

HYDRODYNAMIC STUDY OF THREE PHASE FLUIDIZED BED WITH MODERATELY VISCOUS SOLUTIONS-CFD ANALYSIS

A Project Report submitted by

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*In partial fulfillment of the requirements
of the degree of*

Bachelor of Technology in Chemical Engineering

Under the guidance of

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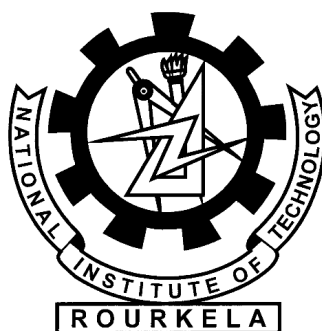


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CERTIFICATE

This is to certify that the report entitled “Hydrodynamic Study of Three Phase Fluidized Bed with Moderately Viscous Solutions-CFD Analysis”, submitted by **RAHUL NAIR**, ROLL NO-**107CH033** to National Institute of Technology, Rourkela is a record of bonafide project work under my supervision and is worthy for the partial fulfillment of the degree of Bachelor of Technology (Chemical Engineering) of the Institute. It is based on candidate’s own work and has not been submitted elsewhere.

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ABSTRACT

Fluidization basically refers to the process of passing a fluid upwards through a packed bed of solid particles resulting in a pressure drop due to the drag force of fluid. If the fluid velocity is gradually increased then the pressure drop increases as well as the drag force on the particles and after some time the particles will no longer be in a state of rest but will start to move and will remain suspended in the fluid. This condition represents fluidization. Three-phase fluidized beds or slurry bubble columns have gained considerable importance because of the good heat and mass transfer characteristics in their applications in physical, chemical, petrochemical, and biochemical processing. They are operated by a number of industries around the world for carrying out various reactions and for them to be successful their hydrodynamics (phase holdups, bed expansion, pressure drop etc) have to be studied.

To understand better the bed complexities while designing and carrying out reactions CFD-Computational Fluid Dynamics is promoted as a useful tool. The potential of CFD for describing the hydrodynamics and heat and mass transfer of multiphase fluidized beds has been established by several publications. CFD predicts the flow characteristics, bed hydrodynamics, phase holdups and heat and mass transfer happening inside the bed qualitatively.

In the current work an attempt has been made to study the hydrodynamics of three phase fluidized bed with moderately viscous solutions. The simulation is done for a column of 1.88m height and 0.1m diameter filled with 4mm glass beads till a certain height. GAMBIT 2.2.30 is used to develop the computational grid of 0.01m and FLUENT 6.3.26 is used to carry out the simulation. It is observed that the bed expands considerably with increase in glycerol concentration for a constant inlet gas and liquid velocity. The gas holdups as well as liquid holdups are found to increase with glycerol concentrations for constant inlet velocities whereas solid holdup decreases.

Keywords: fluidization, phase holdup, computational fluid dynamics

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NOMENCLATURE

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

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

ϵ = Dissipation rate of turbulent kinetic energy, J

μ_{eff} = Effective viscosity, $kg/m\cdot s$

$M_{i,g}$ = Interphase force term for gas phase

$M_{i,l}$ = Interphase force term for liquid phase

$M_{i,s}$ = Interphase force term for solid phase

P = Pressure, Pa

t = Time, s

K = Turbulent kinetic energy, J

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

ϵ_k = Volume fraction of phase k = g (gas), l (liquid), s (solid)

CHAPTER 1

INTRODUCTION

1.1 Fluidization

Fluidization basically refers to the process of passing a fluid upwards through a packed bed of solid particles resulting in a pressure drop due to the drag force of fluid. If the fluid velocity is gradually increased then the pressure drop increases as well as the drag force on the particles and ultimately after some time a stage comes when the solid particles will no longer be in a state of rest but will start to move and will remain suspended in the fluid medium. The pressure drop now becomes constant but the bed height continues to increase. This condition when solid particles behave as a fluid represents fluidization.

Fluidization has gained wide acceptance in many industrial applications particularly in the fields of catalytic cracking and coal gasification. In a typical gas-liquid-solid fluidized bed solid particles fill the bed to a particular height and gas as well as liquid are sent co-currently to fluidize the solid particles. Here liquid is the continuous phase and gas as dispersed bubbles if the superficial gas velocity is low. Three-phase fluidized beds or slurry bubble columns ($u_t < 0.05$ m/s) have gained considerable importance in their application in physical, chemical, petrochemical, electrochemical and biochemical processing because of the good heat and mass transfer characteristics (Fan, 1989).

Gas-liquid-solid fluidized beds are used extensively in the refining, petrochemical, pharmaceutical, biotechnology, food and environmental industries. Some of these processes use solids whose densities are only slightly higher than the density of water (Bigot et al., 1990; Fan, 1989; Merchant; Nore, 1992). Gas-liquid-solid fluidized beds can be made to operate differently

by changing the velocities of solid and liquid phases and also by changing the properties of any or all phases. Minimum liquid fluidization velocity, U_{Lmf} , and the transition velocity from the coalesced to dispersed bubble regime, U_{cd} are important in determining the operability of the fluidized beds. The minimum liquid fluidization velocity is the superficial liquid velocity at which the bed becomes fluidized for a given superficial gas velocity. In the coalesced bubble regime, bubble size varies as the bubbles continuously coalesce and split, while in the dispersed bubble regime, there is no coalescence and thus the bubble size is more uniform and generally smaller (Luo et al., 1997). Any three phase fluidization systems can be operated in different forms namely:-

- Any of the phases acting like reactants or products.
- Gas-liquid reactions where solid acts as a catalyst.
- Two of them as reacting phases and the third being inert.
- All three as inerts like in unit operations.

Three phase reactors can be operated as slurry bubble column or fluidized bed reactors. In the initial one the particle density is slightly higher than the liquid, size varies from 5-150 μm and volume fraction is less than 0.15 (Krishna et al., 1997). Hence, liquid phase along with solid is treated as homogeneous with mixture density. In the latter one the particle density is much higher than the liquid and size exceeds 150 μm , volume fraction ranges from 0.6(packed stage) to 0.2 as close to dilute transport stage (Panneerselvam et al., 2009).

1.2 Applications of Gas-Liquid-Solid Fluidized Bed

Fluidization has always lived up to the expectations, turning into a well established technology used in chemical, petrochemical and biochemical processing (Muroyama et al., 1985); three phase reactors are nowadays employed in many areas such as coal liquefaction, biomass gasification and fermentation, bio-oxidation process for waste water treatment.

In the biotechnological processes three gas-liquid-solid reactors are used in the production of cell mass and primary and secondary metabolites with microorganisms, and cultivation of animal cell lines (K. Schügerl). Three-phase fluidized beds enjoy widespread use in a number of applications including methanol production, conversion of glucose to ethanol various hydrogenation and oxidation reactions, hydro treating and conversion of heavy petroleum and synthetic crude, coal liquefaction.

Three phase fluidized beds are also used in hydrogenation and hydro de-sulferization of residual oil and Fischer-Tropsch process (Jena et al., 2009). Fluidized beds are also used in facilitating catalytic and non-catalytic reactions, drying and other forms of mass transfer. One of the widespread use is in Fluidized Catalytic Cracking units in the oil refineries for the manufacture of gasoline where fine catalyst particles are used to increase the reactor performance by increasing the available surface area for reaction.

1.3 Modes of Operation and Flow Regimes

Gas-liquid-solid fluidization can be classified mainly into four modes of operation. Two of them in co-current modes and the other two in counter-current modes. Co-current three-phase fluidization is classified as liquid as the continuous phase and co-current three-phase fluidization with gas as the continuous phase. The counter-current modes are divided as inverse three-phase

fluidization and fluidization represented by a turbulent contact absorber (TCA). In inverse three-phase fluidization liquid constitutes the continuous phase whereas gas forms the discrete phase. In this operation the bed of particles with density lower than that of the liquid is fluidized by a downward liquid flow, opposite to the net buoyant force on the particles, while the gas is sent counter currently to that liquid, forming discrete bubbles in the bed. Counter current three phase fluidization with gas as the continuous phase is called turbulent contact absorber, mobile bed or turbulent bed contactor (Epstein., 1981). The gas-liquid contacting is more and the flow rates are much higher as compared to the conventional counter current packed beds.

CHAPTER 2

LITERATURE REVIEW

2.1 Recent Research on Gas-Liquid-Solid Fluidization

Numerous researches have been done in understanding the gas-liquid-solid fluidization characteristics. Most of the previous studies related to three-phase fluidized bed reactors have been directed towards the understanding the complex hydrodynamics, and its influence on the phase holdup and transport properties.

Recent research on fluidized bed reactors focuses on the following topics:

- **Flow structure quantification:** It mainly focuses on local and globally averaged phase holdups and phase velocities for different operating conditions and parameters. Rigby et al.(1970), Muroyama and Fan(1985), Lee and DeLasa(1987), Yu and Kim(1988) used electro-resistivity probe and optical fiber probe for investigating bubble phase holdup and velocity in three-phase fluidized beds for various operating conditions. Recently Warsito and Fan (2001, 2003) quantified the solid and gas holdup in three-phase fluidized bed using the electron capacitance tomography (ECT) (Panneerselvam et al., 2009).
- **Flow regime identification:** Muroyama and Fan (1985) developed the flow regime diagram for air–water–particle fluidized bed for a range of gas and liquid superficial velocities. Chen et al. (1995) investigated the identification of flow regimes by using pressure fluctuations measurements. Briens and Ellis(2005) used spectral analysis of the pressure fluctuation for identifying the flow regime transition from dispersed to coalesced bubbling flow regime based on various data mining methods like fractal and chaos analysis, discrete wake decomposition method etc. Fraguío et al.(2006) used solid phase

tracer experiments for flow regime identification in three phase fluidized beds (Panneerselvam et al., 2009).

- **Advanced modeling approaches:** A large number of experimental studies have been directed towards the quantification of flow structure and flow regime identification for different process parameters and physical properties but still the complex hydrodynamics of these reactors are not well understood due to complicated phenomena such as particle–particle interactions or because of interactions between all the three phases simultaneously. For this reason, computational fluid dynamics (CFD) has been promoted as a useful tool for understanding multiphase reactors (Dudukovic et al., 1999) for precise design and scale up. The two approaches used for this purpose are the Euler–Euler formulation based on the interpenetrating multi-fluid model, and the Euler–Lagrangian approach based on solving Newton's equation of motion for the dispersed phase.

2.2 Hydrodynamics of a Three Phase Fluidized Bed

Hydrodynamic properties of a three phase fluidized bed are important for analyzing their performance. These include mainly bed expansion behaviour, phase holdups and pressure drop. All the three phase holdups should add to give unity as a three phase fluidized bed constitutes of three phases. Bed expansion is important in determining the size of the system while the phase holdups are essential in mixing and studying about the overall performance of the system. For chemical processes where mass transfer is the rate-limiting step, it is important to estimate the gas holdup since this relates directly to the mass transfer (Fan et al., 1987) and (Schweitzer et al., 2001). The gas holdup is found to be influenced by the formation of bubbles by many researchers. Also it is found to be influenced by superficial gas velocities, particle size, liquid velocity etc.

Various investigators have made attempts to simulate the small bubble behaviour of the ebullated bed reactor under atmospheric conditions by the use of a liquid or a liquid solution having special properties in the laboratory experimental systems (Fan et al., 1987), (Safoniuk et al., 2002) and (Song et al., 1989). A high viscous and low surface tension liquid enhances the gas holdup due to the following reasons:

- Higher liquid viscosity exerts higher drag on the gas bubble which in turn lowers bubble rise velocities and hence increases the gas holdup.
- The same is done by lower surface tension of liquid due to formation of surface tension gradient on the bubble surface.
- Presence of surfactants also increases the gas holdup as they increase drag on the gas bubble by decreasing bubble rise velocities due to the formation of a surface tension gradient on the bubble surface (Shah et al., 1985).

2.3 Previous Studies on CFD Modeling of Solid-Liquid-Gas fluidized bed (Panneerselvam et al., 2009):

- Bahary et al. (1994) used Multi fluid Eulerian approach for three phase fluidized bed where Gas phase was treated as a particulate phase having 4mm diameter and a kinetic theory granular flow model applied for solid phase. They verified the different flow regimes in the fluidized bed.
- Grevskott et al. (1996) used two fluid Eulerian–Eulerian model for three phase bubble column. The liquid phase along with the particles is considered pseudo homogeneous by modifying the viscosity and density. They included the bubble size distribution based on the bubble induced turbulent length scale and the local turbulent kinetic energy level.

They studied the variation of bubble size distribution, liquid circulation and solid movement.

- Mitra-Majumdar et al. (1997) used 2-D axis-symmetric, multi-fluid Eulerian approach for three- phase bubble column. They used modified drag correlation between the liquid and the gas phase to account for the effect of solid particles and between the solid of gas bubbles. Axial variation of gas holdup and solid hold up profiles for various range of liquid and gas superficial velocities and solid circulation velocity were the parameters studied.
- Jianping and Shonglin(1998) used 2-D, Eulerian–Eulerian method for three-phase bubble column. Pseudo-two-phase fluid dynamic model. k_{sus} – ε_{sus} – k_b – ε_b turbulence model used for turbulence. They validated local axial liquid velocity and local gas holdup with experimental data.
- Li et al. (1999) used 2-D, Eulerian–Lagrangian model for three-phase fluidization. The Eulerian fluid dynamic method, the dispersed particle method (DPM) and the volume-of-fluid (VOF) method are used to account for the flow of liquid, solid, and gas phases, respectively. A continuum surface force (CSF) model, a surface tension force model and Newton's third law are applied to account for the interphase couplings of gas–liquid, particle–bubble and particle–liquid interactions, respectively. A close distance interaction (CDI) model is included in the particle–particle collision analysis, which considers the liquid interstitial effects between colliding particles. They investigated single bubble rising velocity in a liquid–solid fluidized bed and the bubble wake structure and bubble rise velocity in liquid and liquid–solid medium are simulated.

- Padial et al. (2000) used 3-D, multi-fluid Eulerian approach for three-phase draft- tube bubble column. The drag force between solid particles and gas bubbles was modeled in the same way as that of drag force between liquid and gas bubbles. They simulated gas volume fraction and liquid circulation in draft tube bubble column.
- Matonis et al. (2002) used 3-D, multi-fluid Eulerian approach for slurry bubble column. Kinetic theory granular flow (KTGF) model for describing the particulate phase and a k - ε based turbulence model for liquid phase turbulence was used. Time averaged solid velocity and volume fraction profiles, normal and shear Reynolds stress were studied and compared with experimental data.
- Schallenberg et al. (2005) used 3-D, multi-fluid Eulerian approach for three-phase bubble column. Extended k - ε turbulence model to account for bubble-induced turbulence was used. The interphase momentum between two dispersed phases is included. They validated local gas and solid holdup as well as liquid velocities with experimental data.
- Zhang and Ahmadi (2005) used 2-D, Eulerian-Lagrangian model for three-phase slurry reactor. They included the interactions between bubble-liquid and particle-liquid. The drag, lift, buoyancy, and virtual mass forces are also included. Particle-particle and bubble-bubble interactions are accounted for by the hard sphere model approach. Bubble coalescence is also included in the model. Transient characteristics of gas, liquid, and particle phase flows in terms of flow structure and instantaneous velocities were studied.

2.4 Current Work

There are many literatures available for three phase fluidization with moderately viscous solutions which are mainly based on experimental data and due to complex hydrodynamics involved in them it is difficult to analyze those systems exactly but CFD being a flow modeling software helps us in understanding the behaviour with much accuracy. Also not much work has been done till now using computational methods, the current work is carried out using CFD to analyze hydrodynamics of three phase fluidization with moderately viscous solutions. The simulation is done for a bed of height 1.88m and 0.1m diameter. Glass beads of size 4mm constitute the solid phase. The static bed height is 25.6cm. The gas (air) and liquid (glycerol solution) are sent co currently from the bottom of the bed. Different concentrations of glycerol solutions are used ranging from 6% to 30%. The CFD software package of Fluent 6.3 has been used in running the simulations for the cases while the computational grid has been made using GAMBIT 2.2 and the results obtained are validated from the literature.

CHAPTER 3

NUMERICAL METHODOLOGY IN MULTIPHASE FLOW

3.1 Computational Fluid Dynamics

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

3.2 Advantages of CFD

CFD has seen dramatic growth over the last several decades. This technology has widely been applied to various engineering applications such as automobile and aircraft design, weather science, civil engineering process engineering, and oceanography. The most fundamental consideration in CFD is how one treats a continuous fluid in a discretized fashion on a computer. It allows us to design and simulate any real systems without having to design it practically. CFD predicts performance before modifying or installing systems. The ability to simulate the flow behaviour of any new product or process improves the understanding of fluid behaviour and

hence it reduces the time of prototype production and testing, leading to a successful glitch free design. Using CFD, we can build a computational model that represents a system or device that we want to study. A key advantage of CFD is that it is a very compelling, non-intrusive, virtual modeling technique with powerful visualization capabilities, and researchers can evaluate the performance of any practical system on the computer without the time, expense, and disruption required to make actual changes onsite. After our required design is built, we apply the fluid flow physics and chemistry to this virtual model and correspondingly the software will output a prediction of fluid dynamics and related physical phenomena (Kumar., 2009). Once the simulation is done then various parameters like temperature, pressure, mass fraction etc can be analyzed. Some of the main advantages of CFD can be summarized as:

1. CFD is particularly useful in simulating conditions where it is not possible to take measurements manually.
2. It can predict performance at any scale, thereby minimizing the risk in designing full fledged plants and reducing the number of pilot stages required to scale-up.
3. It provides the much needed flexibility in changing design parameters without the expense of onsite changes. It therefore costs less than laboratory or field experiments, thereby allowing engineers to try and develop something alternate which will be feasible.
4. It produces the results in a relatively short time as compared to the onsite experience.
5. It is also cost effective as it allows testing of a large number of variables without modifying existing processes or plants.

3.3 Governing Equations in Computational Fluid Dynamics

For all flows, conservation equations for mass and momentum are to be solved. For flows involving heat transfer or compressibility, an additional equation for energy conservation is solved.

3.3.1 The Mass Conservation Equation

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

$$\frac{\delta}{\delta t}(\epsilon_k \rho_k) + \nabla(\epsilon_k \rho_k \mathbf{u}_k) = 0$$

Where ρ_k is the density and ϵ_k is the volume fraction of phase $k=g, s, l$ and the volume fraction of the three phases satisfy the following condition:

$$\epsilon_g + \epsilon_l + \epsilon_s = 1$$

3.3.2 Momentum Equations

For liquid phase

$$\frac{\delta}{\delta t}(\rho_l \epsilon_l \mathbf{u}_l) + \nabla(\rho_l \epsilon_l \mathbf{u}_l \mathbf{u}_l) = -\epsilon_l \Delta P + \nabla(\epsilon_l \mu_{\text{eff},l} (\nabla \mathbf{u}_l + \mathbf{u}_l^T)) + \rho_l \epsilon_l \mathbf{g} + M_{i,l}$$

For gas phase

$$\frac{\delta}{\delta t}(\rho_g \epsilon_g \mathbf{u}_g) + \nabla(\rho_g \epsilon_g \mathbf{u}_g \mathbf{u}_g) = -\epsilon_g \Delta P + \nabla(\epsilon_g \mu_{\text{eff},g} (\nabla \mathbf{u}_g + \mathbf{u}_g^T)) + \rho_g \epsilon_g \mathbf{g} + M_{i,g}$$

For solid phase

$$\frac{\delta}{\delta t}(\rho_s \epsilon_s \mathbf{u}_s) + \nabla(\rho_s \epsilon_s \mathbf{u}_s \mathbf{u}_s) = -\epsilon_s \Delta P + \nabla(\epsilon_s \mu_{\text{eff},s} (\nabla \mathbf{u}_s + \mathbf{u}_s^T)) + \rho_s \epsilon_s \mathbf{g} + M_{i,s}$$

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

3.3.3 Boundary Conditions

For any fluid flow problems the governing equations remain same, the difference in solving lies on the boundary conditions. They are quite different for each of the problems. The boundary conditions as well as the initial conditions set by the user decided the fate of the solution obtained from the governing equations. One such example can be when there is no relative motion between the surface and the fluid immediately adjacent to it the slip velocity is taken as zero. This is called the no-slip condition. If the surface is stationary, with the flow moving past it, then $u = v = w = 0$ at the surface for a viscous flow. This is one particular case of a physical boundary condition imposed for the problem.

3.4 How CFD Code Works

There are three steps for solving a CFD problem:

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

3.4.1 Pre-processing

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

- Definition of the geometry of the region: The computational domain.
- Grid generation the subdivision of the domain into a number of smaller, non-overlapping sub domains (or control volumes or elements Selection of physical or chemical phenomena that need to be modeled).
- Definition of fluid properties.

- Specification of appropriate boundary conditions at cells, which coincide with or touch the boundary.

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

3.4.2 Solver

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

ANSYS has developed two solvers namely FLUENT and CFX. They are high precision solvers and rely heavily on a pressure-based solution technique for broad applicability. The CFX solver uses finite elements (cell vertex numerics), similar to those used in mechanical analysis, to discretize the domain. In contrast, the FLUENT solver uses finite volumes (cell centered numerics). CFX software focuses on one approach to solve the governing equations of motion

(coupled algebraic multigrid), while the FLUENT product offers several solution approaches (density-, segregated- and coupled-pressure-based methods) (Kumar., 2009).

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

- (1) Fluid properties are updated in relation to the current solution; if the calculation is at the first iteration, the fluid properties are updated consistent with the initialized solution.
- (2) The three momentum equations are solved consecutively using the current value for pressure so as to update the velocity field.
- (3) Since the velocities obtained in the previous step may not satisfy the continuity equation, one more equation for the pressure correction is derived from the continuity equation and the linearized momentum equations: once solved, it gives the correct pressure so that continuity is satisfied. The pressure–velocity coupling is made by the SIMPLE algorithm, as in FLUENT default options.
- (4) Other equations for scalar quantities such as turbulence, chemical species and radiation are solved using the previously updated value of the other variables; when inter-phase coupling is to be considered, the source terms in the appropriate continuous phase equations have to be updated with a discrete phase trajectory calculation.
- (5) Finally, the convergence of the equations set is checked and all the procedure is repeated until convergence criteria are met.

3.4.3 Post- processing

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

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

3.5 CFD Approaches in Multiphase Flows

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

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

3.5.1 The Euler-Lagrange Approach

The Lagrangian discrete phase model in FLUENT follows the Euler-Lagrange approach. The fluid phase is treated as a continuum by solving the time-averaged Navier-Stokes equations, while the dispersed phase is solved by tracking a large number of particles, bubbles, or droplets through the calculated flow field. The dispersed phase can exchange momentum, mass, and energy with the fluid phase. A fundamental assumption made in this model is that the dispersed second phase occupies a low volume fraction, even though high mass loading ($m_{\text{particles}} \geq m_{\text{fluid}}$)

is acceptable. The particle or droplet trajectories are computed individually at specified intervals during the fluid phase calculation. This makes the model appropriate for the modeling of spray dryers, coal and liquid fuel combustion, and some particle-laden flows, but inappropriate for the modeling of liquid-liquid mixtures, fluidized beds, or any application where the volume fraction of the second phase is not negligible (Fluent., 2006).

3.5.2 The Euler-Euler Approach

In the Euler-Euler approach, the different phases are treated mathematically as interpenetrating continua. Since the volume of a phase cannot be occupied by the other phases, the concept of phase volume fraction is introduced. These volume fractions are assumed to be continuous functions of space and time and their sum is equal to one. Conservation equations for each phase are derived to obtain a set of equations, which have similar structure for all phases. These equations are closed by providing constitutive relations that are obtained from empirical information, or, in the case of granular flows, by application of kinetic theory. In FLUENT, three different Euler-Euler multiphase models are available: the volume of fluid (VOF) model, the mixture model, and the Eulerian model (Fluent., 2006).

1. The VOF Model

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

prediction of jet breakup (surface tension), and the steady or transient tracking of any liquid-gas interface.

2. The Mixture Model

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

3. The Eulerian Model

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

3.6 Some Multiphase Systems

Some examples of multiphase flow systems are as follows:

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

3.7 Choosing a Multiphase Model

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

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

CHAPTER 4

MODELLING AND SIMULATION OF

THREE PHASE FLUIDIZED BED

WITH MODERATELY VISCOUS SOLUTIONS

4.1 Problem Description

The problem consists of a three phase: gas-liquid-solid fluidized bed. Air and glycerol solutions of varying concentrations constitute the gas phase and liquid phase respectively. Solid phase consists of glass beads of uniform diameter, 4mm in this case. The gas and liquid are sent concurrently from the bottom of the bed while the solid phase is filled till a particular height called the static bed height.

Table 1 Properties of air and glass beads

Phases	Density, Kg/m³	Viscosity, kg/m-s
Air	1.166	1.789*10-05
Glass beads	2470	0.001003

Table 2 Properties of glycerol solutions

% Glycerol by weight	Density, Kg/m³	Viscosity, kg/m-s
6	1009.7	0.000984
12	1024	0.001082
18	1039	0.001268
24	1054	0.001567
30	1068.6	0.001852

4.2 Experimental Setup

Column specifications: 0.1m diameter

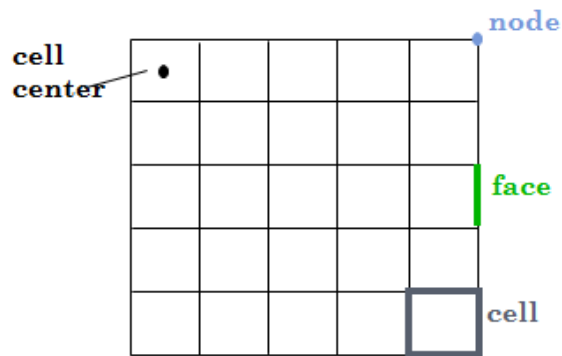
1.88m height

Static bed height= 25.6cm

4.3 Geometry and mesh

GAMBIT 2.2.30 was used for making 2D rectangular geometry of width of 0.1m and height 1.88m. Coarse mesh size of 0.01m is used for the whole geometry. It consists of 1880 quadrilateral cells, 376 -2D wall faces, 3562 -2D interior faces.

A typical 2D rectangular mesh is shown in the Figure1.



Simple 2D Mesh

Figure 1: 2D Mesh



4.4 Simulation and Models Used

Fluent 6.3.26 is used for running the simulations. 2D segregated 1st order implicit unsteady solver is used (the segregated solver must be used for multiphase calculations). Standard k- ϵ dispersed eulerian multiphase model with standard wall functions were used.

The model constants used during simulation are given in the table below.

Table 3: Model constants used for simulation

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

4.4.1 Turbulence Modeling

Standard k- ϵ model is used which is a de facto standard version of the two-equation model that involves transport equations for the turbulent kinetic energy, k and its dissipation rate, ϵ . At high Reynolds numbers the rate of dissipation of kinetic energy ϵ is equal to the viscosity multiplied by the fluctuating vorticity. An exact transport equation for the fluctuating vorticity, and thus the dissipation rate, can be derived from the Navier Stokes equation. The k - epsilon model consists of the turbulent kinetic energy equation. Its popularity in industrial flow and heat transfer simulations is because of robustness, economy, and reasonable accuracy for a wide range of

turbulent flows. It is a semi-empirical model, and the derivation of the model equations relies on phenomenological considerations and empiricism (Fluent., 2006).

4.4.2 Discretization

FLUENT uses a control-volume-based technique to convert the governing equations to algebraic equations that can be solved numerically. This control volume technique consists of integrating the governing equations about each control volume, yielding discrete equations that conserve each quantity on a control-volume basis (Fluent., 2006). In the current work First Order Upwind discretization scheme is used to discretize momentum, volume fraction, turbulent kinetic energy and turbulent dissipation rate. In this scheme quantities at cell faces are determined by assuming that the cell-center values of any field variable represent a cell-average value and hold throughout the entire cell; the face quantities are identical to the cell quantities. The main advantage is that it is easy to implement and gives stable results with reasonable accuracy and takes less computational time (Fluent., 2006). For pressure-velocity coupling Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) is used. It is one of the most commonly used methods. It is based on the premise that fluid flows from regions with high pressure to low pressure.

Table 4: Models used for considering interactions among phases.

Interactions	Model
Solid-Air	Gidaspow
Solid-Glycerol solution	Gidaspow
Air- Glycerol solution	Schiller-Naumann

- Water is taken as continuous phase while glass and air as dispersed phase.
- Interphase interaction models considered are tabulated below:
- Velocity Inlet Boundary Conditions: Air velocity was varied as 0.02123 m/s, 0.04246 m/s, 0.06369 m/s and 0.08492 m/s while liquid velocity was varied from 0.05 to 0.15 m/s in multiples of 0.0125 and inlet air volume fractions obtained as fraction of air entering in a mixture of gas and liquid.
- Pressure outlet boundary conditions:
Mixture Gauge Pressure- 0 Pascal
Backflow volume fraction for air = 0
- Specified shear was set as $X=0$ and $Y=0$ for gas and solid whereas no slip condition for water was used.

4.4.2 Solution Controls

Segregated solver is used which solves the equations individually unlike coupled solver. 1st order implicit unsteady formulation used. Velocity formulation is taken as absolute. Multiphase model is taken as Eulerian. Standard k-epsilon dispersed multiphase model with standard wall functions is used. Under relaxation factor for pressure, momentum and volume fraction were taken as 0.3, 0.2, and 0.5 respectively. The discretization scheme for momentum, volume fraction, turbulence kinetic energy and turbulence dissipation rate were all first order upwind. Pressure-velocity coupling scheme was Phase Coupled SIMPLE. Convergence criteria of 0.001 was used and iterations were carried with time step size of 0.001.

CHAPTER 5

RESULTS AND DISCUSSION

Simulations have been carried out for a three phase fluidized bed of 1.88m height and 0.1m diameter. It is done for a static bed height of 25.6cm. The simulations are done till a quasi steady state is obtained, that is, there is no further change in the bed, be it contours or bed height. The following figure indicates the bed behavior in course of time.

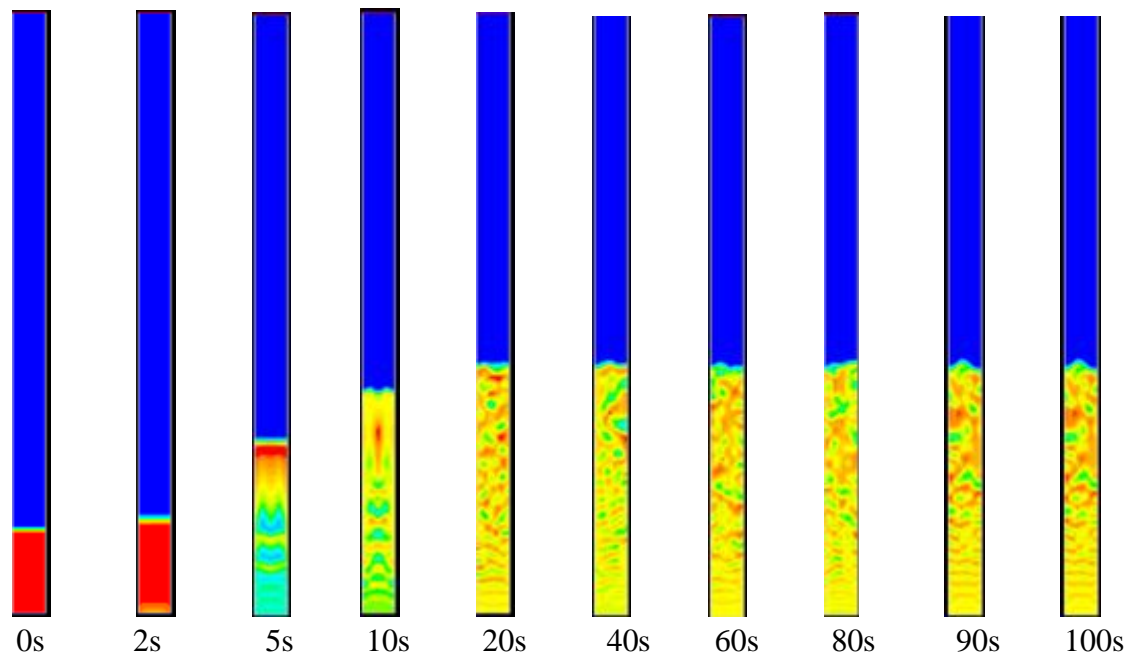


Figure 2: Contours of volume fraction of glass beads for air velocity of 0.02123m/s and liquid velocity of 0.15 m/s for 24% glycerol solution.

Above figure illustrates how the solid phase volume fraction changes in due course of time. Initially there is ver little change but when fluidization starts gradually the volume fraction of glass beads changes and after a quasi steady state is obtained there is no further change in the bed.

5.1 Phase Dynamics

All the three phases can be represented by contour plots. The following figure shows the contours of glass beads, air and glycerol solution after achieving a quasi steady state. The color scale given to the left of each contours gives the value of volume fraction corresponding to the color. The contour of water indicates that the volume fraction of water or liquid holdup is less in the fluidized part of the column as compared to the remaining part. The contour of air indicates that the gas holdup is significantly more in fluidized part of the bed as compared to the remaining part.

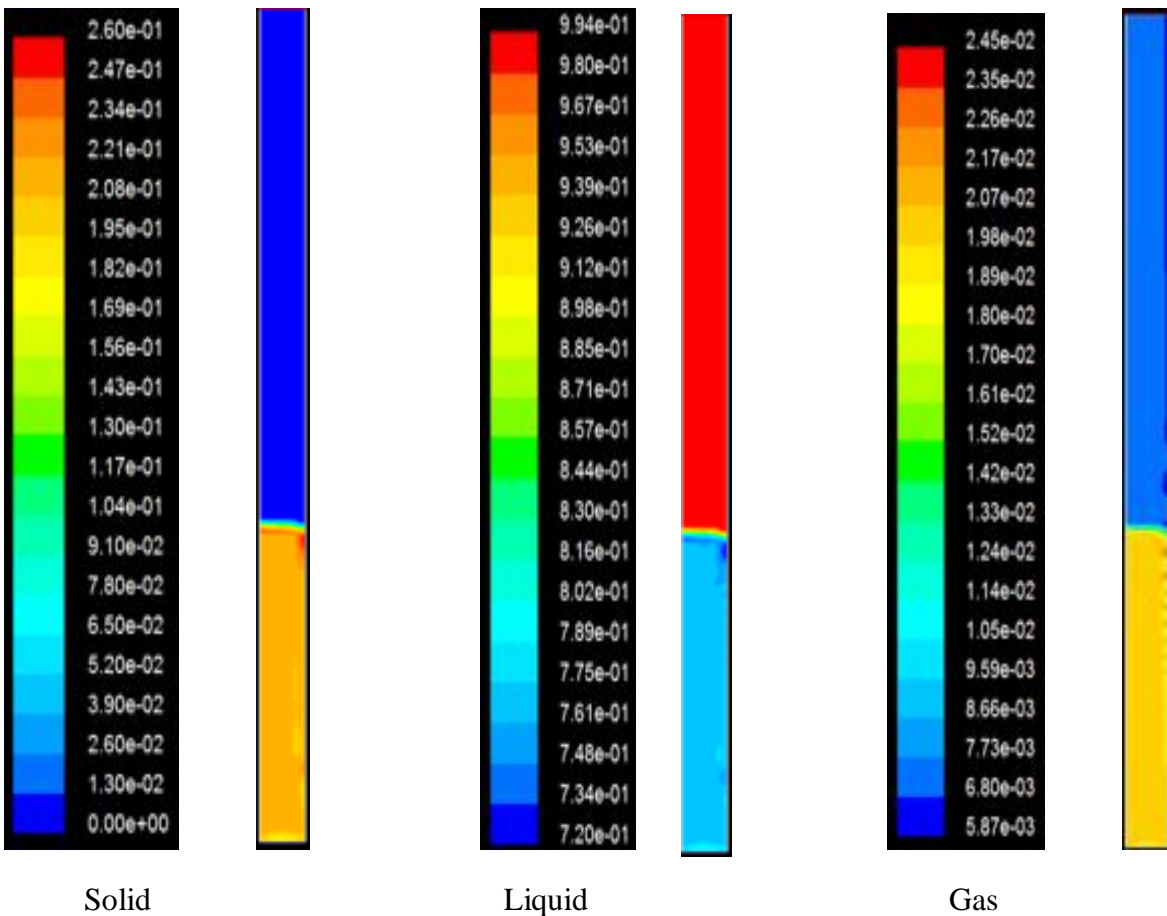


Figure 3: Contours of volume fractions of solid, liquid and gas at liquid velocity of 0.125m/s and gas velocity of 0.02123m/s for 30% glycerol solution.

The following figure shows the velocity vector of glass beads for 30% glycerol solution and for inlet gas velocity of 0.06369 m/s and liquid velocity of 0.15 m/s.

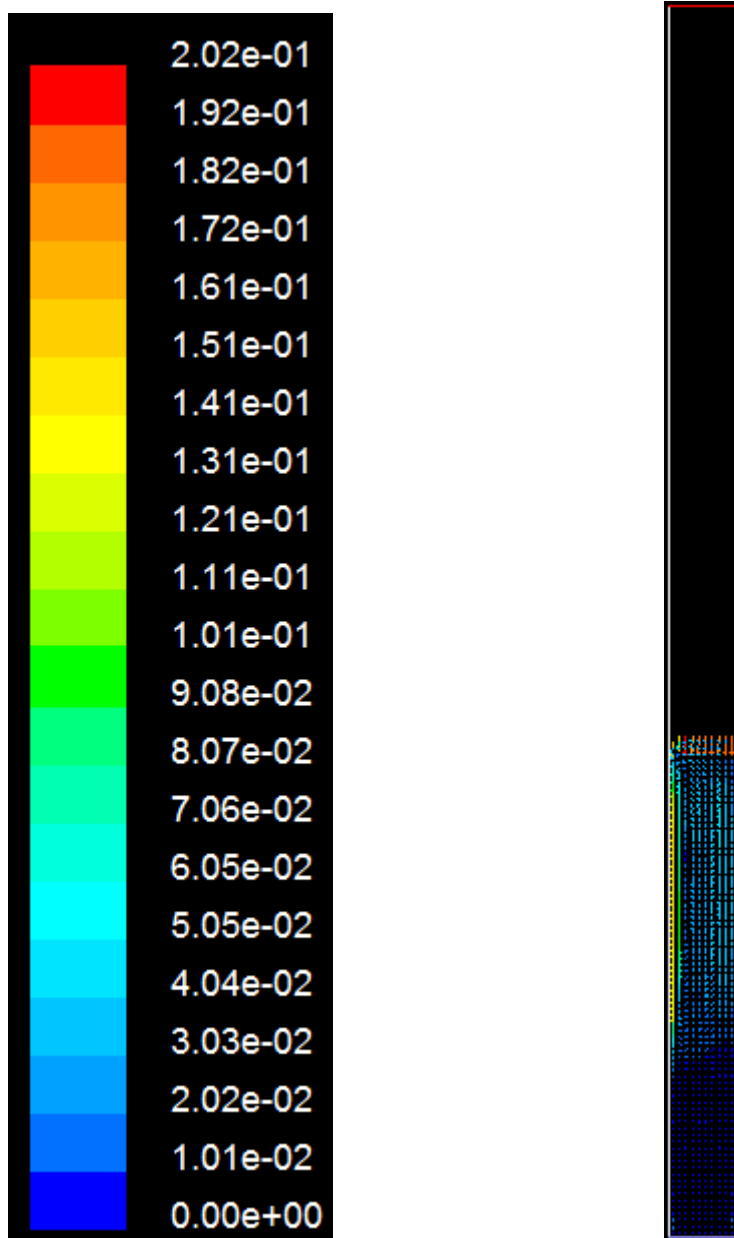


Figure 4: Velocity vector of glass beads (actual)

The following figure shows the magnified version of the velocity vector of the previous figure.

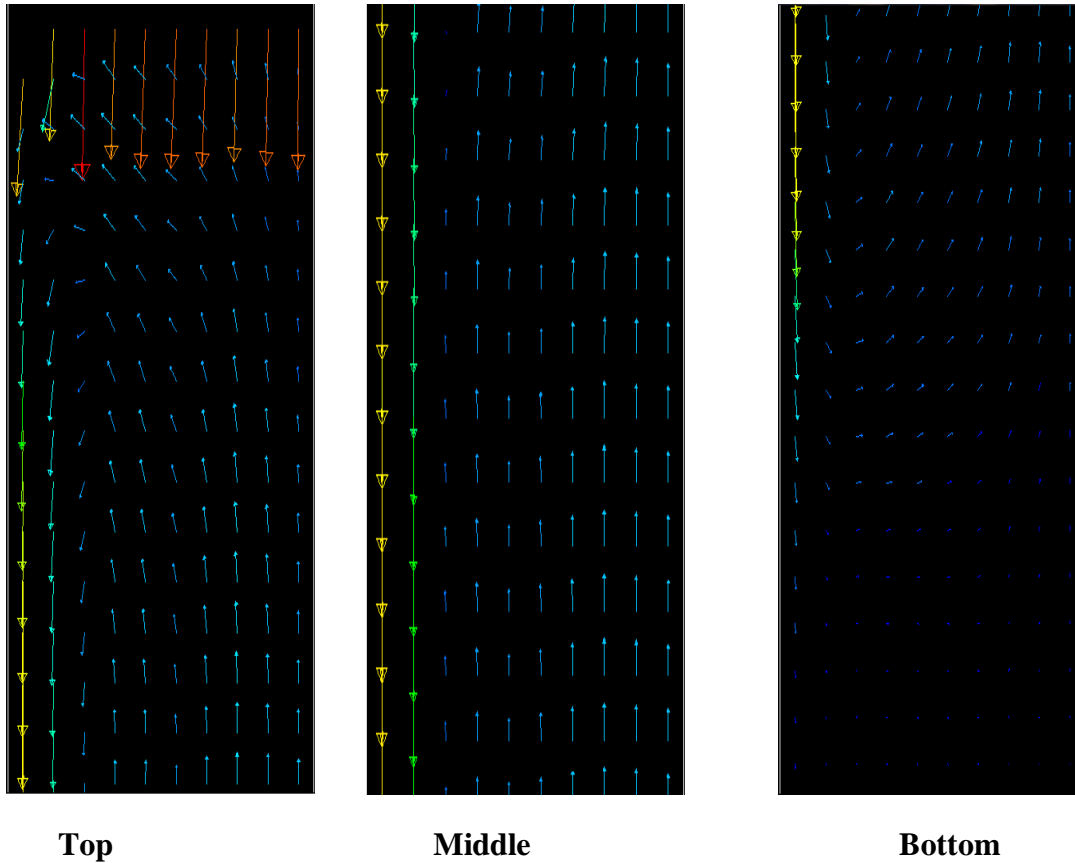


Figure 5: Velocity vectors (magnified)

It can be seen that at the upper sections vectors are absent because of absence of glass beads while at the top of the fluidized part the vectors are downward. At the middle the arrows are downward near the wall because the movement of glass beads is towards downward direction. At the bottom part the vectors are small because of less velocity of glass beads.

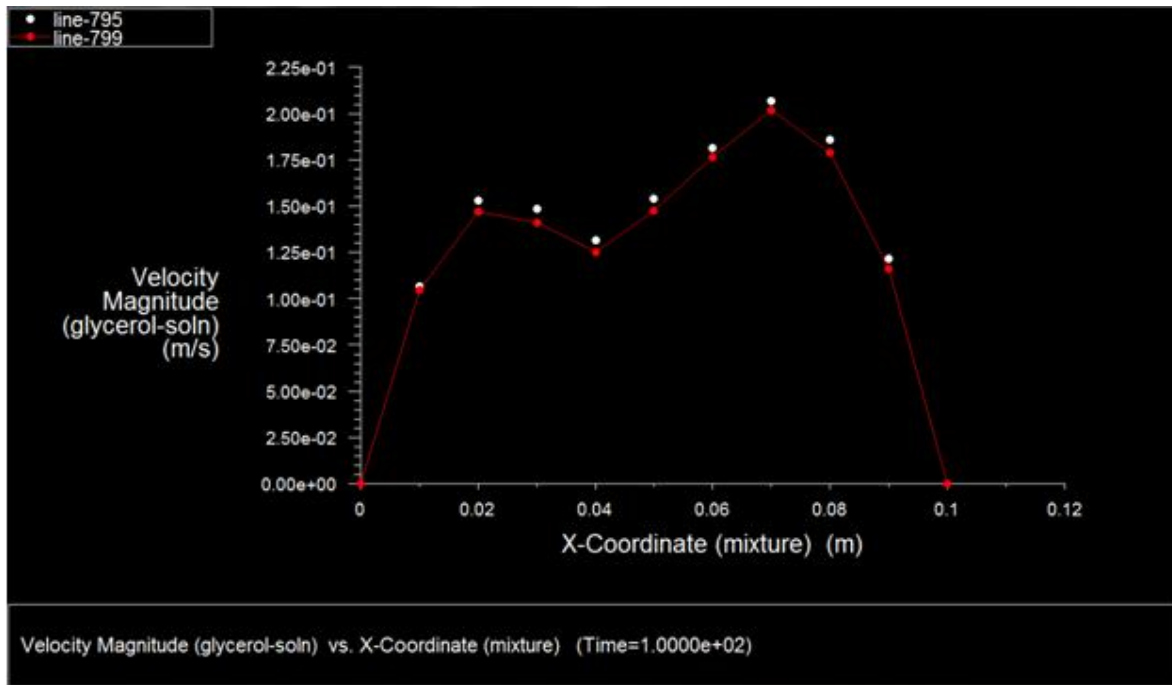


Figure 6: X-Y plot for velocity magnitude of glycerol solution

The above plot indicates the velocity profile of glycerol solution inside the bed. It can be seen that the average velocity is near 0.15 m/s. The inlet air velocity is 0.02123 m/s and the concentration of the glycerol solution is 30%. A parabolic profile is desired after fully developed flow.

5.2 Bed Expansion

The bed behavior can be seen and determined by the contour plots and X-Y plots. Following contour plots tell about the change in bed for different glycerol solutions.

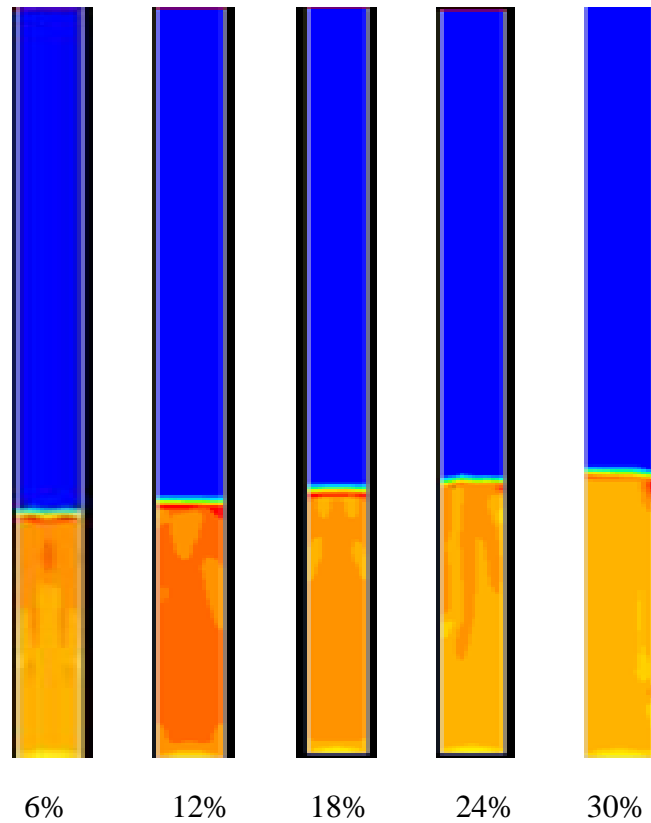


Figure 7: Contours of volume fraction of glass beads at liquid velocity 0.125m/s and gas velocity 0.02123m/s.

Above figure illustrates how the bed changes for different concentrations of glycerol solutions. It can be seen that the bed height increases with increase in glycerol concentration. The fluidization is more prominent in higher concentrations of glycerol.

The following figure shows the expansion of bed with varying liquid velocity for a constant gas velocity for 6% glycerol solution. It shows that the bed height increases with increase in liquid velocity.

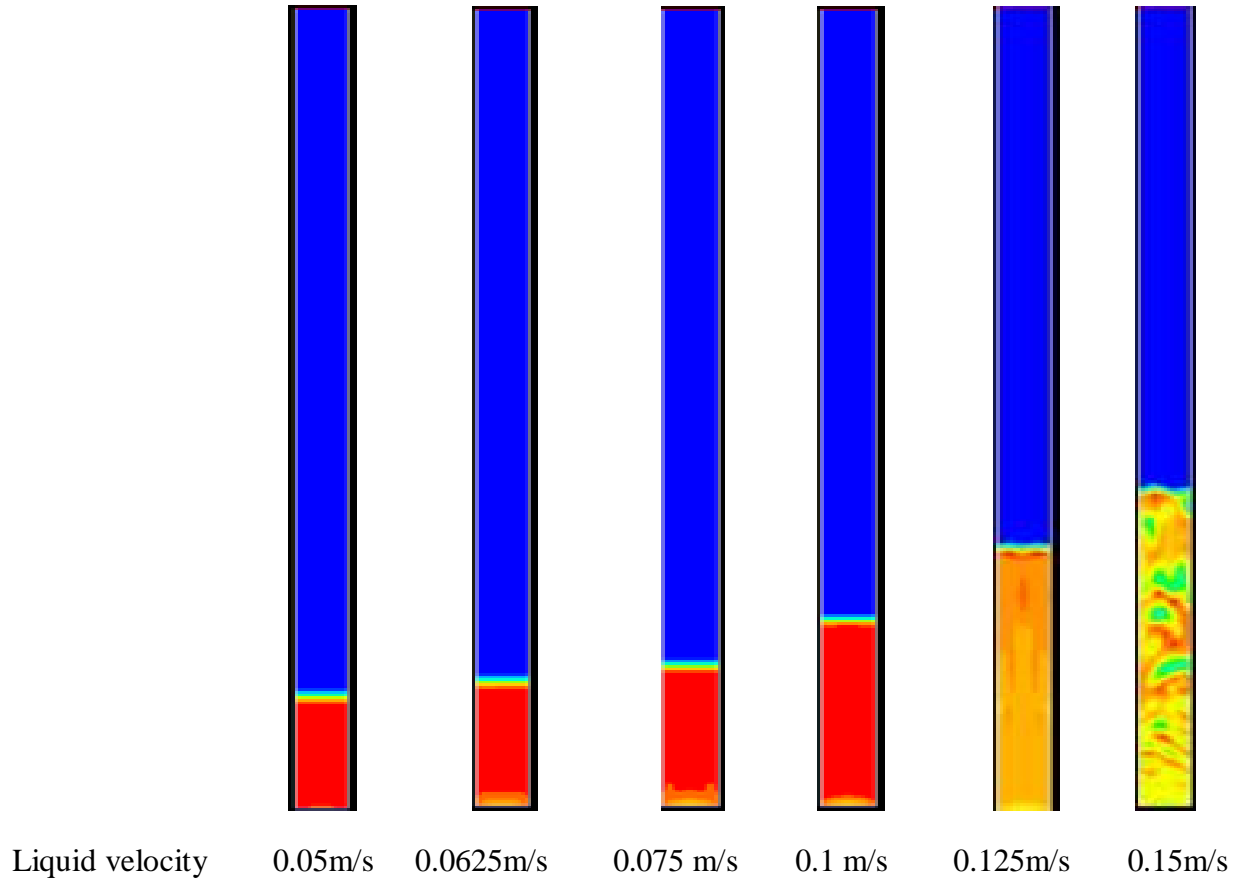


Figure 8: Variation in volume fraction of glass beads at constant inlet air velocity of 0.02123m/s and varying glycerol solution velocity for 6% glycerol solution.

The above contours are obtained after a quasi steady state is reached and there is no further change in the bed. It can be seen that initially there is almost no change in the bed but when the velocity of glycerol solution is increased the bed starts to expand at higher velocities the bed has risen by a considerable amount.

The bed height can be determined by the X-Y plot (as shown below) of volume fraction of glass beads on Y-axis while height of the column at X-axis.

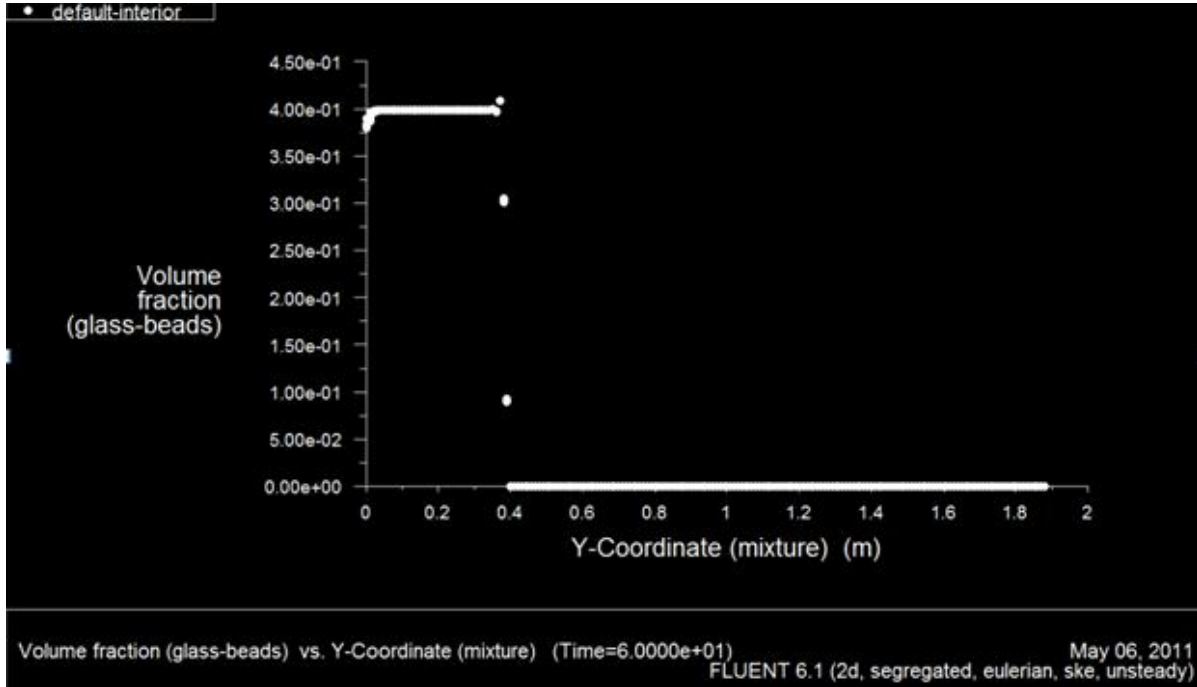


Figure 9: X-Y plot 30% glycerol solution.

The above plot is obtained for air velocity of 0.06369 m/s and glycerol solution velocity of 0.1 m/s. The maximum bed height is taken at that point at which the volume fraction of the glass beads suddenly reduces to zero.

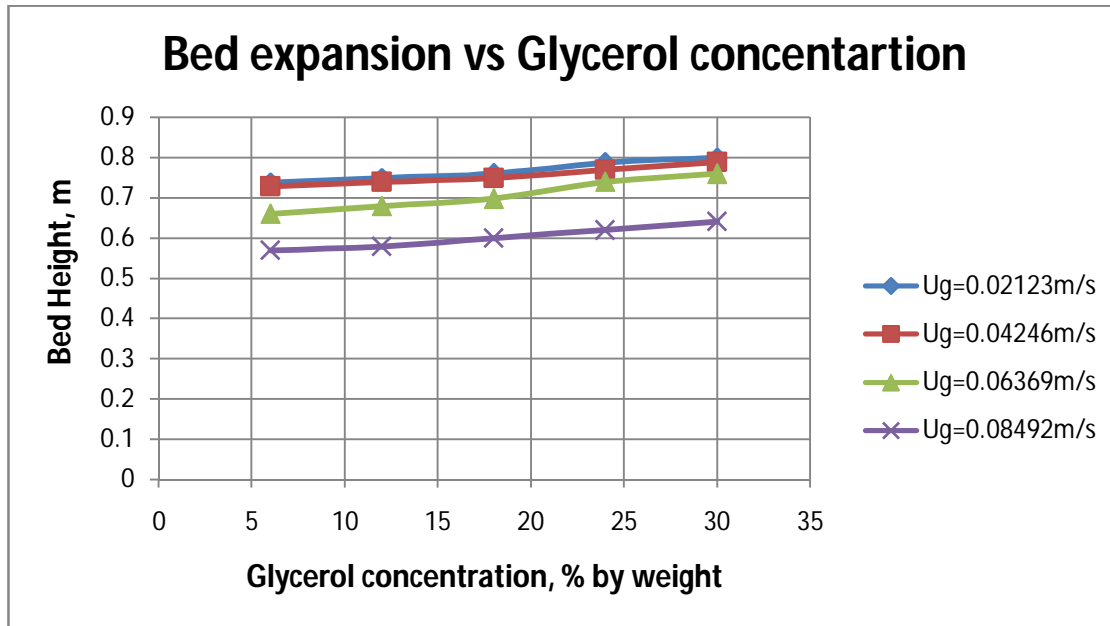


Figure 10: Bed expansion for different glycerol solutions for different gas velocities and constant liquid velocity of 0.15m/s.

The above plots are obtained for constant velocity of glycerol solution at 0.15 m/s and for a particular air velocity. The increase in bed height can be observed in the above plots.

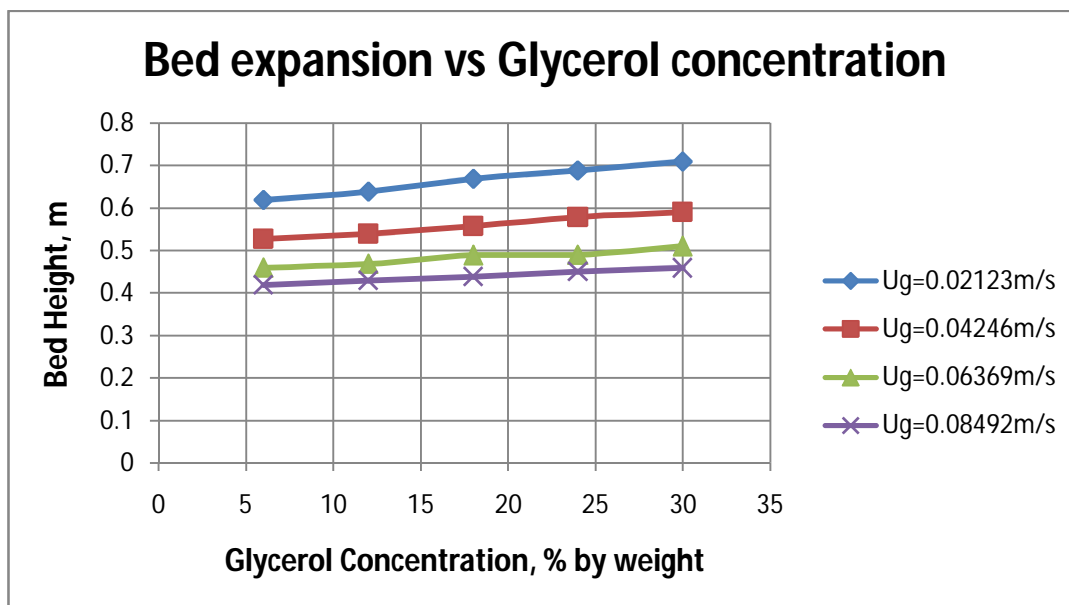


Figure 11: Bed expansion for different glycerol solutions for different gas velocities and constant liquid velocity of 0.125m/s.

It is clear from the previous figures that the bed expands considerably as the concentration of glycerol solution is increased from 6% by weight to 30% by weight for a constant inlet air velocity and glycerol solution velocity.

The following figure illustrates the bed expansion behavior of three phase fluidized bed with the variation in liquid velocity for a constant inlet gas velocity.

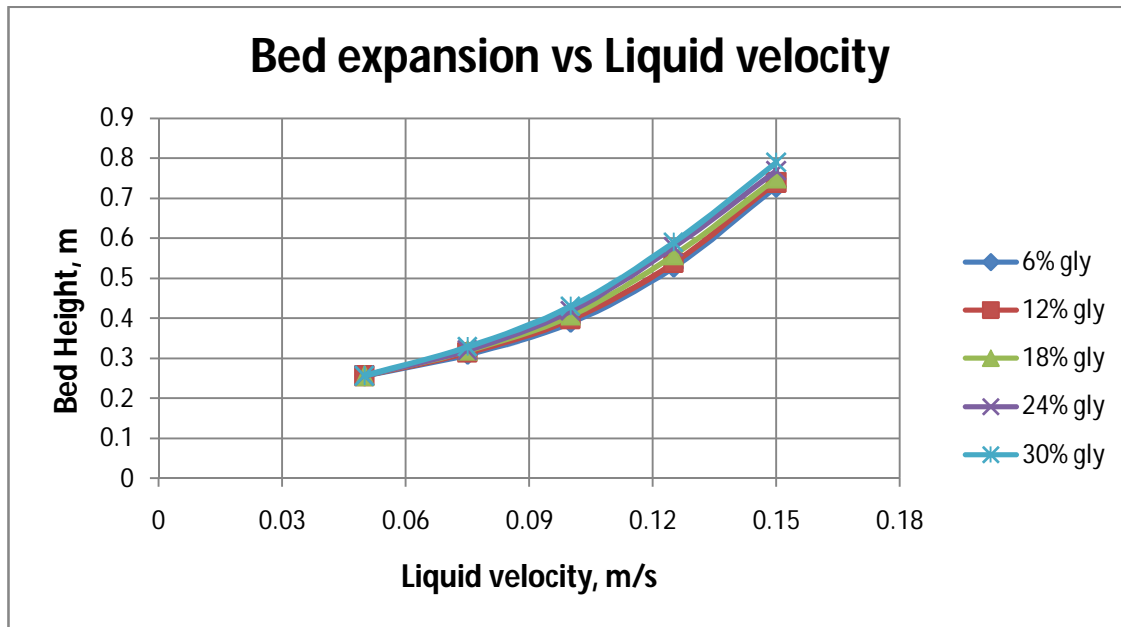


Figure 12: Bed expansion vs liquid velocity for a constant air velocity of 0.04246 m/s for different glycerol solutions.

It is observed that the bed expands considerably with the increase in the velocity of glycerol solution and the increase is more for higher concentrations of glycerol.

5.3 Phase Holdup

Phase holdup is obtained as mean area-weighted average of volume fraction of any phase at different points in fluidized part of the bed. It is done so because the volume fraction of phases are different at different points in the fluidized bed and hence area weighted average of volume fraction is determined at heights 10cm, 20 cm 30 cm etc till fluidized part is over and the average of these values provides us with the phase hold up.

Following figures illustrates the variations in gas holdup at different inlet velocities.

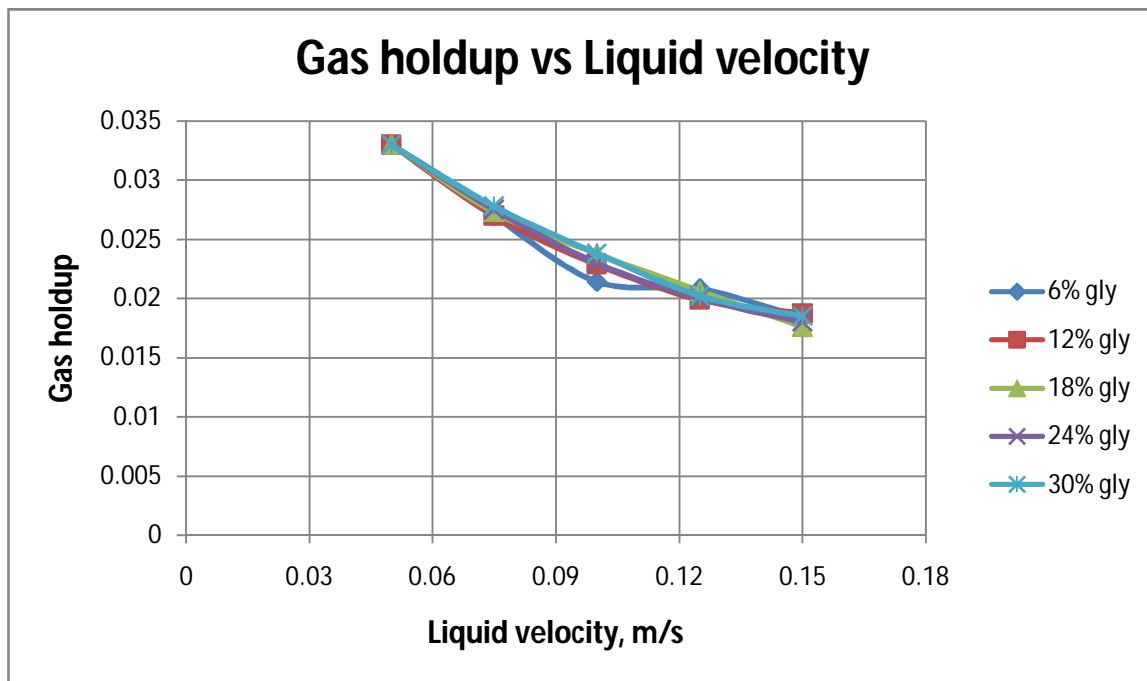


Figure 13: Gas holdup vs velocity of glycerol solution at constant air velocity of 0.02123 m/s for different glycerol solutions.

Above figure illustrates that as the liquid velocity is increased for a particular glycerol solution the gas holdup decreases for a constant air velocity.

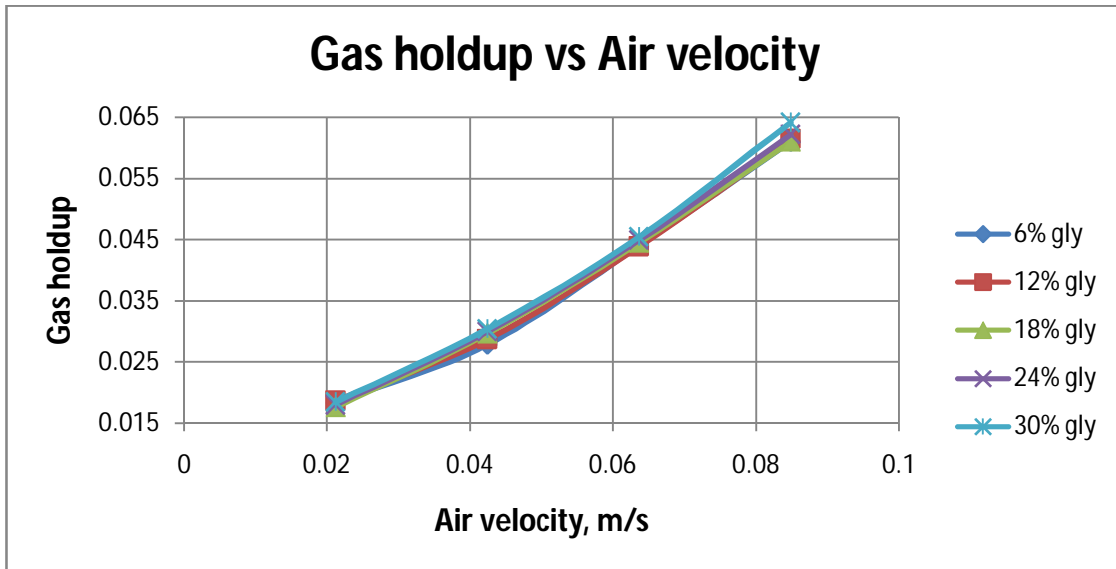


Figure 14: Gas holdup vs air velocity at constant liquid velocity of 0.15m/s for different glycerol solutions.

The above figure illustrates that the gas holdup increases with increase in air velocity for a particular glycerol solution.

Following figure illustrates the variation of gas holdup with increase in glycerol concentration.

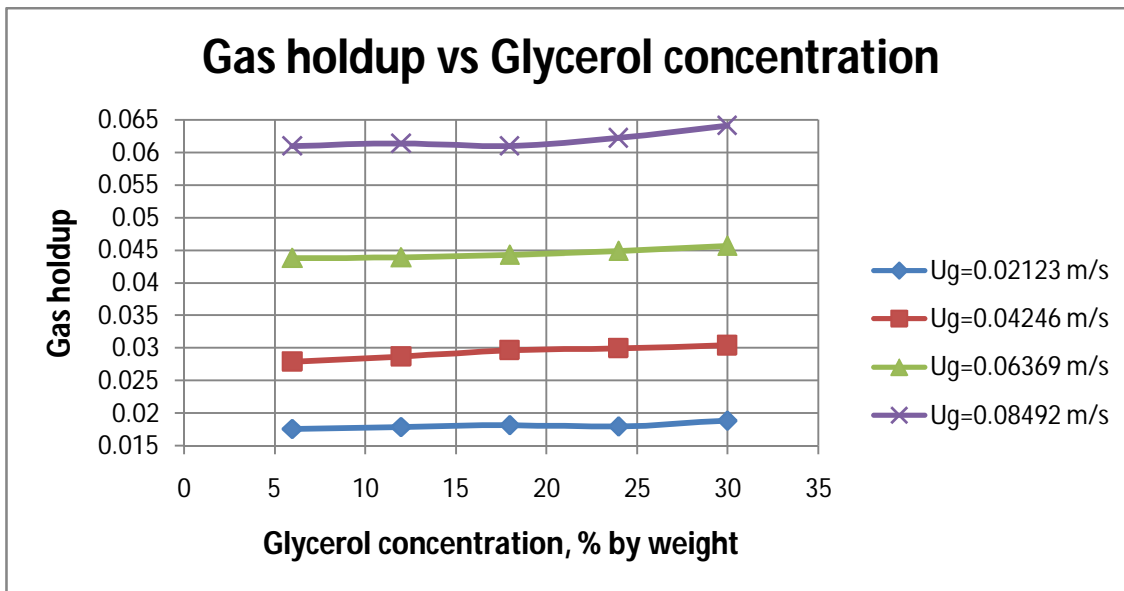


Figure 15: Gas holdup vs glycerol concentration for constant liquid velocity of 0.15m/s.

The figure tells about the variation in gas holdup with glycerol concentration and it is seen that the gas holdup increases with the increase in glycerol concentration. The increase is fairly more for higher gas velocity as compared to the lower velocities. It is seen that initially the increase is less or almost same but as the concentration increases the gas holdup starts to increase more. It is so because as the glycerol concentration increases the viscosity of the solution increases and hence the bubble rise velocities decrease there by increasing the gas holdup.

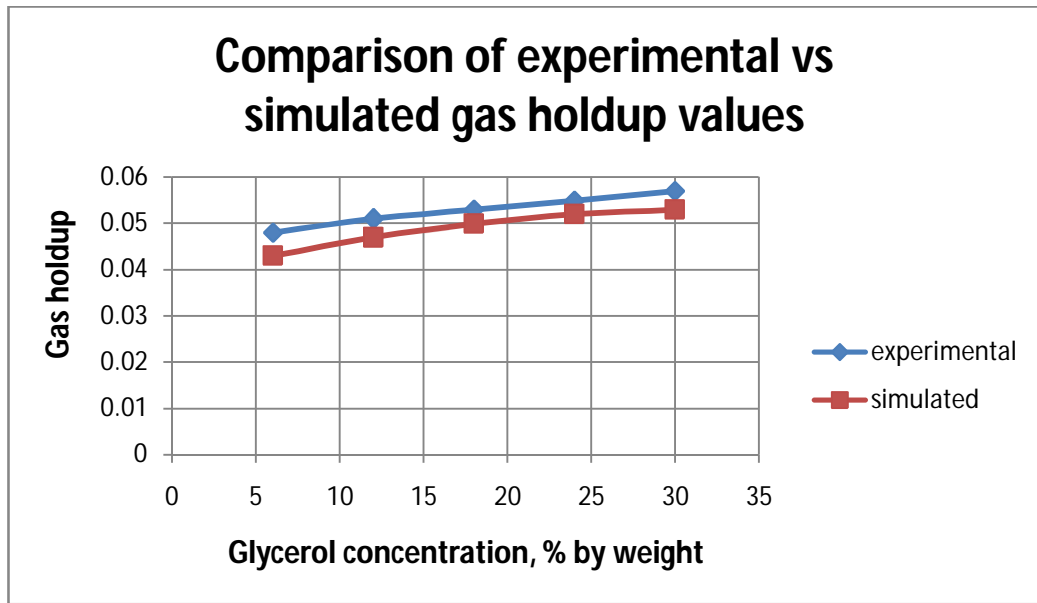


Figure 16: Comparison of experimental vs simulated gas holdup

The above plots are done for comparing the simulated and experimentally obtained values for constant inlet liquid velocity of 0.06369 m/s and air velocity of 0.02123 m/s for different concentrations of glycerol solutions and are found to be in good agreement with one another. The reason for small deviation may be that the glass beads used in experiment have a range of diameters while in the simulation all glass beads are taken to be of the uniform diameter.

The following plots show the variations of liquid holdup and solid holdup with glycerol concentration.

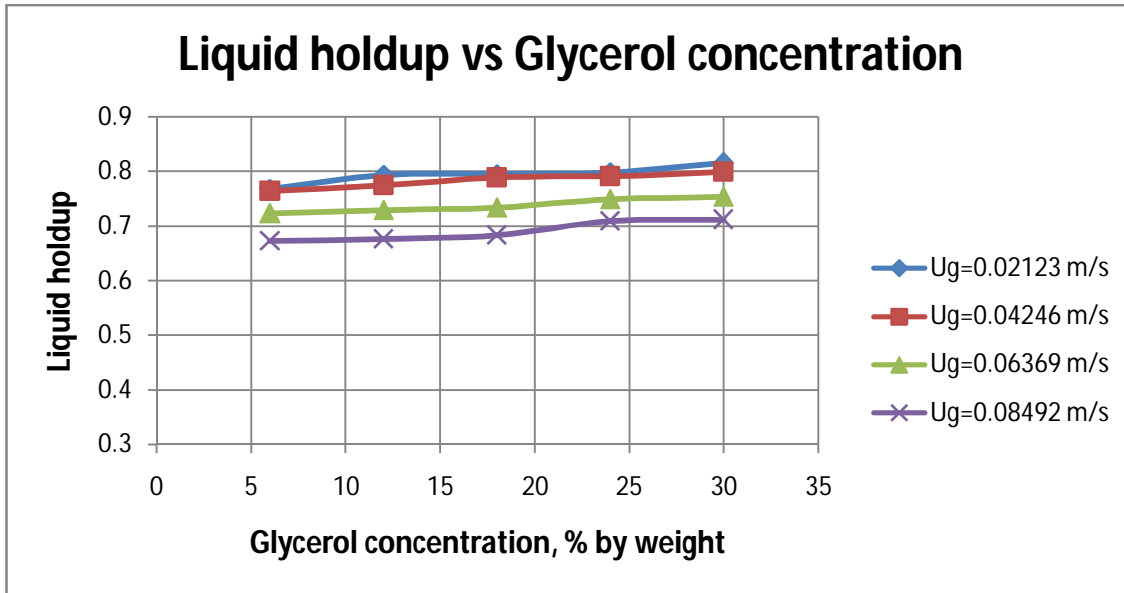


Figure 17: Variation of liquid holdup with glycerol concentration for a particular inlet air velocity and constant liquid velocity of 0.15 m/s.

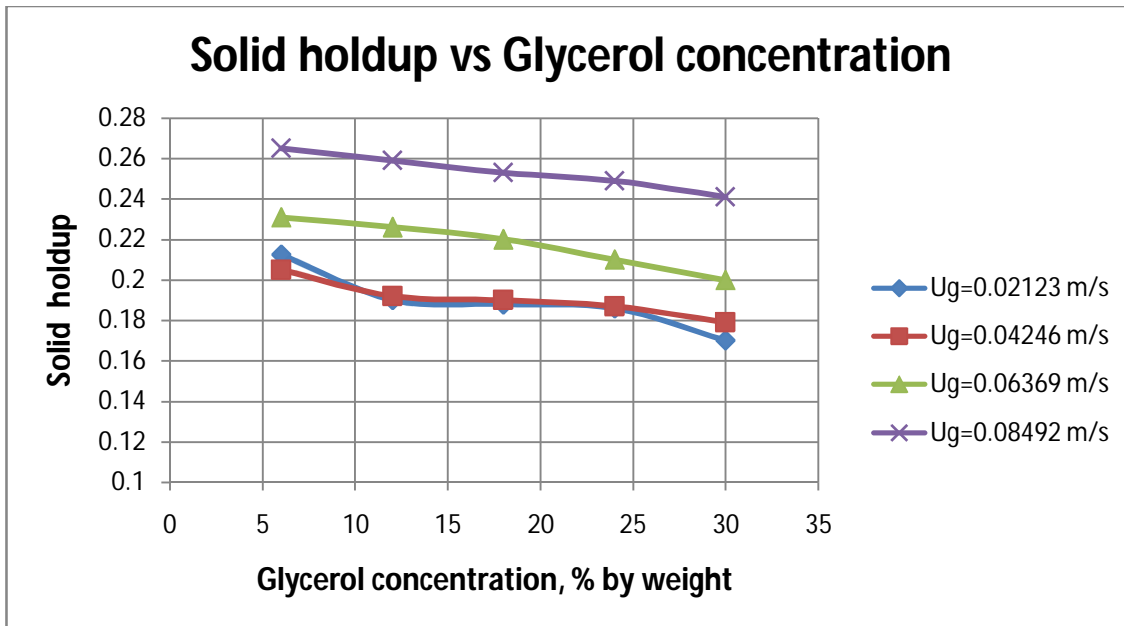


Figure 18: Variation of solid holdup for different glycerol solutions for inlet liquid velocity of 0.15 m/s and a particular gas velocity.

It is seen from the Figure 17 that the liquid holdup rises slightly with the increase in concentration of glycerol solution for a particular inlet velocity of gas and liquid. Since liquid as well as gas holdup is increasing with the increase in concentration of the glycerol solution so arithmetically the solid holdup has to decrease as all the three phases sum up to unity in terms of volume fraction which is observed in the previous figure.

5.4 Pressure Drop Variations

The following contour shows the variation in the static gauge pressure (mixture phase) in the column for 30% glycerol solution at inlet gas velocity of 0.04246 m/s and liquid velocity of 0.075 m/s.

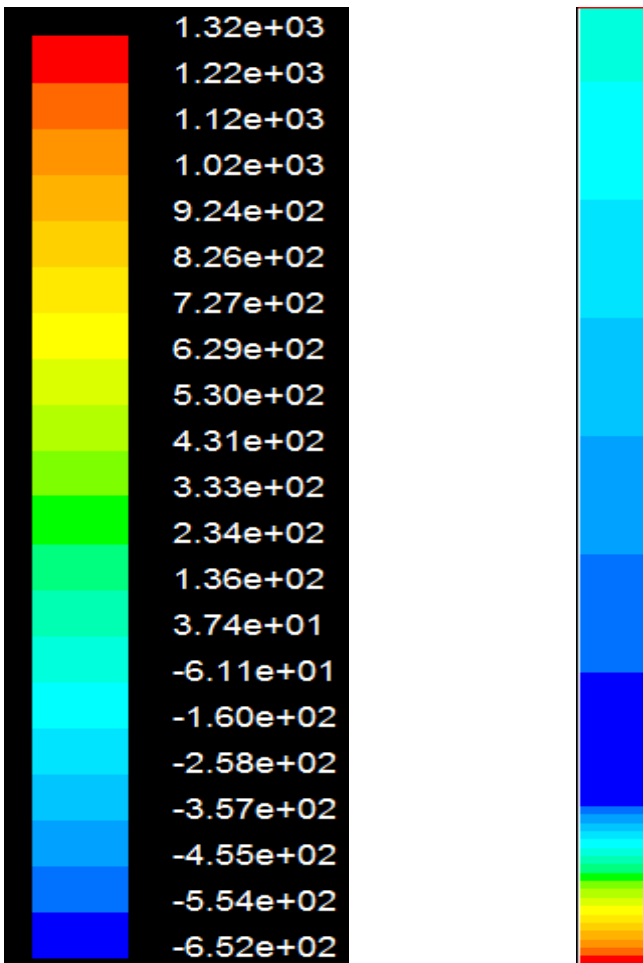


Figure 19: Contours of static gauge pressure (mixture phase) in the column for 30% glycerol solution at inlet gas velocity of 0.04246 m/s and liquid velocity of 0.075 m/s.

The following plot shows the variation of pressure drop with the concentration of glycerol solution.

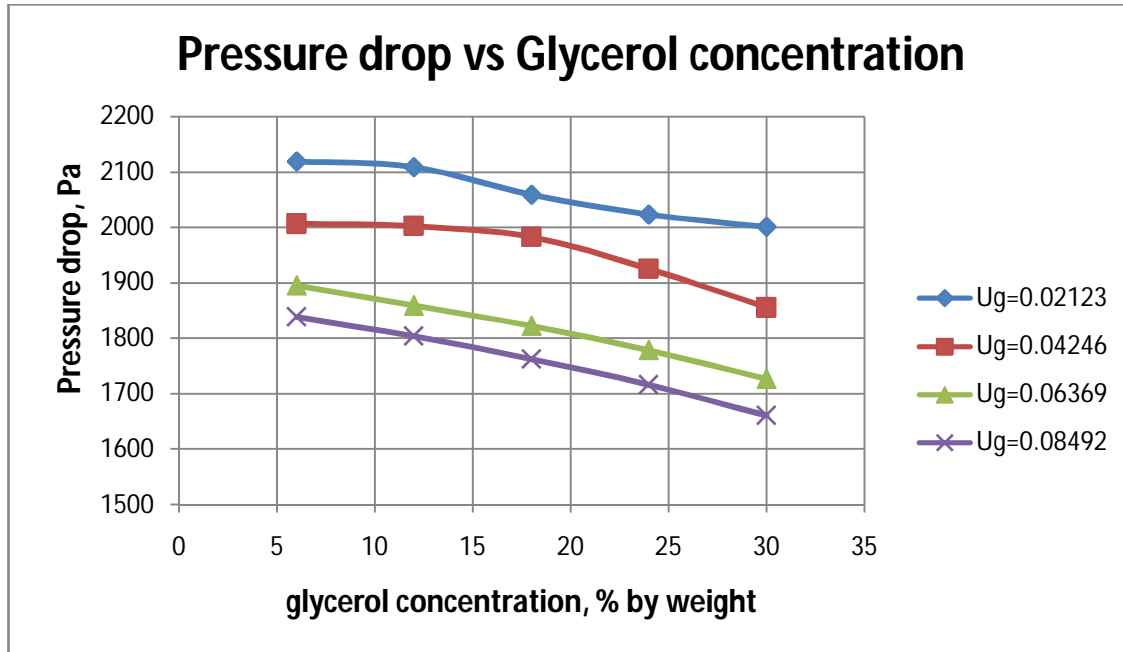


Figure 20: Variation of pressure drop with respect to glycerol concentration for uniform liquid velocity of 0.15 m/s and uniform inlet gas velocities.

The above plots are for a constant velocity of glycerol solution at 0.15 m/s and it is seen that as the concentration of glycerol solution is increased from 6% by weight to 30% by weight the static pressure drop decreases for a particular inlet velocity of air.

The following are the trends of static pressure drop with gas velocity.

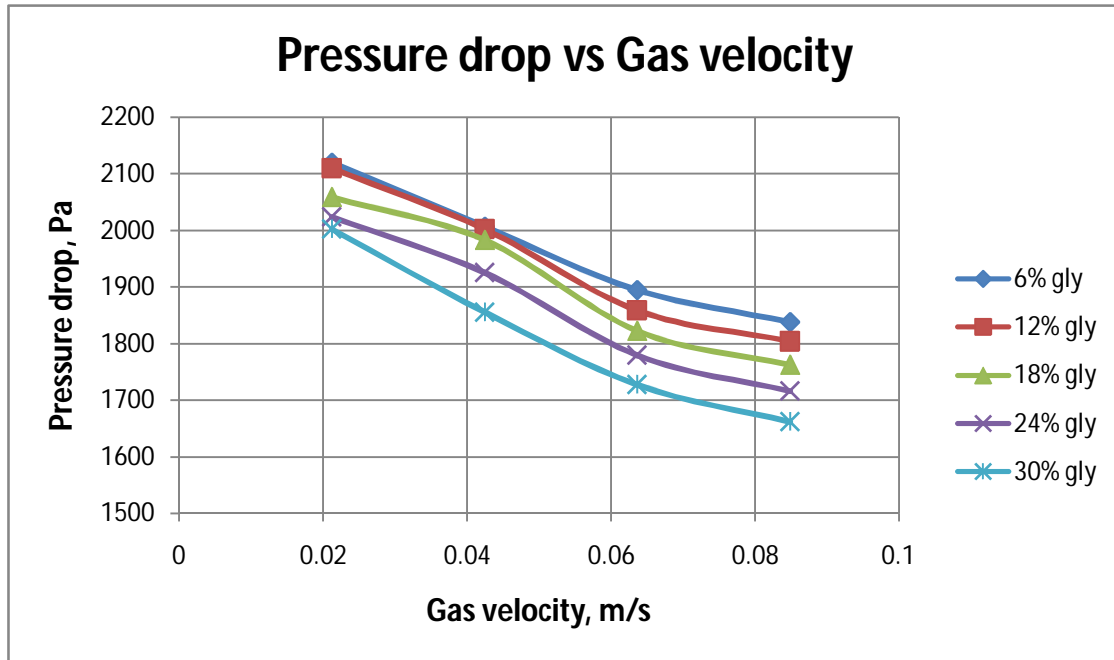


Figure 21: Variation of pressure drop with gas velocity for constant liquid velocity of 0.15 m/s for particular glycerol solutions.

It can be seen that the static pressure drop decreases for a particular concentration of glycerol with the increase in inlet air velocity for a constant liquid velocity i.e velocity of glycerol solution.

CHAPTER 6

CONCLUSIONS

Simulations have been carried out successfully for a three phase co current fluidized bed of 1.88m height and 0.1m diameter in which glass beads of 4mm diameter filled to a height of 25.6cm constitute the solid phase. Air and different concentrations of glycerol solutions are passed from the bottom of the domain to fluidize the bed. The aim was to observe the bed expansion for different glycerol solutions along with the phase holdup and pressure drop. Some of the conclusions obtained from the simulations are as follows:

- I. The fluidization is found to be more prominent in higher concentrations of glycerol solutions.
- II. The bed height is found to increase with the increase in concentrations of glycerol solutions for a particular inlet air and liquid velocity.
- III. The bed height is also found to increase with the increase in liquid velocity for a particular glycerol concentration for a constant air velocity.
- IV. Gas holdup is showing an increasing trend with increase in concentrations of glycerol for a particular inlet air and liquid velocity.
- V. Gas holdup is also increasing with increase in gas velocity for any concentrations of the glycerol solutions taken for a constant liquid velocity.
- VI. It is found that the gas holdup decreases with the increase in liquid velocity for any concentrations of the glycerol solutions taken for a constant air velocity.
- VII. It is found that the liquid holdup increases with increase in glycerol concentration for constant inlet gas and liquid velocity.

- VIII. It is also observed that the solid holdup decreases with increase in glycerol concentration for constant inlet gas and liquid velocity.
- IX. The pressure drop is decreasing with increase in glycerol concentration for constant inlet gas and liquid velocity.
- X. The pressure drop is also decreasing with increase in air velocity for any glycerol concentration for a particular liquid velocity.

The results obtained from the simulations have been compared from the literature Jena et al., 2009 and they are found to be in good agreement with each other.

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