reactor

1.3 Flow Regimes

Based on different gas and liquid flow rate (also method of packing, particle size and shape and bed dimensions), four flow regimes exists (Chaudhari & Ramachandran, 1983):

- Trickle flow (Continuous gas phase and semi-continuous liquid phase):
  Low gas and liquid velocity results in low gas-liquid interaction enabling films and rivulets to be formed on solid particles as the liquid trickle downwards. Thus, it is known as low interaction regime. Low liquid flux exhibit lower inertial forces juxtaposed against local surface forces while capillary pressure dictating the liquid spreading over catalyst surface thus forming rivulets. At higher flux, inertial forces become appreciable with surface forces forming films.
- Pulse Flow (Dispersed gas phase with dispersed liquid phase):
  The moderate gas and liquid velocities enhances phase interaction and the liquid phase occupies entire flow cross-section thereby forming a sandwiched gas-liquid-gas-liquid enriched zones. Transition from trickle to pulse can happen wither from increased liquid or increased gas velocities. In this regime, liquid pockets obstructs local gas flow path forming alternate gas and liquid-rich zones. Liquid rich zone completely wets the solid particles.
- Spray Flow (Continuous gas phase with dispersed liquid phase):
  Low liquid and high gas velocity favors a continuous gas phase dispersed with liquid droplets just like a spray.
- Bubble Flow(Dispersed gas phase interspersed within continuous liquid phase):
  Low gas flux and high liquid flux creates a zone of continuous liquid zone with gas bubbles descending at low velocities.



(a) Film Flow: Continuous phase-Gas; Liquid form film over solid
(b) Trickle flow: Continuous phase-gas; Liquid partially supported on solid and partially on gas
(c) Spray regime: Continuous phase- Gas, Dispersed phase- Liquid
(d) Bubbly regime: Continuous phase- Liquid, Dispersed phase- gas

Figure 1.2: Flow Regime in gas-liquid contact (Gunjal et al., 2005)

Industrial trickle bed reactor (TBR) are operated in proximity to tickle/pulse transition regime thus getting the best of both regimes- better wetting, effective catalyst utilization, higher mass and heat transfer rates from pulse regime; and low pressure drop, low gas-liquid throughputs, less catalyst attrition, suitability for foaming liquids from trickle flow regime.

1.4 Performance Indicators of Trickle Bed Reactor

A plethora of parameters dictates the performance criteria of a trickle bed reactor. Thus, a critical analysis of trickle bed reactor usually involves an in-depth study of these parameters:

- Hydrodynamics and flow pattern, flow maldistribution, liquid backmixing, RTD and axial dispersion.
- Phase pressure drop and mixture pressure drop.
- Catalyst bed packing nature, orientation, tortuosity of channels, porosity, particle shape and size distribution
- Wettability of solid catalyst particles.
- Local heat and mass transfer, axial dispersion.
- Chemical kinetics.

1.5 Advantages and Disadvantages of Trickle Bed Reactor

Many chemical industries rely on trickle bed reactor (TBR) because:

- It's simple design and operation procedure under severe environment is its forte making it suitable for industrial-scale production (Ranade et al.,2011).
- No need for additional catalyst separation unit also minimizes catalyst attrition.
- It can accept solid catalyst with a wider range of size and shape which makes it versatile.
- The design of trickle-bed helps in exploiting the benefits of plug flow scenario better than slurry bubble or packed or stirred reactor leading to higher conversion and selectivity.
- Large-scale operation is more economical in trickle bed reactor than any other type of reactors.
- No concern for flooding has to be considered because of concurrent gas and liquid flow.
- Lower liquid holdup (or higher catalyst holdup) favors minimizing homogeneous liquid phase reaction which is attained in trickle bed reactor as compared to ebulliating bed or slurry bed reactor. This also leads to higher throughput per unit volume of reactor for large catalyst holdup.
- Unlike fluidized bed, slurry bed or stirred reactor, power consumption is quite lower as there is no need for solid to be suspended.
- It has lesser pressure drop and lesser back-mixing than packed beds.

Still there are some shortcomings restricting the extensive use of trickle bed reactor which are:

- Lower intraparticle and interphase mass and heat transfer limits reaction rate.
- Incomplete wetting and liquid maldistribution as a result from low liquid velocity decreases overall performance of reactor. Liquid maldistribution may results from- improper initial feed distribution, randomness in local properties of packing, wall effects, wetting properties of catalyst, intrinsic properties of liquid and severity of operating conditions (Schwidder & Schnitzlein, 2012).
- Partial wetting of catalyst can wreak havoc in trickle bed reactor operations by causing undesirable gas phase side reactions, hot-spot formation or temperature runaways. This issue can be mitigated by using intermediate cooling, excess solvent and liquid distributors. This limits the use of trickle bed reactor in slower reactions requiring high catalyst loading.
- Radial heat and mass flux may seem to be a problem.

However, there is further scope of optimization of trickle bed reactor performance which can be realized with more comprehensive research works.

1.6 Applications of Trickle Bed Reactor

Table 1.1:Industrial Applications of Trickle Bed Reactors (Ranade et al., 2011)

Type	Chemicals involved
Oxidation	Phenol, ethanol, formic acid, organic matter in wastewater, SO_2 to SO_3 conversion.
Petroleum Processing	Hydrodesulphurization, hydrodenitrogenation, hydrodemetalization, catalytic hydrocracking/hydrofinishing, manufacturing lube oils, catalytic dewaxing of lube-stocks cut.
Hydrogenation	Petroleum fractions, nitro- and carbonyl- compounds, carboxylic acids to alcohol conversion, C_2H_2 to separate compound from C_4 fraction in the presence of butadiene, 2-butyne-1,4-diol, caprolactone, adipic acid, butadiene to butane, vinyl acetylene to butadiene, alkylanthraquinone to hydroquinone, aniline to cyclohexylaniline , glucose-sorbitol conversion. Conversion of benzoic acid to hydrobenzoic acid, caprolactone to hexanediol, maleic anhydride.
Pollution abatement	Waste water treatment, VOC removal from industrial flue gas, removal of CO_2 and H_2S from caustic alkali solution.
Biochemical	Immobilized enzyme reactions, Bio fermentation.
Miscellaneous	Fischer-Tropsch process, Acetone and butanol esterification.

1.7 Objective and Scope of the Work

Most of the literature (Gunjal et al., 2003, Atta et al., 2007a ,Atta et al., 2007b, Bazmi et al., 2011) is based on the application of one model without any modification of solution control in the simulation of trickle bed reactor (TBR). In the present work, an attempt has been made to study the effect of patching using different pressure values on simulation results. This will help in understanding the sensitivity of iterative schemes with varying initial guess. The objective of the project is briefly stated in the following points:

- Comparison of axial variation of pressure, radial variation and axial variation of liquid holdup in trickle bed reactor.
- Comparison of effects of different pressure patching values on pressure drop and liquid holdup.

CHAPTER 2

LITERATURE REVIEW

2.1 Computational studies on Trickle Bed Reactor

CFD simulation provide an easy yet cost effective approach in design as has been used by Foumeny & Benyahia, 1993 and Ranade et al., 1994 for optimizing internals of packed bed reactors. After Attou and Ferschneider, 2000 came up with a 1-D model for analyzing hydrodynamics. Calis et al., 2001 applied CFD techniques to analyze flow profile in catalyst packed reactor. Jiang et al., 2002 formulated a 2-D CFD model with varying porosity. Nature of solid catalyst surface in the packing and its wettability influences the liquid spreading over the catalyst surface in trickle flow regime. On the other hand, pulse flow, pulse frequency and holdup controls hydrodynamic properties of trickle bed reactor operating in pulse flow regime. Gunjal et al., 2003 analyzed the RTD using both experimental and CFD simulation while Gunjal et al., 2005 studied the hydrodynamics using CFD simulation. Our area of interest is the trickle flow and the gas and liquid velocities required for operation of trickle bed reactor in trickle flow regime is referred from Gunjal et al., 2007. CFD modeling was used for trickle bed reactor (operating at 170-200^0 C and 10-20 bar pressure) using catalytic oxidation of phenolic acids by Lopes & Quinta-Ferreira, 2007.

2.2 Drag Force Models used in CFD

Out of multitude of drag force models used in CFD simulation, they can be categorized into two groups:

2.2.1 Empirical/phenomenological models

They represent a set of correlations derived from analyzing experimental data obtained from cold flow experiments, laboratory or pilot-scale trickle bed reactor. Al-Dahan & Dudukovic, 1994 studying gas density effect on hydrodynamics of trickle bed reactor running at atmospheric pressure using water/hexane (liquid phase) and N_2/He (gas phase) with extrudates/porous/ non-porous spherical catalyst of Pd/alumina; Attou et.al, 1999 working on trickle-pulse transition; Wammes et al.,1991 using nitrogen-water system with glass beads; Larachi et al. 1991 operating trickle bed reactor at 2.1 MPa and using N_2-water system with glass beads; Ellman et al., 1998devised the 4 adjusted parameters-correlation of pressure gradient with liquid saturation; Holub et al., 1991and Holub, 1993 using single flat-slit model for a packed bed.

2.2.2 Semi-empirical models

Attou et al., 1999 proposed this model to describe the hydrodynamics involved in trickle bed reactor and is based on macroscopic ensemble-average mass and momentum conservation laws. Interphase drag is calculated from theoretical standpoint. However, the weak point of the model is that it underestimates the pressure gradient at higher superficial gas velocities.

Succinctly, there are three widely adopted models used for calculating drag force expression. As stated by Carbonell, 2000, they are as follows:

- Relative permeability model by Saez and Carbonell, 1985
- The slit model by Holub et al., 1992 and 1993
- Fluid-fluid interaction model by Attou and Boyer, 1999

2.2.2.1 Relative Permeability model

Derived by Saez and Carbonell,1985 this model has gain a wide acceptance in many engineering fields like soil science, textile engineering, pollution abatement and environmental science, chemical science, reservoir engineering, fuel cells, subsurface environmental engineering and has an ever-increasing popularity in research community (Xiao et al., 2012). Relative permeability of phase is considered as the tendency of one fluid to flow with respect to motion of another fluid and thus modifies drag force expression for on phase flow. Relative permeability is dependent on phase holdup and saturation of corresponding phase.

2.2.2.2 Slit Model

Representing the fluid flow around solid packing of trickle-bed as flow through a rectangular slit, this model also include slip effect to calculate velocity and stress fields. As Holub et al., 1992, 1993 states that the slit gap depends on voidage of porous medium, and the orientation of slit is related to tortuosity factor for the packed bed.

2.2.2.3 Fluid-Fluid Interaction Model

Macroscopic mass and momentum balance is applicable over control volume in interstitial space between solid particles. This model is consistent for incompressible two-phase, two species concurrent gas-liquid trickle flow; 1-D, steady state, 2-phase flow with Newtonian fluids. Momentum exchange terms are calculated from Ergun's equation (modified form for multiphase flow).

CHAPTER 3

CFD Modeling

3.1 Definition of CFD

CFD is a novel technique to simulate fluid engineering system and involves predicting fluid flow, heat transfer, mass transfer, chemical reactions and related phenomena by solving governing mathematical equations by numerical methods.

Results from CFD helps in achieving some of the required objectives like:

- Conceptual study of new design
- Detailed product development
- Troubleshooting
- Redesign

3.2 Basic Governing Equations

Mathematical modeling of any physical system involves a set of characteristic equations like:

- Conservative form of equations
- Equations based on basic thermodynamic laws
- Equation of state
- Equations relating intrinsic properties of the system (like Newton's law of motion, Newton's viscosity relation, Fourier law of heat conduction, Law of gravitation)

Out of which the conservative equations play a central role and are indispensible to any physical system. And for fluid flow system, they are:

- Equation of continuity:

$$\frac{\partial \rho_m}{\partial t} + \nabla.(\rho_m v_m) = 0 \tag{3.1}$$

- Equation of motion:

$$\frac{\partial}{\partial t}(\rho_m v_m) + \nabla.(\rho_m v_m v_m) = -\nabla p + \nabla.[\mu_m(\nabla v_m + \nabla v_m^T)] + \rho_m g + F + \nabla.(\sum_{k=1}^{n} \alpha_k \rho_k v_{dr,k} . v_{dr,k}) \tag{3.2}$$

- Equation of energy:

$$\frac{\partial}{\partial t}(\sum_{k=1}^{n}\alpha_k\rho_k E_k) + \nabla.(\sum_{k=1}^{n}\alpha_k v_k(\rho_k E_k + p)) = \nabla.(k_{eff}\nabla T) + S_E \tag{3.3}$$

In the above set of equations,

p=local pressure at a point

$$\mu_m = \sum_{k=1}^{n}\alpha_k \mu_k \tag{3.4}$$

ρ_m is mixture density,

$$\rho_m = \sum_{k=1}^{n}\alpha_k\rho_k \tag{3.5}$$

α_k= volume fraction of k phase

F= body force

$v_{dr,k} = v_k - v_m$, is the drift velocity for k phase (3.6)

k_{eff}= effective thermal conductivity($\sum_k \alpha_k(k_k + k_t)$, where k_t= turbulent conductivity)

S_E = any other volumetric heat source

$$E_k = h_k - \frac{\rho}{\rho_k} + \frac{v_k^2}{2} \tag{3.7}$$

For a compressible phase, E_k=h_k

for incompressible phase; h_k=sensible enthalpy for phase k

3.3 Basic Fluid Flow Models

Based on the continuum hypothesis of fluid, basic modeling equations employs either of the two techniques for study of multiphase flow system as described in Verlag & Mueller, 2011:

3.3.1 Euler- Lagrangian approach

Fluid phase is considered to be conforming with the continuum hypothesis so that Navier-Stokes equation is applicable to the fluid flow system. The other phase is treated as a discrete phase and is modeled by keeping track of each of the particles, bubbles, droplets through the calculated flow field. The dispersed phase can exchange momentum, mass and energy with the fluid phase.

The basic yet rudimentary assumption considered for this model is that the dispersed phase is present in low volume fraction in spite of acceptable high mass loading. Particles or droplets trajectories are computed individually at specified intervals during fluid phase calculation.

Scope of applications:

- Spray dryers

- Coal and liquid fuel combustion
- Particle-laden flow but not for liquid-liquid mixtures, fluidized beds or any application where volume fraction of second phase

3.3.2 Euler- Euler approach:

Different phases are represented in mathematical modeling as interpenetrating continua where any space in computational domain is exclusively occupied by either one of the many phases. This gives rise to the concept of phasic volume fraction, which itself are a continuous spatial-temporal functions and sums up to unity. Conservation equations are formulated for each phases which in turns yields a set of equations. The closure of the equations is provided from using empirical information, or in case of granular flows, by implementing kinetic theory.

Out of the above two approaches, we adopt the second one for the reason of

Three forms of Euler-Euler approach of modeling:

- Volume of Fluid (VOF) model
- Mixture model
- Eulerian model

3.3.2.1 Volume of Fluid Model

For a system of immiscible fluids, VOF model is used which solves a set of momentum equation and analyzing the surface volume fraction of the fluids used in computational domain. While VOF model finds wide application in case of time-dependent solution, the steady stated from is also used. This model assumes the non-penetrating nature of the fluids. Area of application if the model includes liquid jet breakup prediction, motion of large bubbles inside liquid, stratified flows, liquid flow after dam break, steady or transient tracking of nay gas-liquid interface. Some of its limitation includes:

- Available only for pressure-based solver.
- Inability to model streamwise periodic flow.
- Second-order implicit time-splitting step cannot run in this model.

3.3.2.2 Mixture Model

On the assumption of two fluids behaving as interpenetrating continua moving at different velocities, mixture model calculates relative velocities for dispersed phases to model homogeneous flow. However, it also assumes local equilibrium over short length scales. Applications include particle-laden flow with low loading, sedimentation, cyclone separator.

3.3.2.3 Eulerian Model

The Eulerian model solves n sets of equations for each phase. The pressure and interphase exchange coefficients incorporates the coupling effects. The nature of phases involved dictates the mode of handling coupling by this model. There is a separate technique for handling granular and non-granular flows. The properties of phases described as "granular" flow are derived from kinetic theory. Momentum exchange between the phases is influenced by the nature of the phases. UDF (User-defined functions) also comes handy when momentum exchange is to be calculated. Eulerian models mostly find use in areas such as bubble columns, risers, particle suspension and fluidized beds, packed beds and trickle bed reactors. A detailed guideline and criterions are listed in the ANSYS theory guide to help choose which model can be used in a particular scenario.

3.4 Drag Force Calculation:

This project deals with gas-liquid system and as common perception, gas phase should travel faster than the liquid phase. This results in phase slippage and culminates into interphase drag force, a parameter that plays a pivotal role in turbulence modeling. To understand this concept, the term relative velocity has been introduced; which is defined as difference between primary phase and secondary phase velocity (that is p and q); also

$$v_{pq} = v_p - v_q \tag{3.8}$$

For the multiphase system, we have the following options for drag force calculation:

- Schiller-Nauman model which calculates the drag coefficients based on the range of Reynolds number and then calculate the friction factor from Drag coefficient. This is generally used in case of fluid-fluid drag function.
- Gidaspow et al. calculates the momentum exchange coefficients for each pair of phases using the drag coeeficients. It uses Ergun type equations for packing with bed voidage less than 0.8 while Wen yu equation is used for higher bed voidage.

3.5 Turbulence Model (the k- ε model)

Due to chaotic nature of turbulence, there has to be a multitude of models to represent the exact nature of turbulent flow for each specific scenario. Dealing with RANS-based turbulence model is comparatively easy for CFD simulation and is widely applicable in many scenarios. Sophisticated models like LES, DES and DNS models are applicable for highly sophisticated problems dealing with big data. The linear, non-linear eddy viscosity models and Reynolds Stress Model forms the RANS-based model. While the non-linear eddy viscosity models (EVM) can truly represent turbulence in the system, they are most complex and hence less popular in CFD. Our main focus in CFD is the linear eddy viscosity models which are available in different forms as shown in Figure 3.1.

The two-equation model computes two parameters- turbulent length and time-scale from two different transport equations. The standard k-ε model belongs to the two-equation model category. Proposed by Launder and Spalding, it is based on kinetic energy (k) and its dissipation (ε). Basic assumptions considered are: a fully turbulent flow and miniscule effect of molecular viscosity.
It suffers from the disadvantage of high insensitivity to abnormal pressure gradient and boundary layer separation. They prognosticate a deferred and condensed separation with respect to observer leading to overly optimistic modeling. The turbulence kinetic energy arises from two effects: from the mean velocity gradient and the buoyancy effects. While the RNG form of k- ε model uses the statistical approach called the renormalized group, the Realizable form solves equations within constraints put on Reynolds stresses.

3.6 Porous Media Model:

It finds application in packed beds, tube banks, perforated plates, catalytic convertors, mixing tank problems and many more scenarios. Initially, the phase (cell zone) on which porous media model is to be applied is specified. Pressure loss is calculated too based on the inputs like the Superficial Velocity Porous Formulation (indication of bulk pressure loss). Superficial velocity is same whether the region is inside the porous zone or outside of it. This curtails its velocity increase computation capability to some extent and hence limits its accuracy. This model incorporates an additional term- a momentum source term to transport equations. This source term comprises of two parts: a viscous resistance term (Darcy's term) and an inertial resistance term (Forschneider term).The present problem in focus is a case of homogeneous porous media where porous media model is of the form:

$S_i = -(\frac{\mu}{\alpha} v_i + C_2 \frac{1}{2} \rho |v| v_i)$, where α= permeability and C_2= internal resistance factor. (3.9)

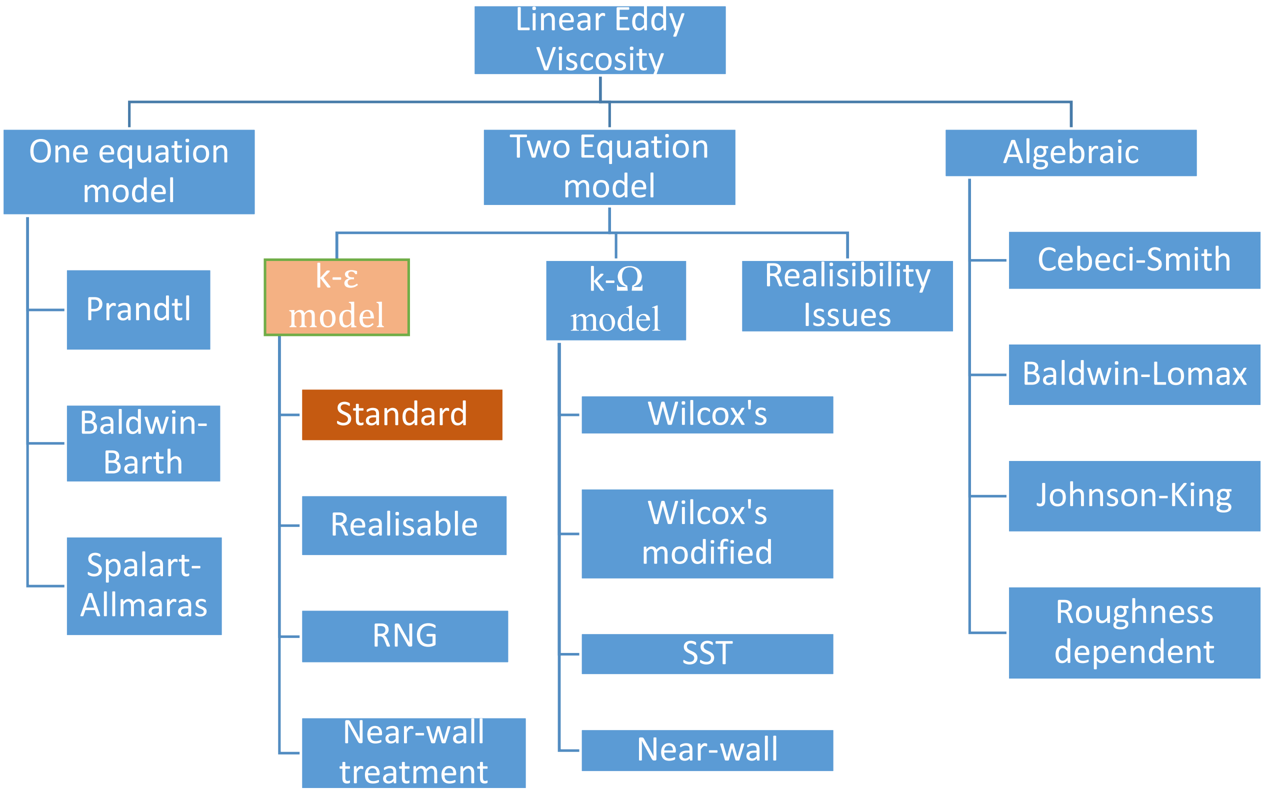


Figure 3.1:Various Linear Eddy Viscosity Models

(*http://www.cfd-online.com/Wiki/RANS-based_turbulence_models)*

Another provision for modeling source term is also used in ANSYS FLUENT, known as the power law of velocity magnitude.

$S_i = -C_0|v|^{C_1}$, where C_0 and C_1 are user-defined empirical constants. (3.10)

α and C_2 can be calculated from the following relations:

$$\alpha = \frac{d_p^2}{150} \cdot \frac{\varepsilon^3}{(1-\varepsilon)^2} \quad (3.11)$$

$$\text{and} C_2 = \frac{3.5}{d_p} \cdot \frac{(1-\varepsilon)}{\varepsilon^3} \quad (3.12)$$

CHAPTER 4

CFD SIMULATION

The geometry is prepared using ANSYS Design Modeler. Subsequently, mesh is prepared with the help of ANSYS Meshing application and then run in ANSYS® FLUENT 15.0. A comparison is drawn on the results (obtained from ANSYS CFD-Post) of various models and varying phasic velocities. Results are analyzed and plotted using Origin Pro 2015. The whole project focuses on trickle flow regime only.

4.1 Geometry and Mesh

Table 4.1: Geometry specifications of trickle bed reactor

Variables and conditions	Specifications
Height of column	128 cm
Inner diameter	91 mm
Packing material	9.81 mm raschig rings
Voidage	0.44
Phases (Primary-Secondary)	Air-water

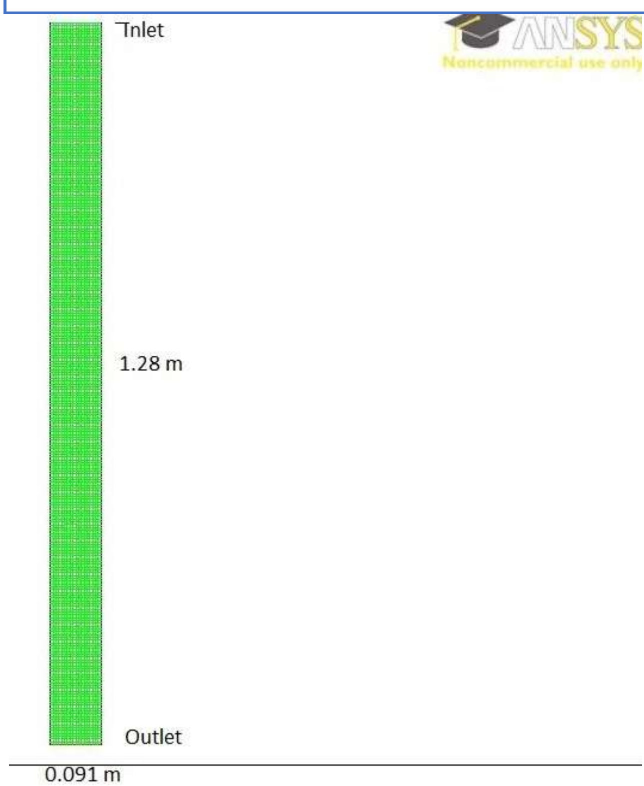


Figure 4.1: Structured grid for simulation

Table 4.2 Mesh report

Parameters	values
Cells	4608
Faces	9490
Nodes	4883
Partitions	1
Cell size	0.005 units
Meshing method	Uniform Quad/Tri
Min Orthogonal Quality	0.99965
Max Aspect ratio	1.4617

4.2 Assumptions:

Based on the following assumptions, CFD modeling of trickle bed reactor is done:

- The two fluids involved in simulation are treated as incompressible
- Operation is strictly in the trickle flow regime, that is gas-liquid interaction is so little that capillary forces can be ignored. Thus our assumption of same uniform pressure throughout space and time remains valid.
- No interphase mass transfer is occurring
- Porosity is uniform and constant
- An isotropic porosity in the phase indicating uniform permeability throughout the phase
- Overall equation of motion is not influenced by the effect of turbulent stress terms

4.3 Boundary conditions and Numerical Solutions

A two-dimensional double precision, serial processing ANSYS Solver is opened. Pressure-based type solver runs a transient fluid flow process on a planar geometry with the gravity (9.81 m/s^2 downward acting) taken into consideration. Now there are two scenarios used for modeling:

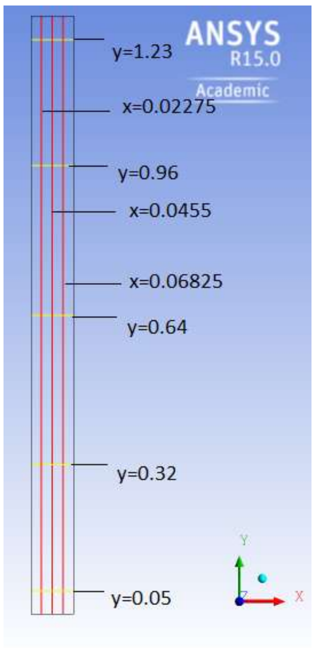
Table 4.3: Operating conditions and model used

Specifications	Values
Primary phase	Air
Secondary phase	Water, Raschig rings
Multiphase Model	Eulerian 3-phase
Interactions: **Air-water** **Solid-water, Solid-air**	 Gidaspow et al. Schiller-Naumann
Superficial gas velocity	0.22 m/s, 0.33 m/s
Superficial liquid velocity	0.0025,0.0035,0.0050,0.0065, 0.0075 m/s
Pressure-velocity coupling	SIMPLE algorithm

Different simulation conditions:

I. Different superficial gas and liquid velocities

II. Non-porous with granular packing with patching of surface body done at 3000 Pa, 5000 Pa, 10000 Pa



Given alongside is the figure 4.2, depicting the lines along which results are displayed in the following section. All these line partitions the geometry into equal segments. The complete results is shown in the last section, that is 5.4. While for the first three sections, we have chosen x=0.0455 m line for displaying the axial variation of properties and y=0.64 m line for the radial variation. These results were obtained from the ANSYS CFD-Post Processing. Table 4.4 shows the values inputted for solution controls.

Figure 4.2: Lines on geometry for retrieving information on pressure drop and liquid holdup (from ANSYS-CFD Post Processing)

Table 4.4: Solutions settings

Simulation parameters	
Discretization scheme	First Order Upwind
Pressure velocity coupling	Phase coupled SIMPLE
Convergence criteria	10^{-3}
Time step size	0.005 s
Number of time steps	12000
Discretization gradient	Least Square Cell based
Initialization type	Standard
Relaxation Factors	
Pressure	0.1-0.3
Density	0.7-1.0
Body Force	0.7-1.0
Momentum	0.3-0.7
Volume Fraction	0.2-0.4

RESULTS AND DISCUSSION

CFD simulation is performed on three-phase concurrent air-water Trickle Bed Reactor with 9.81 mm ceramic raschig rings as explained in Table 4.1, in previous section. Uniform gas and liquid distribution is assumed at the inlet of two-dimensional model of trickle bed reactor and a flat velocity profile is considered for the fluids. No-slip condition is activated on the wall with roughness factor set to 0.5. Simulation is run for 60 seconds with 0.005 s time steps. As seen in Figure 5.1, there is sharp variations in scaled residual up to 750 iterations and subsequently shows gradual decrease upto 2500 iterations, showing the quasi-steady state region. Steady state is attained in 3000 iterations or 15 s.

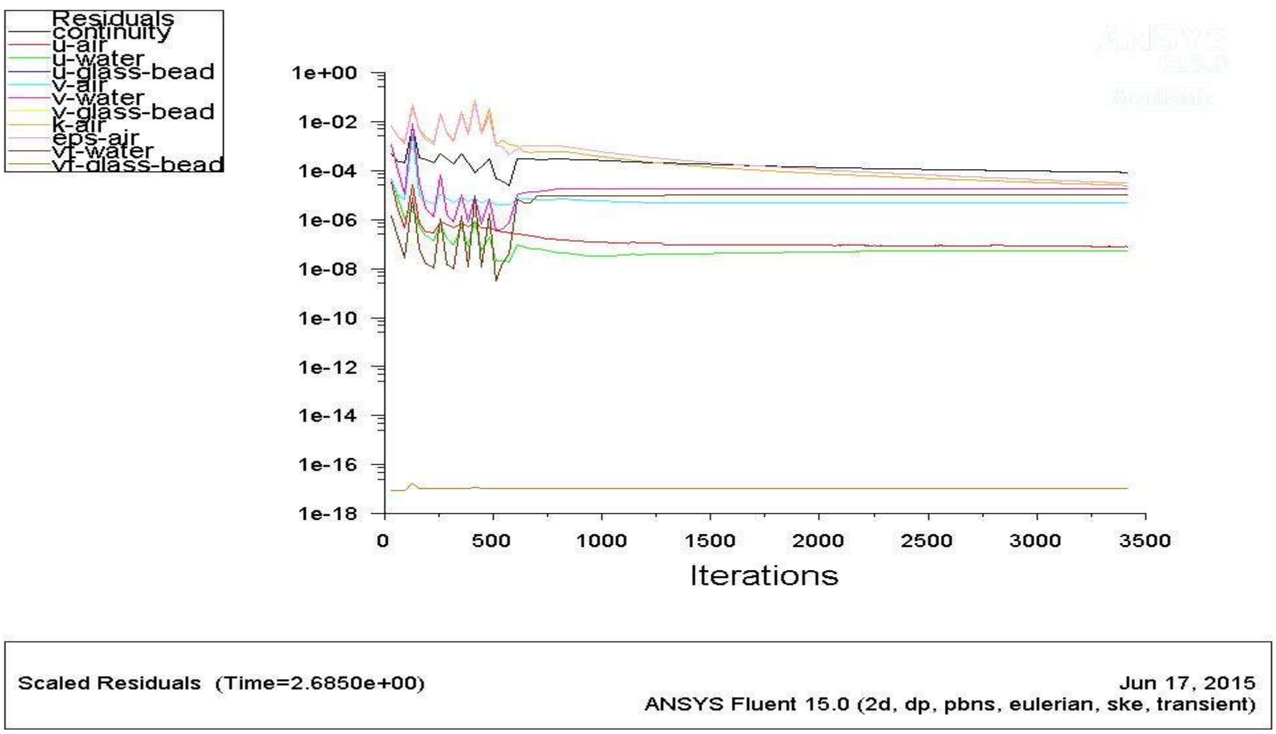
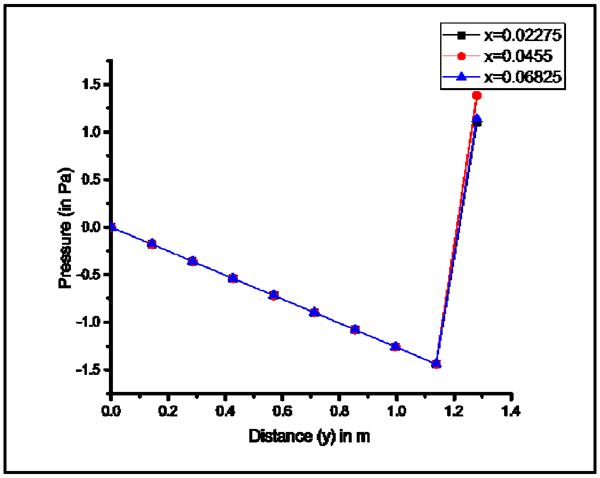


Figure 5.1: Scaled Residual plot showing convergence

5.1 Transverse and longitudinal variation of pressure and liquid holdup for Ug=0.22 m/s and Ul=0.0025 m/s

The graph in figure 5.2 shows the expected linear drop in pressure across the length of reactor with maximum pressure drop of 1.384 Pa. Figure 5.2 shows liquid holdup variation across the length of the reactor showing steep decrease near the inlet and then nearly remains constant thereafter. As shown, maximum liquid holdup of 0.01152 is obtained at the inlet of reactor.



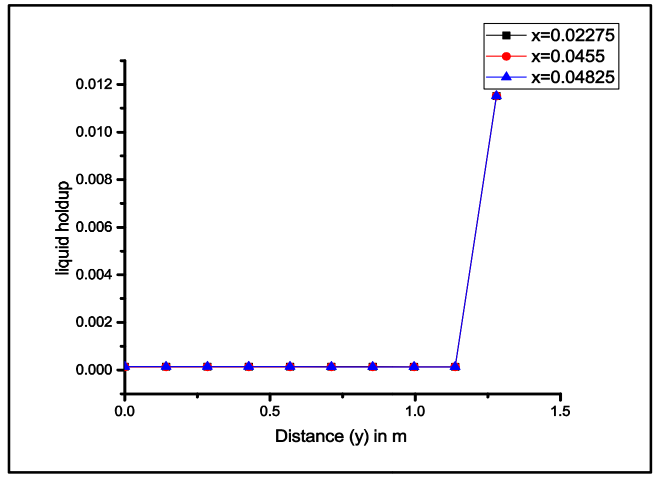


Figure 5.2: Axial variation of Pressure drop **Figure 5.3: Axial variation of Liquid holdup**

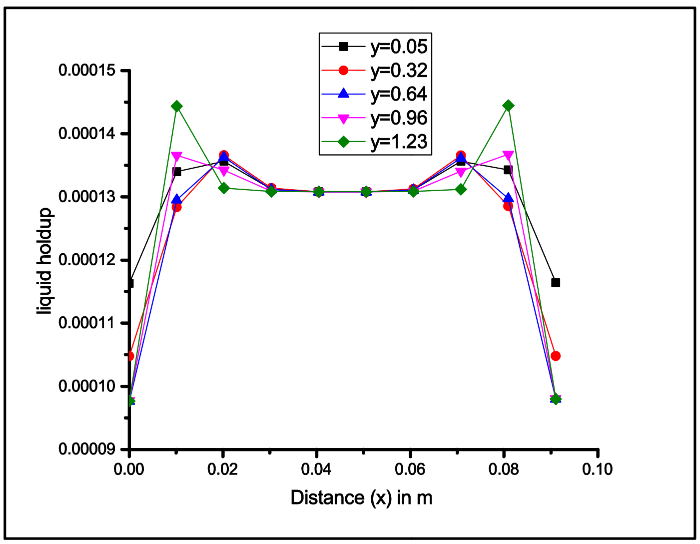


Figure 5.4: Radial variation of Liquid holdup

Figure 5.3 shows the transverse variation of liquid holdup which follows closely to the shape of boundary layer while it flattens out near the centre indicating that behaves according to a fully developed flow. This graph also points out that up to 0.05 m from the inlet, liquid holdup is high (0.0144) as compared to downstream portion, like at height y=0.96 m, 0.64 m and the rest (showing a value of 0.0135-0.0138).

5.2 Effect of patching with different pressure on the solution

The iterative methods employed for the prediction of pressure drop and liquid holdup exploits the Gauss-Seidel method or ILU method which commences its calculation from an initial guess (may be zero or non-zero number). But choosing an initial guess closer to local solution can help in achieving stable solution and even eliminating the chances of solution divergence. From various literature works, experimental work on atmospheric pressure operation of trickle bed reactor has been carried at a gauge pressure range of 0-15000 Pa. Hence, we use gauge pressure values of 3000 Pa, 5000 Pa and 10000 Pa to patch the mesh. The results are then compared with the values at 0 Pa pressure. It is observed that the plots for different patching values follow a similar trend, with slight differences in their values. Significant difference arises in the case of transverse variation of liquid holdup closer to the wall which gradually diminishes in the centre. Due to pressure-velocity coupling involved in SIMPLE algorithm, solution of different pressure patching shows different response to velocity fluctuations arising due to boundary layer. This may indicate to the varying sensitivity of different pressure patching values due to boundary effect. This also explains the difference in liquid holdup vales at x=0.01 m and x=0.08 m along the diameter.

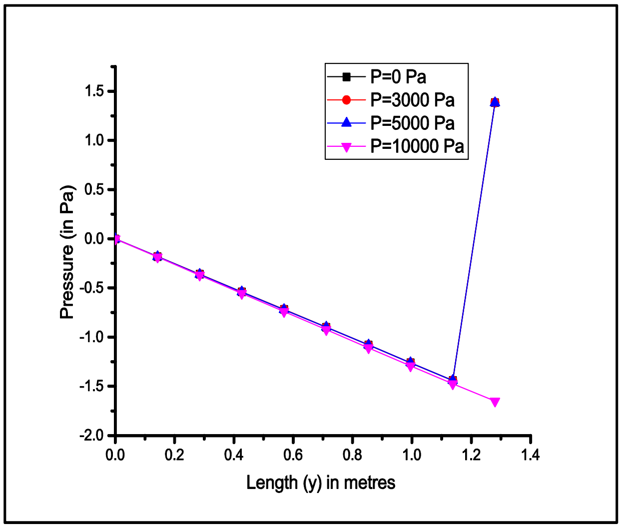


Figure 5.5: Axial variation of Pressure drop for different pressure patching

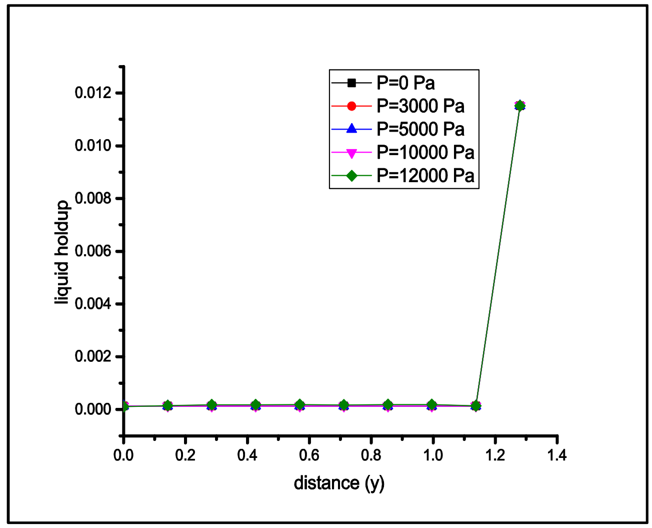


Figure 5.6: Axial variation of liquid holdup for for different pressure patching

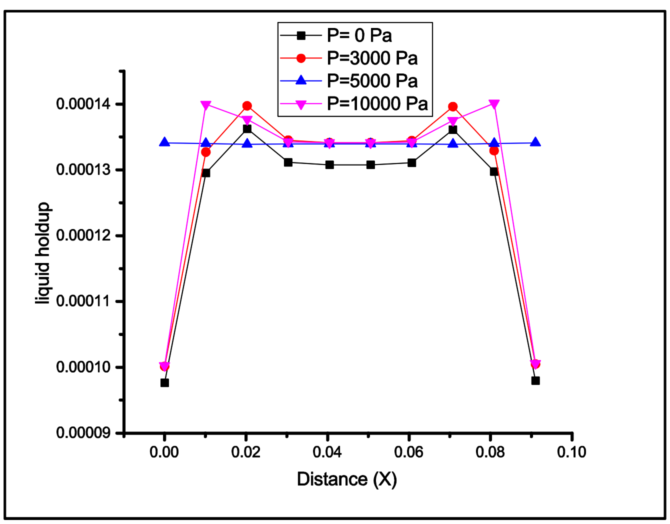


Figure 5.4 shows the axial variation of pressure drop for different values of pressure patching. Figure 5.5 shows the axial variation of liquid holdup while Figure 5.6 shows the radial variation of liquid holdup for pressure patching 0 Pa, 3000 Pa, 5000 Pa and 10000 Pa. Simulation with 12000 Pa, 14000 Pa and 15000 Pa were also performed which resulted with divergence

Figure 5.7: Radial variation of Liquid holdup for different pressure patching

5.3 Different gas and liquid velocities:

The right half part of the page shows variation of two parameters (pressure drop and liquid holdup) at gas velocity of 0.22 m/s while left half shows the same at gas velocity of 0.33 m/s. As seen from

Figure 5.7, with increase in liquid velocity the pressure gradient increases as expected with the pressure drop more steep for higher liquid velocity. There is maximum pressure drop of 1.439 Pa for u_l=0.0025 m/s while it is 4.275 Pa drop for u_l=0.0075 m/s. An increase in liquid volume fraction is expected from increased liquid velocity which in turns increases the interphase drag force and hence the pressure drop. At u_l=0.005 m/s,pressure drop is 1.875 Pa for u_g=0.33 m/s while it is 2.83 Pa for u_g=0.22 m/s (shown in Figure 5.8). This suggest that increasing gas velocity has reverse effect than increasing the liquid flow velocity. Figure 5.9 shows the maximum liquid holdup as 0.01152 which is same for different liquid velocity at gas velocity of 0.22 m/s. Even liquid holdup is 0.01152 for gas velocity if 0.33 m/s (Figure 5.10). Figure 5.11 shows the radial variation of liquid holdup, indicating liquid holdup of 0.0001 for u_l=0.0025 m/s, 0.00014 for u_l=0.0035 m/s, 0.00019 for u_l=0.005 m/s, 0.00026 for u_l=0.0065 m/s and 0.0003 for u_l=0.0075 m/s. As expected, maximum liquid holdup at height y=0.64 m (middle of the length of reactor) increases as liquid velocity increases. This trend is followed at all different heights of the bed. Figure 5.12.

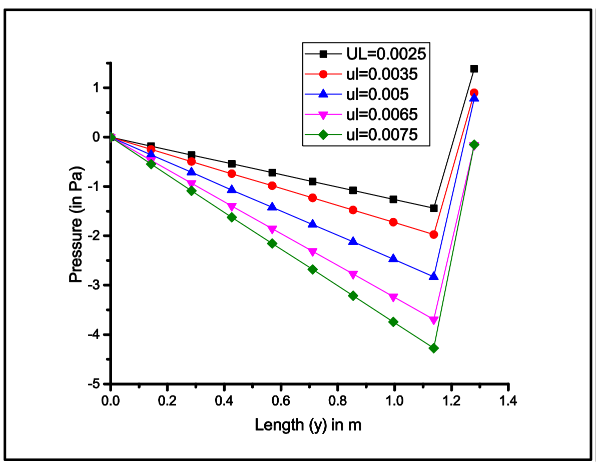


Figure 5.8:Axial variation of Pressure variation at different liquid velocity and U_g=0.22 m/s

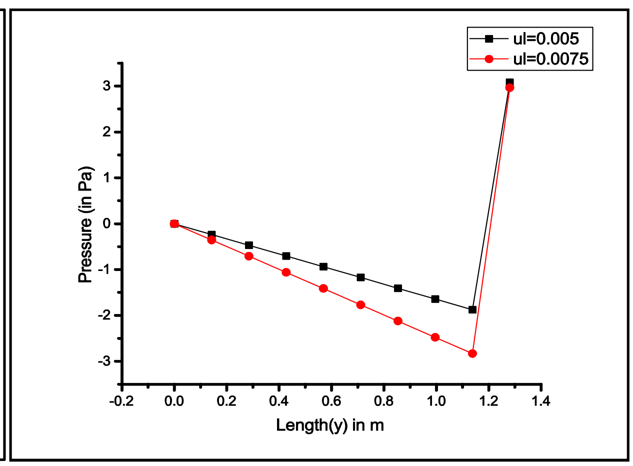
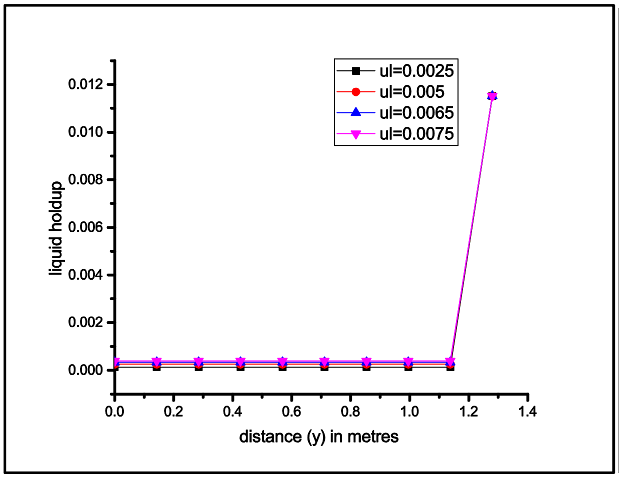


Figure 5.9: Axial variation of Pressure variation at different liquid velocity and U_g=0.33 m/s



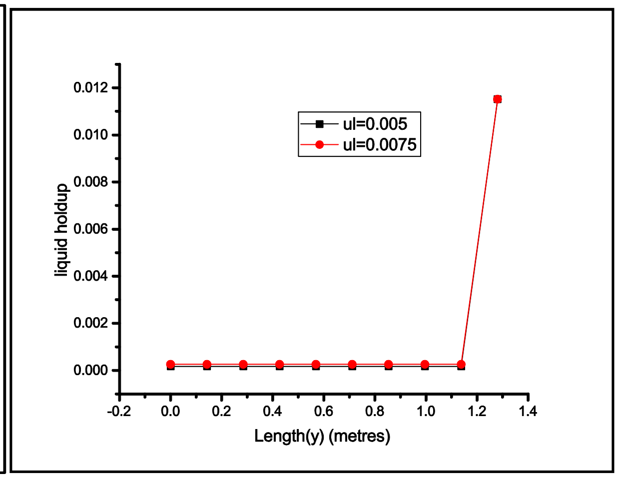
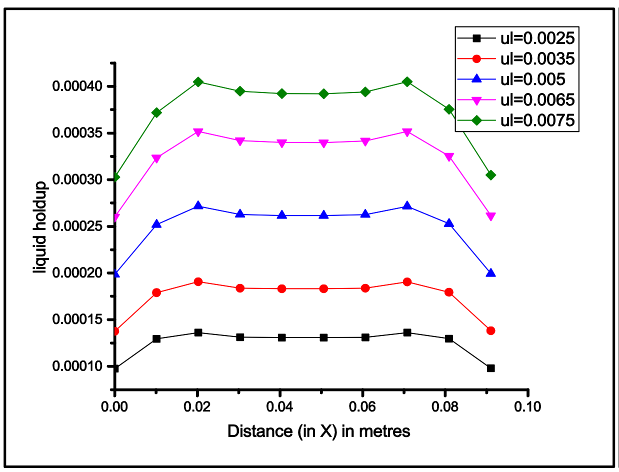


Figure 5.11: Axial variation of liquid holdup at different liquid velocity and U_g=0.22 m/s

Figure 5.11: Axial variation of liquid holdup at different liquid velocity and U_g=0.33 m/s



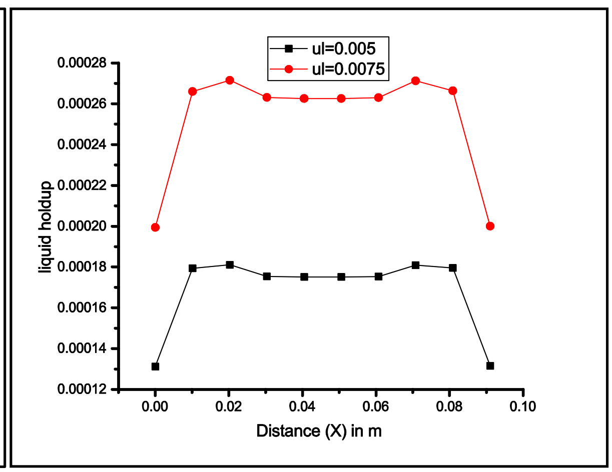


Figure 5.12: Radial variation of liquid holdup at different liquid velocity and U_g=0.22 m/s

Figure 5.12: Radial variation of liquid holdup at different liquid velocity and U_g=0.33 m/s

CHAPTER 6

CONCLUSION

A two-dimensional model for trickle bed reactor is solved using ANSYS employing the Eulerian-Eulerian model with specifications of the trickle bed reactor as mentioned in Table 4.1 in previous section. For gas velocity of 0.22 m/s, we run simulation for different liquid velocities of 0.0025 m/s, 0.0035 m/s, 0.005 m/s, 0.0065 m/s and 0.0075 m/s. On the other hand, for gas velocity of 0.33 m/s, we have results for 0.005 m/s and 0.0075 m/s liquid velocities. From the different case scenario of the ANSYS simulation of trickle bed reactor, we can infer that:

- Pressure decreases linearly along length of the reactor and more is the liquid velocity, steeper is the pressure drop. Pressure drop increases with decreasing gas velocity and increasing liquid velocity. Patching values have no effect up to a certain range, which is 10000 Pa. Beyond the 10000 Pa value, the solution becomes instable as is expected from the limitations of iterative schemes. Divergence is detected which cannot be eliminated. The sharp increase in pressure drop close to the inlet is maybe due to excessive pressure loss in the entrance length.
- Liquid holdup has strong variation in transverse section, following the usual fully developed turbulent flow regime. This is shown by the two portion of the radial liquid holdup variation plot, one in which consists of flatter region (within 0.03-0.06 m) resembling the turbulent core section of fully developed flow; the second one is the sharply varying hump like section within 0.03 m from the wall resembling the boundary layer. Axial variation shows that liquid holdup decreases steeply (from 0.01152 to 0.00026) close to the inlet than in any other portion of the reactor. For different patching pressure values, the radial variation of liquid holdup follows the same line, while the radial variation of liquid holdup shows slight deviation at x=0.03 and x=0.06 m.

Future scope of the work

For an extensive study of hydrodynamics of trickle bed reactors, a comparison of all the three models (relative permeability, slit model, fluid-fluid interaction model) on a Trickle-Bed reactor operating at high pressure high temperature can be carried out and their applicability can be studied. Two cases of CFD simulation, one including porous media and the other excluding porous media can also be studied. Comparative studies on various models for trickle bed reactor operating in different operating condition can help us gain a better understanding of the limitations of these models. This will enable is us to introduce further modifications in these models which in turn, can help us in more accurate hydrodynamic study of trickle bed reactor.

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