Numerical Investigations of Bubble Column Equipped with Vertical Internals in Different Arrangements

Tuntun Gaurav
The University of Western Ontario

Supervisor
Prakash, Anand
The University of Western Ontario Co-Supervisor
Zhang, Chao
The University of Western Ontario

Graduate Program in Chemical and Biochemical Engineering
A thesis submitted in partial fulfillment of the requirements for the degree in Master of Engineering Science
© Tuntun Gaurav 2018

Follow this and additional works at: https://ir.lib.uwo.ca/etd

Part of the Catalysis and Reaction Engineering Commons, and the Other Chemical Engineering Commons

Recommended Citation
https://ir.lib.uwo.ca/etd/5607

This Dissertation/Thesis is brought to you for free and open access by Scholarship@Western. It has been accepted for inclusion in Electronic Thesis and Dissertation Repository by an authorized administrator of Scholarship@Western. For more information, please contact wlswadmin@uwo.ca.
Abstract

Bubble columns are multiphase contactors with wide applications in industrial processes. Often they are equipped with longitudinal tube bundles to facilitate heat exchange. Studying effects of these internals on column hydrodynamics is vital for the design of these internals. Computational Fluid Dynamic (CFD) simulations provide an understanding of the complex two-phase flow enabling the study of the effects of the internals on the column hydrodynamics. In the present work, an Eulerian-Eulerian based two-fluid model (TFM) coupled with a population balance model (PBM) is used to simulate the gas-liquid two-phase flows in bubble columns. The models studied were validated using experimental data from the literature. The selected model was used to simulate the effects of the tube-to-tube distance and height of the internals on the hydrodynamics in the column. It was found that the tube-to-tube distance has a significant impact on the liquid axial velocity distribution and flow recirculation. Decreasing the tube-to-tube space reduces the axial liquid flow and the height of internals affects the liquid recirculation only in homogeneous flow regime.

Keywords

Co-Authorship Statement

The thesis contains material that is in preparation for submission in peer reviewed journals as listed below.

Chapter 3: CFD Modelling of the Hydrodynamic Characteristics of a Bubble Column

The simulations conducted for this study were designed and carried out by T. Gaurav, with the guidance from Dr. Anand Prakash and Dr. Chao Zhang. The analysis, interpretation and manuscript drafting was conducted by Gaurav while critical revision was provided by Prakash, A and Zhang, C.

Chapter 3 will be submitted for publication under the co-authorship of Gaurav, T, Prakash, A and Zhang C.

Chapter 4: Numerical Studies on Effects of Geometrical Modifications of Internals on Bubble Column Hydrodynamics

The simulations performed for this study were designed and carried out by T. Gaurav, with the guidance from Dr. Anand Prakash and Dr. Chao Zhang. The analysis, interpretation and manuscript drafting was conducted by Gaurav while critical revision and analysis was provided by Prakash, A and Zhang, C.

Chapter 4 will be submitted for publication under the co-authorship of Gaurav, T, Prakash, A and Zhang C.
Acknowledgement

Foremost, I am grateful to the God, for the successful completion of this work.

I would like to express my sincere gratitude to my supervisors Dr. Anand Prakash and Dr. Chao Zhang for their relentless support and patience in the completion of this work. I thank Dr. Prakash for his consistent encouragement and pushing me to challenge myself while allowing me to pursue different endeavors while keeping me on the path to a successful completion of the study. Furthermore, I am truly thankful for the constructive discussions, valuable insights and personal guidance that he has provided me. I’d like to thank to Dr. Zhang for her resourcefulness in supporting me and for providing insightful knowledge throughout the program.

I am also thankful to Dr. Anil Jhawar for his guidance at various instances and help with acclimatizing with the environment in a new country.

I would like to thank the Shared Hierarchical Academic Research Computing Network (www.sharcnet.ca), Compute/Calcul Canada and Western Engineering for their facilities.

I have great gratitude to my father who has always taught me the lines below. I would like to thank my mother, sister and their families for their consistent support throughout the entire process. I’d like to dedicate this thesis to my niece, Myra on her birthday, who has come as a light in our lives. Finally, I’d like to thank all my friends back in India and here for keeping me motivated along the way.

“शक्तिः दुददम्येच्छाशक्तिः आगच्छति”
“What’s strength come from indomitable will”.

iii
# Table of Contents

Abstract..........................................................................................................................i

Co-Authorship Statement.................................................................................................iii

Acknowledgments............................................................................................................iv

Table of Contents...........................................................................................................v

List of Tables..................................................................................................................viii

List of Figures................................................................................................................ix

List of Appendices.........................................................................................................xii

Nomenclature................................................................................................................xiii

Chapter 1.........................................................................................................................1

  1. Introduction..............................................................................................................1
    1.1. Objective of the thesis.......................................................................................3
    1.2. Thesis Structure...............................................................................................3

References......................................................................................................................5

Chapter 2.........................................................................................................................7

  2. Literature Review.....................................................................................................7
    2.1. Effects of Internals Design on Column Hydrodynamics.................................14
    2.2. Effects of Internals on Local Holdups.............................................................16
    2.3. Effect on Bubble Chord Length and Rise Velocity.........................................18
    2.4. Effects on Liquid Flow Patterns......................................................................18
    2.5. Effects on Internals on Liquid Phase Axial Dispersion.................................20
    2.6. Summary Comments.......................................................................................21
    2.7. Numerical Modeling of Bubble Column with Internals...............................21
    2.8. Discussion on numerical model......................................................................30
      2.8.1. Drag Force...............................................................................................31
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.8.2.</td>
<td>Lift Force</td>
</tr>
<tr>
<td>2.8.3.</td>
<td>Turbulent Dispersion</td>
</tr>
<tr>
<td>2.8.4.</td>
<td>Turbulence</td>
</tr>
<tr>
<td>2.8.5.</td>
<td>Population Balance Model (PBM)</td>
</tr>
<tr>
<td>2.8.6.</td>
<td>Wall Lubrication Force</td>
</tr>
<tr>
<td>2.9.</td>
<td>Summary Contents</td>
</tr>
</tbody>
</table>

References

Chapter 3

3. CFD Modelling of the Hydrodynamic Characteristics of a Bubble Column

3.1. Introduction

3.2. Objectives of this study

3.3. Mathematical Model

3.3.1. Governing equations

3.3.2. Interfacial forces

3.3.3. Turbulence equations

3.3.3.1. RNG k-ε Turbulence Model

3.3.3.2. RSM Turbulence Model

3.3.4. Population balance equations

3.3.4.1. Breakup model

3.3.4.2. Coalescence model

3.4. Numerical method

3.5. Results and Discussions

3.6. Conclusions

References

Chapter 4
4. Numerical Studies on Effects of Geometrical Parameters of Internals on Bubble Column Hydrodynamics ................................................................. 105
   4.1. Introduction .................................................................................. 105
   4.2. Numerical Method ...................................................................... 110
   4.3. Results and Discussions ................................................................. 111
   4.4. Conclusions ................................................................................ 142

References .......................................................................................... 144
Chapter 5 ............................................................................................ 148

5. Conclusions and Recommendations .................................................... 148
   5.1. Conclusions ................................................................................ 148
   5.2. Recommendations ...................................................................... 150

Appendix A .......................................................................................... 152
Appendix B .......................................................................................... 156
Curriculum Vitae .................................................................................. 160
List of Tables

Table 2.1 Summary of experimental investigations on bubble column with vertical tube internals……………………………………..9

Table 2.2 Summary of Computational work done on bubble columns with vertical tube internals………………………………………………………..25

Table 3.1 Summary of previous work on bubble column modelling with PBM……56

Table 3.2 Different drag model equations from literature…………………………………60

Table 3.3 List of constants and their values for the two turbulence model…………65

Table 3.4 Population balance aggregation and breakage kernels…………………………68

Table 3.5 Numerical model used in the present work…………………………………74

Table 3.6 Experimental data used from literature studies for comparison………….77

Table 3.7 List of bubble sizes for PBM model……………………………………….79

Table 3.8 Division of gas inlet fraction…………………………………………….81

Table 4.1 Dimensions and grid resolutions for each case used in the simulations…..117
List of Figures

Figure 1.1. Fluid dynamic parameters selection and internals design variables for simulating a bubble column with internals…………………………………………………………2

Figure 2.1. Schematic of bubble column with vertical tube internals………………8

Figure 2.2 Typical profiles in the presence of internals (F. Möller, Lau, Seiler, Hampel, & Schubert, 2018)…………………………………………………………………………………15

Figure 3.1 Flow of simulations performed (abbreviations taken from the Table 1)…78

Figure 3.2 Instantaneous bubble diameter along the centerline at Ug = 0.12 m/s (Case S12) ………………………………………………………………………………………………84

Figure 3.3 Comparison of the bubble size distributions using different models………85

Figure 3.4 Comparison of the predicted time averaged radial profiles of air volume fraction and liquid velocity using different models with the experimental data from Bhole et al. (2008) …………………………………………………………………………88

Figure 3.5 Comparison of the predicted time averaged radial profiles of air volume fraction and axial liquid velocity using different models with the experimental data from Sanyal et al. (1999) at Ug = 0.12 m/s …………………………………………………………89

Figure 3.6 Comparison of the time averaged radial profiles of gas volume fraction and axial liquid velocity using different drag correlations with experimental results from Sanyal et al. (1999) at Ug = 0.12 m/s …………………………………………………………92

Figure 3.7 Grid independent test: Time averaged radial profiles of air volume fraction and axial liquid velocity ………………………………………………………………………94

Figure 3.8 Mesh (i) Hollow (Medium), (ii) With internals……………………………94
Figure 3.9 Comparison of time averaged radial profiles gas volume fraction and gas axial velocity of Case JH with similar inlet superficial gas velocities from Xue et al. (2008) (Case X) .................................................................96

Figure 3.10 Comparison between gas volume fraction results from 2D and 3D geometry from Jhawar et al (2011) (for case JH). .................................................................97

Figure 4.1 Schematic of the experimental setup of the bubble column with 15 vertical tubes (From Jhawar et al. (2014)) .................................................................113

Figure 4.2 Geometries of different tube-to-tube spacing ........................................115

Figure 4.3 Comparison between the numerical results and the experimental data from Jhawar et al. (2014) of the time averaged overall gas holdup and centerline liquid axial velocity (for Cases JH and 15T) .................................................................117

Figure 4.4 Comparison of the time averaged radial profiles of the gas holdup with the inlet gas velocity for the columns with and without internals based on setup from Jhawar et al. (2014) (Cases 15T and JH) .................................................................118

Figure 4.5 Comparison of the time averaged radial distributions of small and large gas bubble fractions for the columns with and without internals (Cases JH and 15T) at z/D = 4 for Ug = 0.042 m/s and Ug = 0.147 m/s .................................................................119

Figure 4.6 Comparison of the liquid velocity contours and velocity vectors for the columns with and without internals (Cases JH and 15T) (a) Ug = 0.020 m/s (b) Ug = 0.147 m/s .................................................................122

Figure 4.7 Comparison of the RMSE radial and axial velocities for Cases JH and 15T at Ug = 0.042 m/s and Ug = 0.147 m/s .................................................................123

Figure 4.8 Comparison of turbulent kinetic energy and turbulent Reynolds number for “Case JH” and “Case 15T” at Ug = 0.042 m/s and Ug = 0.147 m/s .................................................................124
Figure 4.9 Comparison of gas volume fraction for Case 12T, Case 15T and Case 18T at Ug = 0.042 m/s and Ug = 0.147 m/s………………………………………………………………………………126

Figure 4.10 Comparison of axial liquid velocity for Case 12T, Case 15T and Case 18T at Ug = 0.042 m/s and Ug = 0.147 m/s………………………………………………………………………………127

Figure 4.11 Comparison of liquid axial velocity contours and velocity vector for (a) Case 12T, (b) Case 15T and (c) Case 18T at Ug = 0.042 m/s, 0.097 m/s and 0.147 m/s …………………………………………………………………………………136

Figure 4.12 Comparison of radial profiles of gas volume fraction for internal at 0.3 m, 0.5 m and 0.7 m from the gas distributor at Ug = 0.042 m/s and Ug = 0.147 m/s at z/D = 5………………………………………………………………………………137

Figure 4.13 Comparison of axial profiles of gas volume fraction and axial liquid velocity for internal at 0.3 m, 0.5 m and 0.7 m from the gas distributor………………138

Figure 4.14 Comparison of radial profiles of turbulent kinetic energy at Ug = 0.042 m/s at z/D = 5 (0.75 m) for internal at 0.3 m, 0.5 m and 0.7 m from the gas distributor…138

Figure 4.15 Comparisons of radial profiles of axial liquid velocity at Ug = 0.042 m/s and Ug = 0.147 m/s at z/D = 5 for internal at 0.3 m, 0.5 m and 0.7 m from the gas distributor………………………………………………………………………………140

Figure 4.16. Comparison of liquid axial velocity contours and velocity vectors for internals at (a) 0.3 m, (b) 0.5 m and (c) 0.7 m from the gas distributor at Ug = 0.042 m/s………………………………………………………………………………141

Figure 4.17 Comparison of radial profiles of gas volume fraction for internal height of 0.9 and 2 m at Ug = 0.042 m/s and Ug = 0.147 m/s at z/D = 8………………142
Figure 4.18 Comparison of axial liquid velocity contours and velocity vectors for different total height of internals (a) Total height = 0.9 m; (b) Total height = 1.4 m
List of Appendices

Appendix A – UDF for Drag laws..........................................................152

Appendix B – Contour figures showing the effect of internals..................... 156
Nomenclature

\( A_i \) interfacial area, \( m^2 \)

\( B_b \) birth term due to breakage (number of particles/time)

\( B_c \) birth term due to aggregation (number of particles/time)

\( C \) coefficient, dimensionless

\( c_f \) increase coefficient of bubble surface area

\( C_{ij} \) convection term in turbulence model

\( C_{\mu} \) model constant in k-\( \varepsilon \) turbulence model, dimensionless

\( C_{1\varepsilon} \) model constant in k-\( \varepsilon \) turbulence model, dimensionless

\( C_{2\varepsilon} \) model constant in k-\( \varepsilon \) turbulence model, dimensionless

\( C_{3\varepsilon} \) model constant in k-\( \varepsilon \) turbulence model, dimensionless

\( C_D \) drag coefficient, dimensionless

\( C_L \) lift coefficient, dimensionless

\( d, d_b, d_g \) bubble diameter, m

\( D_b \) death term due to breakage (number of particles/time)

\( D_c \) death term due to aggregation (number of particles/time)

\( d_{g,s} \) Sauteur mean bubble diameter of the distribution, m

\( d_i, d_j \) diameter of bubble represented by index-‘i’, ‘j’, m

\( D_{L,ij} \) molecular diffusion term in turbulence model, kg/ms³
\( D_{T,ij} \)  
\text{turbulent diffusion term in turbulence model, kg/ms}^3

\( Eo \)  
\text{Eotvos number, dimensionless}

\( f_{BV} \)  
\text{fraction describing the daughter bubbles, dimensionless}

\( \vec{F}_D \)  
\text{drag force per unit volume, N/m}^3

\( \vec{F}_{lift} \)  
\text{lift force per unit volume, N/m}^3

\( \vec{F}_{TD} \)  
\text{turbulent Dispersion per unit volume, N/m}^3

\( \vec{g} \)  
\text{gravity, ms}^{-2}

\( G \)  
\text{production of turbulent energy, Wm}^3

\( I \)  
\text{identity matrix}

\( k \)  
\text{turbulent kinetic energy per unit mass, m}^2\text{s}^{-2}

\( K_{pk} \)  
\text{momentum exchange coefficient among phases p and k (p\neq k), Nsm}^{-4}

\( m_{kp} \)  
\text{mass transfer from phase ‘p’ to phase ‘k’, kgm}^{-1}

\( \vec{n} \)  
\text{normal unit vector, dimensionless}

\( P_{ij} \)  
\text{stress production term in turbulence model}

\( P_c \)  
\text{probability of collision for bubble coalescence}

\( R_{pk} \)  
\text{drag force per unit volume between the phases p and k (p\neq k)}

\( \text{Re} \)  
\text{Reynolds number, dimensionless}

\( R_\varepsilon \)  
\text{RNG k-\(\varepsilon\) specific strain rate, Wm}^3\text{s}^{-1}

\( t \)  
\text{time of flow, s}
\( \bar{u}_i \) velocity fluctuation in ‘i’ coordinate, m/s

\( \bar{u}_k \) velocity vector of \( k^{th} \) phase, m/s

\( \bar{U}_k \) Reynolds-averaged velocity of \( k^{th} \) phase, m/s

\( u_g \) inlet superficial velocity, m/s

\( u_{g,i} \) fluctuating bubble velocity in ‘i’ coordinate direction, m/s

**Greek Letters**

\( \alpha_k \) volume fraction of the \( k^{th} \) phase

\( \bar{\tau}_k \) Reynolds stress tensor for phase \( k \), Pa

\( \rho_k \) density of the \( k^{th} \) phase

\( \lambda_k \) shear Viscosity for the \( k^{th} \) phase

\( \mu_k \) bulk viscosity of the \( k^{th} \) phase

\( \sigma_k \) Prandtl number for turbulent kinetic energy (dimensionless)

\( \sigma_\varepsilon \) Prandtl number for turbulent energy dissipation rate (dimensionless)

\( \Pi_{\varepsilon,l}, \Pi_{k,l} \) source terms due to presence of bubble induced turbulence

\( \varphi_{ij} \) pressure strain term in turbulence model, kg/ms³

\( \varepsilon_{ij} \) dissipation term in turbulence model, kg/ms³

\( \beta(v,v') \) probability distribution function of generating a daughter droplet of size \( v' \) from parent droplet of size \( v \)

\( n(v) \) number size distribution of bubble of size \( v \)
\[ \xi = \frac{\lambda}{d_i} \] size ratio of eddy and a particle in the inertial subrange

\[ \Omega \] breakup rate of bubbles

\[ \omega_c \] collision frequency for bubble coalescence

**Subscripts**

\[ k \] phase (\( k: g \)-gas phase, \( l \)-liquid phase)

**Abbreviations**

2PH Homogenous discrete PBM with one gas velocity group

3PIH Inhomogeneous discrete PBM with two gas velocity group

3PIHM Inhomogeneous discrete PBM with two gas velocity group and modified inlet condition

4PIH Inhomogeneous discrete PBM with three gas velocity group

CFD Computational Fluid Dynamics

PBM Population balance model

LES Large Eddy Simulation

RANS Reynolds-Averaged Navier Stokes

RNG Re-normalization Group method

RSM Reynolds Stress Model

TKE Turbulent Kinetic Energy

CSA Cross-Sectional Area
Chapter 1

1 Introduction

Bubble columns are becoming reactors of choice for a number of industrial applications due to a combination of desirable features, which include excellent thermal management properties, low maintenance cost due to simple construction and absence of any moving parts (Deckwer, 1992; Larachi et al., 2006; Li et al., 2003; Li and Prakash, 2002; Deckwer and Schumpe, 1993). In addition, these reactor systems offer good mass transfer rates, high selectivity and conversion per pass and online catalyst addition and withdrawal. These benefits have led to a variety of industrial applications of bubble columns such as Fischer-Tropsch synthesis for clean fuels, methanol synthesis, dimethyl ether production (DME), fermentation, and biological waste water treatment, heavy oil upgrading etc. (Duduković et al., 2002; Prakash et al., 1999; Deckwer and Schumpe, 1993; Duduković and Devanathan, 1992; Shah et al., 1982).

In order to obtain desired performance for a given application, bubble columns often need to be equipped with different types of internals. These internals include heat transfer tubes, different types of baffles, and gas/liquid distributors with different configurations. The internals in bubble columns would affect hydrodynamics and mixing pattern, thereby affecting the reactor performance and productivity. Only a limited studies have been conducted to investigate the effects of internals on bubble column hydrodynamics (Jhawar and Prakash, 2014; Youssef and Al-Dahhan, 2009; Larachi et al., 2006; Chen et al., 1999; Schlüter et al., 1995; Saxena et al., 1992). These studies found alterations in flow pattern, mixing intensities and general hydrodynamics due to the insertion of internals in a hollow bubble column. Since there can be a number of alternative configurations, it is not always feasible to conduct large set of experiments with different types of internals to determine the optimum configurations.
However, there is need to quantify the effects of internals arrangements on important parameters such as liquid backmixing and interfacial area for mass transfer. For some applications, the choice of internals is based on considerations such as occupation of small cross-sectional area by the internals to have minimal impact on reactor volume and low-pressure drop to minimize operating costs.

![Figure 1.1. Fluid dynamic parameters selection and internals design variables for simulating a bubble column with internals](image)

In recent years, Computational Fluid Dynamic (CFD) has emerged as a promising tool to study the hydrodynamic characteristics including gas holdup profiles, liquid velocity profiles, mixing time and shear stress profiles of multiphase flow in a bubble column reactor (Joshi & Nandakumar, 2015; Jakobsen et al., 2005; Joshi, 2001). While a number of literature studies used CFD to investigate hydrodynamics of a hollow bubble column, only a few recent studies applied it to bubble column with internals (Guan and Yang, 2017; Guo and Chen, 2017; Guan et al., 2014; Larachi et al., 2006). These
studies provided some information on the performance of the column in the presence of internals as well limitations and challenges due to additional complexity in presence of internals. Figure 1.1 shows that there can be a number of factors associated with the numerical simulation of the column hydrodynamics with internals.

1.1 Objective of the thesis
In this study, the objectives are (1) to develop a suitable numerical model to simulation the gas-liquid two-phase flows in bubble columns including selecting appropriate turbulence model, drag model, bubble population balance model to account for and the bubble coalescence and break up, (2) to validate the proposed numerical model against experimental data, (3) to numerically study the effect of vertical tubes internal arranged concentrically and the role of the tube-to-tube gap on the hydrodynamics and performance of the bubble columns using the proposed numerical model.

The work is aimed at optimizing the internal geometry in order to decrease the phenomena of back-mixing, and increasing the axial and radial mixing in the column.

1.2 Thesis Structure
This thesis consists of 7 chapters and follows the “integrated-article” format as outlined by the Master’s Programs of GENERAL THESIS REGULATIONS by the School of Graduate and Postdoctoral Studies (SGPS) in the University of Western Ontario. A summary of each chapter is listed below:

In Chapter 1, a general introduction to the bubble column reactor is provided. The motivation for this work as well as its contributions are stated. Finally, the thesis structure is outlined.

In Chapter 2, the research available in literature on the experimental studies and CFD simulations to investigate the effects of internals on different hydrodynamic parameters
such as average gas holdup, radial profiles of gas holdup and liquid velocity etc. are summarized. Results of numerical simulation reported in literatures are analyzed and limitations of selected model parameters are discussed. Measurement techniques to determine gas holdup, bubble size distribution, liquid mixing time/axial dispersion are reviewed.

In Chapter 3, a numerical model for the simulation of gas-liquid two-phase flows in bubble columns is presented. Different turbulence models and interfacial closures are evaluated, moreover the bubble population model is extended to cover a wider range of bubble size distribution as observed in experiments. In the heterogeneous flow regime, the inlet boundary condition for the bubble size are modified based on experimentally observed two main fractions i.e. small and large bubbles (Krishna et al., 1999). The model with modified inlet boundary condition is validated against different experimental studies.

In Chapter 4, the numerical model developed and validated in chapter 4 is used to investigate the effects of different arrangements of the vertical tube internals on the performance of the column. The numerical results are validated by comparing them with available experimental data. The simulations are carried out for different internals arrangements to find out the optimum one.

In Chapter 5, the conclusions and recommendations for this study are summarized.
References


Chapter 2

2. Literature Review

Bubble column reactors find applications in chemical and biochemical industries as gas-liquid and gas-liquid-solid contactors for their advantages of simple construction, low maintenance, high mixing effects, and mass and heat transfer. Although bubble columns are relatively simple to construct, the interactions between the liquid and gaseous phases contained within are complex, intimate and difficult to predict or scale. For these reasons, characterization and quantification of the gaseous and liquid phase interactions is of great importance. There are two different methods that can be used to gain an understanding of bubble column systems. The first category refers to empirically-based methods in which rules and guidelines for bubble column design and scale-up are derived from trends in experimental data (Deckwer and Schumpe, 1993). The second category refers to model-based methods in which theoretical models are applied to the system of interest after flow regime analysis has been carried out (Deckwer and Schumpe, 1993). It is not uncommon to find a mix of both methods in an industrial setting. However, a greater dependence on model-base methods is encouraged as they provide additional insight to a reactor’s performance and a basis for reactor design.

In order to obtain desired performance for a given application, bubble columns often need to be equipped with internals of different types. These include baffles, heat transfer tubes and gas/liquid distributors of different configurations. The internals presence and arrangement in bubble columns would affect hydrodynamics and mixing pattern, thereby affecting the reactor performance and heat transfer characteristics. Only a limited number of literature studies have investigated effects of internals on bubble column hydrodynamics (Jhawar and Prakash, 2014; Youssef and Al-Dahhan, 2009;
Larachi et al., 2006; Chen et al., 1999; Schlüter et al., 1995; Saxena et al., 1992). These studies point to alterations in flow pattern, mixing intensities and general hydrodynamics due to insertion of internals in a hollow bubble column. However, there is need to quantify the effects of internals arrangements on important design parameters such as phase holdups, liquid back-mixing and interfacial area for mass transfer.

A common type of internal is a set of vertical tubes providing heat transfer surface for temperature control as shown schematically in Figure 2.1. In-situ installation of these internals provides multiple advantages including higher heat transfer rate, better control of reactor temperature reducing the need for an external exchanger (Schlüter et al., 1995). The presence of internals, however, affect phase holdups, flow patterns and phase mixing.

Figure 2.1. Schematic of bubble column with vertical tube internals
The selection of the number of tubes or the cross-sectional area (CSA) occluded by the tubes, and the configuration of the tubes (i.e. the diameter, pitch and arrangement) are decided by the surface area necessary for the heat transfer. This mainly depends on the exothermic nature of the reaction and the overall heat transfer coefficient. The modifications for different CSA or tube size and configurations have significant effect on the hydrodynamics. Experimental studies on the effects of longitudinal flow tube bundle on column hydrodynamics have been reported in several literature studies (Schlüter et al., 1995; Jinwen Chen et al., 1999; Youssef & Al-Dahhan, 2009; Youssef et al., 2013; Jhawar & Prakash, 2014; Kagumba & Al-Dahhan, 2015; Al Mesfer & Al-Dahhan, 2016; George et al., 2017; Mesfer et al., 2017; Sultan et al., 2018). Table 2.1 summarizes these contributions for quick reference.

Table 2.1. Summary of experimental investigations on bubble column with vertical tube internals

<table>
<thead>
<tr>
<th>Authors</th>
<th>Inner Diameter ($D_c$, mm); Sparger Type($d_s$, mm); Range of Inlet velocity($u_g$, $u_l$, cms$^{-1}$); Gas – Liquid System</th>
<th>Experiment technique</th>
<th>Internals details (i) CSA (%); (ii) Configuration; (iii) Size of Tubes ($d_t$, mm); (iv) Pitch (Inter-tube distance)(mm); (v) Height from gas distributor</th>
<th>Parameters investigated</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yamashita, (1987)</td>
<td>(i) $D_c$ = 80, 160, 310 (ii) $H_s$ = 1.65, 1.3-1.4, 1.3-1.4 (iii) Single Nozzle ($d_s$=10, 27.6, 60 mm); (iv) $u_g$ = 1.66-66.3, 1.66-47.0, 0.883-35.3, $u_l$=0 (v) Air-tap water</td>
<td>Manometric method</td>
<td>(i) CSA: 0-56.2, 0-51.7, 0-74.7 (ii) Multiple arrangements (iii) ($d_t$=14-60) (iv) Pitch = 20-85;</td>
<td>Effect of single and multiple vinyl chloride resin pipe and iron rod internals with different size and arrangements of internals on gas holdup</td>
</tr>
<tr>
<td>Pradhan et al. (1993)</td>
<td>(i) $D_c$ = 102 (ii) $H_s$ = 1.30 (iii) Multi-orifice (64 holes of $d_s$=1.5 mm, triangular pitch (1.2 cm))</td>
<td>Manometric method: 10 Pressure drop measurements</td>
<td>(i) Volume Fraction by internals: 0 – 19.3 (ii) Helical coils (iii) ($d_t$=6) (iv) Pitch = 25;</td>
<td>Effect of superficial velocity, CSA of internals</td>
</tr>
<tr>
<td>Study</td>
<td>Conditions</td>
<td>Methodology</td>
<td>Key Results</td>
<td>Notes</td>
</tr>
<tr>
<td>-------</td>
<td>-------------</td>
<td>-------------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>Schlüter et al. (1995)</td>
<td>(D_c = 190, 290, 450)</td>
<td>Straight tube</td>
<td>Effect of longitudinal and cross-flow tube bundle heat exchangers on heat transfer coefficient</td>
<td></td>
</tr>
<tr>
<td>Chen et al. (1999)</td>
<td>(D_c = 440)</td>
<td>Computed Tomography, Radioactive Particle Tracking</td>
<td>Effect of internals on gas distribution, liquid recirculation and turbulent parameters.</td>
<td></td>
</tr>
<tr>
<td>Forret et al. (2003)</td>
<td>(D_c = 1000)</td>
<td>Pitot tube, tracer method based on Conductivity probes</td>
<td>Study of hydrodynamics (liquid velocity profile, axial dispersion) in a large diameter column with and without internals.</td>
<td></td>
</tr>
<tr>
<td>Youssef &amp; Al-Dahhan (2009)</td>
<td>(D_c = 190)</td>
<td>Four point Optical Probe and Visual Observations</td>
<td>Effects on local gas holdup, gas-liquid interfacial area, bubble chord length, and bubble velocity distributions.</td>
<td></td>
</tr>
<tr>
<td>(A. Youssef, 2010)</td>
<td>(D_c = 445)</td>
<td>Four point Optical Probe and conductivity probe</td>
<td>Effect of internals on Variation of CSA and configuration of internals gas holdup and bubble dynamics. Additionally, Liquid mixing is investigated.</td>
<td></td>
</tr>
<tr>
<td>Balamurugan et al. (2010)</td>
<td>(D_c = 150)</td>
<td>Manometer</td>
<td>Gas Holdup</td>
<td></td>
</tr>
</tbody>
</table>

- \(u_g = 0 - 9, \ u_l = 0\)
- \(u_g = 1 - 65, \ u_l = 0\)
- \(u_g = 1 - 6, \ u_l = 0\)
- \(u_g = 2 - 65, \ u_l = 0\)
<table>
<thead>
<tr>
<th>Authors</th>
<th>(Year)</th>
<th>Details</th>
<th>Methodology</th>
<th>Notes</th>
</tr>
</thead>
</table>
| Hamed  | 2012   | (i) $D_c = 190, 458$  
(ii) $h = 1.60, 266$  
(iii) Perforated plate  
(225 holes of $d_h=1.32$, triangular pitch)  
(iv) $u_l = 5 - 45$, $u_0=0$  
(v) Air-Water | Four Point optical probe | Investigate and model Gas hydrodynamics, Gas mixing, and mass transfer with and without internals |
| Abdulmohsin & Al-Dahhan, 2012 | (i) $D_c = 190$  
(ii) $h = 1.60$  
(iii) Multi-orifice  
(225 holes of $d_h=1.32$, triangular pitch)  
(iv) $u_l = 3 - 20$, $u_0=0$  
(v) Air-Water | Fast response heat-transfer probe | Investigate impact of internals on heat transfer |
| Guan et al., 2014 | (i) $D_c = 800$  
(ii) $h = 4.00$  
(iii) Perforated plate  
(174, 160, 147 and 129 holes of $d_h=2.5$, triangular pitch)  
(iv) $u_l = 8, 12$ and $19$, $u_0=0$  
(v) Air-Water | Double conductivity probe and Pavlov tube | Effect of gas distributor configuration on hydrodynamics in bubble column with internals |
| Jhawar & Prakash 2014 | (i) $D_c = 150$  
(ii) $h = 1.45$  
(iii) Sparger (7 downward facing orifice, $d_h=1.9$, on four arms)  
(iv) $u_l = 0.03-0.35$, $u_0=0$  
(v) Air-Water | Fast response heat flux probe, pressure transducers | Effect of tube and baffle type internals on gas holdup, bubble fraction holdups, heat transfer coefficient and local liquid velocity. |
| Kagumba & Al-Dahhan, 2015 | (i) $D_c = 140$  
(ii) $h_{dynamic} = 1.56$  
(iii) Perforated plate  
(121 holes of $d_h=1.32$, triangular pitch)  
(iv) $u_l = 3 - 45$, $u_0=0$  
(v) Air-Water | Four Point optical probe | Investigate effect of size and configuration of internals on overall gas holdup, bubble passage frequency, bubble sizes, and bubble velocity |
| Guan et al. 2015 | (i) $D_c = 760$  
(ii) $h_{dynamic} = 4.10$  
(iii) Perforated plate  
(492 holes of $d_h=2.5$, triangular pitch)  
(iv) $u_l = 8 - 62$, $u_0=0$  
(v) Air-Water | Electrical resistivity probe and Pavlov tube | Effect of pin-fin tube internals on gas holdup and liquid velocity |
<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Details</th>
</tr>
</thead>
</table>
| Jasim, (2016)                     | (i) \(D_c = 140\)  
(ii) \(H_{dynamic} = 1.56\) 
(iii) Perforated plate (121 holes of \(d_N=1.32\), triangular pitch) 
(iv) \(u_g = 2-45, u_l=0\) 
(v) Air-Water  
Four point Optical Probe  
(i) CSA: 25  
(ii) Three arrangements: Two Circular with 8 of \(d_r=25.6\) with one at center and 30 tubes of \(d_r=12.7\) Hexagonal with 30 tubes of \(d_r=12.8\) and 25.6  
(iv)Pitch = 37.8, 21.4  
Effect of internal configuration and size on gas holdup distribution, specific gas-liquid area, bubble chord length, and bubble rise velocity |
| Al Mesfer, & Al-Dahhan, (2016)    | (i) \(D_c = 140\)  
(ii) \(H_{dynamic} = 1.56\) 
(iii) Perforated plate (121 holes of \(d_N=1.32\), triangular pitch) 
(iv) \(u_g = 5, 45, u_l=0\) 
(v) Air-Water  
\(\gamma\)-ray Computed Tomography  
(i) CSA: 25  
(ii) Triangular with 30 tubes 
(iii) \(d_r=12.8\)  
(iv)Pitch = 21.4  
Effect of dense internals on gas holdup with gas inlet velocity based on free CSA |
| Besagni & Inzoli (2016)           | (i) \(D_c = 240\)  
(ii) \(H_{dynamic} = 1.6\) 
(iii) \(d_N=3.5\)  
(iv) \(u_g = 23(AG), 20 u_l=11(AG), 9.2\) 
(v) Air-Water  
Manometer, double-fiber optical probe  
(ii) Two internal pipes – one centrally (\(d_r=60\)) and one asymmetrically (\(d_r=75\))  
Effect of open tube (OT) and annular gap (AG) configurations on holdup and flow regime transitions in a counter-current bubble column |
| Sultan, & Al-Dahhan, (2017a)      | (i) \(D_c = 152.4\)  
(ii) \(H_{dynamic} = 1.6\) 
(iii) Perforated plate (121 holes of \(d_N=1.32\), triangular pitch) 
(iv) \(u_g = 5, 45, u_l=0\) 
(v) Air-Water  
\(\gamma\)-ray Computed Tomography  
(i) CSA: 25  
(ii) Three arrangements: Two Circular with 30 tubes and one at center, Circular with 30 tubes and hexagonal with 30 tubes  
(iii) \(d_r=12.7\)  
(iv)Pitch = 21.4  
Effect of different configurations of internals on gas holdup distribution |
| Al Mesfer, Sultan, & Al-Dahhan, (2017) | (i) \(D_c = 140\)  
(ii) \(H_{dynamic} = 1.4\) 
(iii) Perforated plate (121 holes of \(d_N=1.32\), triangular pitch) 
(iv) \(u_g = 8, 20, 45\) (free CSA), \(u_l=0\) 
(v) Air-Water  
Radioactiv e particle tracking technique  
(i) CSA: 25  
(ii) Triangular with 30 tubes 
(iii) \(d_r=12.7\)  
(iv)Pitch = 21.4  
Investigate the effects of internals on liquid velocity fields and turbulence parameters |
| Kalaga, Yadav, et al., (2017)     | (i) \(D_c = 120\)  
(ii) \(H_{s} = 0.67\) 
(iv) \(u_g = 4.4-26.5\) \(u_l=5-14\) 
(v) Air-Water  
Radiotracin g, Radioactiv e particle tracking  
(i) CSA: 0-63  
(ii) Multiple configurations: One tube at center (\(d_r=36\)) and three  
Study the hydrodynamic characteristics in co-current bubble column equipped with dense internals |
<table>
<thead>
<tr>
<th>Author(s)</th>
<th>Description</th>
<th>Operating Conditions</th>
<th>Flow Visualization Technique(s)</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>Kalaga, Pant, Dalvi, Joshi, &amp; Roy, (2017)</td>
<td>Concentric bundles ((d_t=12)) over wide range of operating conditions</td>
<td>Radioactive particle tracking</td>
<td>(i) CSA: 0, 9, 11.7 (ii) Two configurations: One tube at center ((d_t=36)) and four concentric tubes ((d_t=12))</td>
<td>Quantify hydrodynamic parameters in bubble column with and without internals</td>
</tr>
<tr>
<td>George, (2015) and George, Jhawar, &amp; Prakash, (2017)</td>
<td>(i) (D_c = 120) (H_s = 0.67) (u_g = 14-26.5, u_l = 0) (v) Air-Water</td>
<td>Camera, conductivity probes, flow visualization, heat flux probe</td>
<td>(i) CSA: 10.75 (ii) Circular tube bundle (15 tubes) with baffles at two heights ((d_t=9.55)) ((iv)) Pitch = 4.4</td>
<td>Investigate the effects of internals on flow structure and mixing.</td>
</tr>
<tr>
<td>Sultan, Sabri, &amp; Al-Dahhan, (2018a)</td>
<td>(i) (D_c = 140) (H_{\text{dynamic}} = 1.58) (u_g = 5 - 45, u_l = 0) (v) Air-Water</td>
<td>(\gamma)-ray Computed Tomography</td>
<td>(i) CSA: 25 (ii) Two arrangements: Circular with 30 tubes, Circular with 7 tubes and one at center ((d_t=12.7, 25.6)) ((iv)) Pitch = 21.4, 37.8</td>
<td>Effect of size of internals on gas holdup distribution</td>
</tr>
<tr>
<td>Sultan, Sabri, &amp; Al-Dahhan, (2018b)</td>
<td>(i) (D_c = 440) (H_{\text{dynamic}} = 2.67) (u_g = 5 - 45, u_l = 0) (v) Air-Water</td>
<td>(\gamma)-ray Computed Tomography</td>
<td>(i) CSA: 25 (ii) Two arrangements: Circular (five concentric circles) and hexagonal (75 tubes) ((iii)) (d_t=25.4) ((iv)) Pitch = 50, 45-triangular</td>
<td>Effect of configuration of internals and column size on gas holdup distribution</td>
</tr>
<tr>
<td>Taofeeq &amp; Al-Dahhan, (2018)</td>
<td>(i) (D_c = 140) (H_{\text{dynamic}} = 1.56) (u_g = 1.4-2.5, u_l = 0) (v) Air-Water</td>
<td>Fast response heat transfer probe, optical fiber probe</td>
<td>(i) CSA: 25 (ii) Circular with 30 tubes ((iii)) (d_t=12.7) ((iv)) Pitch = 21.4</td>
<td>Investigate the effect of internals on heat transfer coefficient and related gas hydrodynamics</td>
</tr>
<tr>
<td>Felix Möller et al., (2018)</td>
<td>(i) (D_c = 100) (H_l = 1.10) (u_g = 2 - 20) (v) Air-Water</td>
<td>Wire Mesh sensors, fast respond oxygen needle probe</td>
<td>(i) CSA: 25 (ii) Four arrangements: Two each of triangular (37, 13 tubes) and square (37, 13 tubes). Additionally,</td>
<td>Study and model the effect of vertical internals on liquid dispersion, gas-liquid mass transfer in bubble column</td>
</tr>
</tbody>
</table>
2.1 Effects of Internals Design on Column Hydrodynamics

The internals design parameters mostly investigated in literature studies include, number and size of tubes, cross-sectional area (CSA) of column occupied and different arrangements of tubes. Presence of internals can further complicate, the complex hydrodynamics of bubble column. The hydrodynamic parameters affected include phase holdup profiles, flow patterns, liquid velocity profile etc. Figure 2.2 shows a representation of typical profiles as an effect of internals in the column. Further details of the effect of different internals reported in experimental literature studies have been discussed in the following sections.

A number of literature studies have reported increase in gas holdups in the presence of internals (Al Mesfer et al., 2016; Youssef and Al-Dahhan, 2009; Pardhan et al., 1993; Yamashita, 1987). The extent of increase, however, has been found to depend on the
size and number of tubes and their layout. Yamashita (1987) reported an increase in gas holdup with diameter of single and multiple internals with number and size of internals while remaining same for different arrangements of the internals. The earliest explanations of these observations in various studies reasoned that the increase in gas holdup was solely due to decrease in free surface area for gas phase in the presence of internals resulting in a higher gas velocity. This was further supported by the work of Bernemann (1989). This theory was, however, contested by Al Mesfer et al. (2016) by plotting the gas-holdup based on both total and free surface area. It was reported that the gas holdup at the center can be extrapolated from that of column without internals at higher inlet superficial velocities while an increase near the wall region was observed as an effect of internals. However, this phenomena is observed more with asymmetrically arranged internals than with circular tube bundles which cause bubbles to coalesce at the center region. Pradhan et al. (1993) reported higher holdup with

Figure 2.2 Typical profiles in the presence of internals (F. Möller et al., 2018)
helical coils in comparison to vertical internals. The author proposed that with the presence of internals (both helical and vertical), the area for gas phase motion is reduced, as a result the gas phase move more vigorously in radial directions. While the large tube-to-tube space of vertical internals allow large bubble to escape directly, the coils promote smaller bubbles, giving rise to higher gas holdup.

Guan et al. (2015) studied the hydrodynamics in a column with pin fin tube internals. They found that these internals have significant effect on local and overall gas holdup as well as liquid axial velocity. It was also reported that the presence of pin fin tube reduces the gas distributor region in the column. Further, changing the internal configuration, flow with no downward liquid flow can be realized with severe short circuiting. Further work on heat exchanging, RTD and mass transfer was suggested by the authors. Balamurugan et al. (2010) studied the increase in gas holdup on inclusion of a vibrating helical coil type internal. It was reported that these internals increased the gas holdup by 135% from that without internals, due to breakup of bubbles by vibrating spring reducing their rise velocity and increasing the gas holdup.

2.2 Effects of Internals on Local Holdups

Local gas holdup measurements in presence of internals were conducted by Jasim (2016) using a four point optical probe to investigate the effect of configuration (circular and hexagonal) and size of internals in same circular configuration (1.27 and 2.56 cm) on gas holdup and gas phase hydrodynamics with a constant CSA of 25%. A steeper increase and higher local gas holdup with both the circular arrangements was observed in the core region and a decrease at the wall regions. This implies a substantiated flow of gas to the center with circular arrangements. This may arise due to funneling effect causing gas to move at the low pressure core region aided by bubble coalescence due to unrestricted flow at the center. For the smallest tube-to-tube space
being (21.4 mm), the flow of large bubble across the bundle is restricted. While the arrangement with larger internals with a central tube and large tube-to-tube space enhanced the gas holdup and specific interfacial area near the wall regions. An asymmetrical radial profile for gas holdup and specific interfacial area were obtained for the hexagonal arrangement.

The local effects of internals configurations were investigated in more details in a recent work (Möller et al., 2018) using ultrafast X-ray tomography. The study investigated the effects of different configurations and size of internals on gas holdup, bubble size distribution, bubble frequency and flow patterns - see Table 2.1 for details. The radial gas holdup profile showed an oscillatory non-uniform and flat profile in the vicinity of internals, in comparison to the parabolic profile in case of empty bubble column in both the bubbly and churn turbulent regime. They found an increasing gas holdup near the walls (kept free of internals) with decreasing pitch and subchannel area with bubbles preferentially rising in the wall zone with free wall area. Further, a distinction between the profiles for triangular and square profile was observed with considerably lower gas holdup in tube bundles for triangular pitch giving it a non-uniform holdup profile. This is attributed to smaller sub channels for triangular pitch with lower hydraulic diameters for flow in the bundle. A higher holdup with superficial velocity was observed for square configuration (with higher hydraulic diameter) than with triangular (with lower hydraulic diameter). It was reasoned that the large bubbles formed in the triangular configuration move faster compared to the square configuration, where bubbles are trapped in sub-channels having a lower velocity and increasing holdup in the column.

2.3 Effect on Bubble Chord Length and Rise Velocity

The presence of internals affects flow patterns and create new regions for bubbles coalescence and breakup depending on the geometry. Based on the geometry and
configuration, it has been found that different factors can be promoted leading to a higher breakup or coalescence in the column. Möller et al. (2018) found a train of low-interacting bubbles in the homogeneous flow (2 cm$^{-1}$), while formation of Taylor-like bubbles in heterogeneous (20 cm$^{-1}$) forming a slug flow confined by tubes. Youssef & Al-Dahhan (2009) found a lower bubble chord length and decreased bubble rise velocity at the column’s center for the 22% asymmetrically arranged internals. It was reasoned that due to presence of internals smaller bubbles observed moving upwards with lower velocities giving a higher residence time and local holdup. However, this was later examined and compared with different configurations in other work (Jasim, 2016; Sultan et al., 2017). It was concluded that the decrease in bubble velocity at the center was mainly due to the asymmetric configuration of the internals while for a symmetric configuration, the bubble velocity at the center was higher.

2.4 Effects on Liquid Flow Patterns

The gas entering a bubble column moves upwards, preferably along the center, transferring momentum to liquid flow. This upward velocity of liquid phase consequently creates a recirculation in the downward direction in the near wall region. This large scale recirculation is the result of upward liquid velocity at the core region and a negative i.e. downward velocity near the walls in an empty bubble column. The presence of internals, however affect this flow profile. While a circular bundle with no internal in the core region gives an enhanced central liquid velocity and a much more profound recirculation, the presence of a asymmetric internals decreases the magnitude of liquid velocity over the entire column, thus dampening the recirculation and large scale flow patterns. George et al. (2017) performed mixing experiments to examine the effects of internals on liquid recirculation and mixing in the presence of internals. The work examined a tube bundle type internal with a low CSA (approx. 10%) with an
empty core region and a baffle. They reported a reduction in back-mixing effects with inclusion of baffle type internal placed below the tube bundle type internal. Further, studies revealed the affect of internals on time averaged flow patterns. It was reasoned that the presence of baffle type internal divert the large bubbles, creating a stronger vortical flow region that acts against the back-mixing, and enhancing the mixing in distributor region due to lower volume and more energetic flows. Guan et al. (2014) conducted studies with different gas distributors in the presence of internals. They found that the effect of variation of distributor is global in the presence of internals as opposed to local impacts in hollow column. The type of gas distributor employed was able to modify the overall flow pattern of the column including the gas holdup and liquid velocity profiles. This was because with presence of internals, existence of well-developed region is difficult to form, and it was suggested the distributor design can be used as a source of controlling flow pattern in the column.

Forret et al. (2003) reported an increase in axial liquid velocity at the core while the radial profile remained the same. Also, an enhanced large scale recirculation in a large column with internals was observed, due to lower liquid velocity fluctuations with internals which is in agreement with observations of Chen et al. (1999). In a recent study, Möller et al. (2018), discovered that the presence of internals divided the column into section of liquid ascending regions (sub channels) and descending regions (tube bridges and near the wall). Therefore, the liquid circulation eddies formed with dimensions of half the pitch, leading to a dampened liquid turbulence and energy strongly impacting the circulation pattern. It was concluded that the internals shift the gas holdup towards the wall and invert the profile compared to the empty BCR. This is most profound in configurations with highest flow resistance.
Dispersion in bubble column consists of two processes, the large-scale recirculation from upward and downward flow regions and turbulence or fluctuating velocity contributing to radial and axial mixing (Forret et al., 2003). The presence of internals affects the processes responsible for dispersion and promote or dampen them. Generally, it has been reported that the presence of internals increase large scale recirculation and decrease fluctuations (Chen et al., 1999; Forret et al., 2003; George, 2015; A. A. Youssef et al., 2013).

2.5 Effects on Internals on Liquid Phase Axial Dispersion

Some of the earliest investigation on the effect of internals on fluid dynamics and mixing behavior was performed by Bernemann (1989), who reported an increase in the dispersion coefficient due to presence of internals in both small and large diameter columns. The work of Forret et al. (2003) showed the importance of including both axial and radial dispersion coefficients to reproduce effects on internals on liquid mixing thus signifying strong influence of internals on liquid circulation pattern and turbulence. They found a higher value of axial to radial dispersion coefficients due to internals as an effect of subdued radial motion and enhanced liquid circulation in the column. In a recent study, Möller et al. (2018) reported that the radial liquid dispersion was about 200 times lower than the axial dispersion coefficients. The lower value for radial dispersion in the presence of internals stems from suppressed radial movement of bubbles due to internals and causing a liquid confinement to sub-channels thus providing large scale axial liquid circulation and low radial spreading. In their experimental study George et al. (2017) and Jhawar and Prakash (2014) investigated the effects of tube bundle and baffle type internals in the column. They reported that the presence of baffle type internal with tube-bundle alters the strong radial gradient of liquid velocity. While the circular tube-bundle type internal was responsible for
elevated gas holdup and liquid axial velocity, adding the baffle type internal at specific height from distributor reduces back-mixing.

2.6 Summary Comments

Insertion of vertical tube internals in a hollow bubble column affects gas holdups, local holdup profiles and liquid flow patterns. The extent of change depends on the internals design and configuration. The important geometrical parameters are tube diameter, number of tubes and their arrangements. The resultant tube-to-tube distance, free cross-sectional area are shown to affect axial and radial distributions which are can affect the reactor performance adversely. A few studies have shown that a suitable combination of baffle type internals with vertical tubes can mitigate some of the adverse effect. More studies with appropriate combinations of internals is recommended for an optimal design of the bubble column.

2.7 Numerical Modeling of Bubble Column with Internals

Over the years, Computational Fluid Dynamic (CFD) simulations have emerged as a promising tool to investigate bubble hydrodynamics including gas holdup profiles, liquid velocity profiles, mixing time and shear stress profiles (Jakobsen, Lindborg, & Dorao, 2005; Joshi, 2001; Joshi & Nandakumar, 2015). Most of the studies have focused on hollow bubble column and only a few recent CFD simulation studies have been performed in bubble column with internals (Guan and Yang, 2017; Guo and Chen, 2017; Guan et al., 2014; Larachi et al., 2006). The task of simulating the complex hydrodynamics of a bubble column operating in a heterogeneous regime becomes even more challenging in presence of internals. There is need to select appropriate modelling approach and modeling parameters and boundary conditions for more realistic simulation results while maintaining ensuring reasonable computational time.
Two widely used modeling approaches for describing multiphase hydrodynamics in CFD simulations are Eulerian-Eulerian (E-E) and Eulerian-Lagrangian (E-L) (Darmana et al., 2005; van Wachem and Almstedt, 2003; Ranade, 2002). In the E-E model both the dispersed and continuous phases are treated as interpenetrating continuum while the volume-averaged mass and momentum equations describe the time-dependent motion of phases (Ranade, 2002; Dean et al., 2001). The number of bubbles present in a computational cell is represented by a volume fraction in the balance equations. The information of the bubble size distribution can be obtained by incorporating population balance equations to account for bubbles break-up and coalescence (Darmana et al., 2005). The E-L approach tracks motion of dispersed phase particles using Newtonian equation of motion while motion of the continuous phase is modeled using a Eulerian framework. Tracking the motion of dispersed phase particles allows direct consideration of effects related to bubble-bubble and bubble-liquid interactions. Mass transfer with and without chemical reaction, bubble coalescence and re-dispersion can be incorporated directly (Delnoij et al., 1997 and Sokolichin and Eigenberger, 1994). A drawback of E-L model compared to E-E model is significant increase in computational time as number of bubbles (particles) to be simulated increase. Since for each bubble one equation of motion needs to be solved, making the method less attractive for large scale bubble column reactors (Darmana et al., 2005). Since, tracking a huge number of bubbles requires a overwhelming amount of computational time, the Eulerian-Eulerian approach is more popular and used for the purposes discussed in this work. In addition, the high volume fraction of the dispersed phase renders the Lagrangian approach unsuitable for the churn turbulent regime. A two-fluid model based on the Euler-Euler approach treats both the phases as continuum and their mechanics is governed by partial differential equations. The equations are solved where
variables are ensemble averaged over time and space while calculating the point phase fraction. The conservation equations are solved for each phase together with interphase exchange terms. Various interfacial forces are used to solve transport equations as closures for interactions between the phases.

**Eulerian-Eulerian Model**

The basic equation set consists of the continuity (conservation of mass) and momentum equations for \(N_p\) phases as detailed below (from Pfleger and Becker, 2001).

### Conservation of Mass

\[
\frac{\partial}{\partial t} (\rho_k \varepsilon_k) + \frac{\partial}{\partial x_i} (\rho_k \varepsilon_k U_{k,i}) = \sum_{\beta=1}^{N_p-1} \left( m_{k\beta} - m_{\beta k} \right) + \varepsilon_k S_k \quad (2.1)
\]

<table>
<thead>
<tr>
<th>Change of mass</th>
<th>Convection flux</th>
<th>Mass transfer</th>
<th>Source term</th>
</tr>
</thead>
<tbody>
<tr>
<td>over time</td>
<td></td>
<td></td>
<td>(i.e. kinetics)</td>
</tr>
</tbody>
</table>

Here,

\[
\sum_{k=1}^{N_p} \varepsilon_k = 1 \quad (2.2)
\]

### Momentum balance

\[
\frac{\partial}{\partial t} (\rho_k \varepsilon_k U_{k,i}) + \frac{\partial}{\partial x_j} (\rho_k \varepsilon_k U_{k,i} U_{k,j}) =
\]

\[
e_k \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \varepsilon_k \mu_i \left( \frac{\partial U_{k,i}}{\partial x_j} + \frac{\partial U_{k,j}}{\partial x_i} \right) + \rho_k \varepsilon_k g + M_{k,i} \quad (2.3)
\]

<table>
<thead>
<tr>
<th>Pr. gradient</th>
<th>Viscous stresses</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gravit. force</td>
<td>Interphase momentum transfer</td>
</tr>
</tbody>
</table>

Inter phase momentum transfer can be expressed as:
Further details of the model can be found in Pfleger and Becker (2001) and Ranade (2002).

**Eulerian-Lagrangian**

This modeling approach computes the motion of each bubble from bubble mass and momentum equations. The liquid phase contributions are accounted for by the interphase mass transfer rate and the net force experienced by each bubble (Darmana et al., 2005). For an incompressible bubble, the equations can be written as

Bubble mass balance:

\[
\rho_b \frac{d(V_b)}{dt} = (\dot{m}_{l\rightarrow b} - \dot{m}_{b\rightarrow l})
\]  

(2.5)

Here \(V_b\) is bubble volume and \(v\) is bubble velocity. The term on right hand side represents mass transfer.

**Bubble momentum balance:**

\[
\rho_b V_b \frac{dv}{dt} = \Sigma F - \left( \rho_b \frac{dV_b}{dt} \right) v
\]  

(2.6)

\(\Sigma F\) represents the net force experienced by individual bubble which include gravity, pressure, drag, lift force and virtual mass.

\[
\Sigma F = F_G + F_P + F_D + F_L + F_{VM}
\]  

(2.7)

Liquid phase balances:

The liquid phase equations consist of continuity and momentum equations represented by the volume averaged Navier-Stokes equations. The presence of bubbles is reflected
by the liquid phase volume fraction - refer to Darmana et al., 2005 for additional details of model equations.

A summary of the literature studies based on the effect of internal geometries on hydrodynamics in the column using numerical modeling is presented in Table 2.2. The first CFD study of bubble columns with vertical internals was performed by Larachi et al. (2006). The effect of different configurations and covered CSA were simulated. The study revealed effect of arrangements on the liquid circulation pattern, inter-tube gap on growth of flow structures (small scale recirculation) and overall effect of internals on turbulence parameters.

Table 2.2 Summary of Computational work done on bubble columns with vertical tube internals

<table>
<thead>
<tr>
<th>Published Work</th>
<th>Geometry (i) Inner Diameter (Dc, mm); (ii) Height of Liquid (Static Hs, Dynamic Hdynamic, m); Operating Details: (iii) Range of Inlet velocity(ug, cms⁻¹)</th>
<th>Internal Geometries CSA (%): Size of tubes(mm); Configuration;</th>
<th>Numerical Model; Interface Closure; Turbulence Model; PBM –Bubble Size Groups; Bubble Size Range (mm);</th>
</tr>
</thead>
<tbody>
<tr>
<td>Larachi, Desvigne, Donnat, &amp; Schweich, (2006)</td>
<td>(i) Dc = 190, 1000 (ii) Hdynamic = 1.4, 7.5 (iii) ug =12</td>
<td>(i) CSA: 2-16 (ii) Four configurations with triangular pitch(57, 171)-uniform dense and scattered, star with wall clearance and core clearance (iii) dt=25.4</td>
<td>Eulerian-Eulerian D: (Morsi &amp; Alexander, 1972); Turbulence: k-ε; (Dispersed + BIT); dl = 5</td>
</tr>
<tr>
<td>Laborde-Boutet et al., (2010)</td>
<td>(i) Dc = 151 (ii) H = 4.61 (iii) ug =34.3</td>
<td>(i) CSA: 12.5 (ii) Two U-tube internals (iii) dt=26.7</td>
<td>Eulerian-Eulerian D:(Morsi &amp; Alexander, 1972); Turbulence: RNG k-ε (Dispersed + BIT, per-phase); dl = 3.2 (Wilkinson, 1991)</td>
</tr>
<tr>
<td>Guan, Li, Wang, Cheng, &amp; Li, (2014)</td>
<td>-</td>
<td>(i) CSA: 5, 10, 20 (ii) Eight configurations with two pitch type (square, triangular) Pitch = 26.7-54.1</td>
<td>Volume of Fluid</td>
</tr>
<tr>
<td>Authors</td>
<td>Details</td>
<td>Details</td>
<td>Details</td>
</tr>
<tr>
<td>----------------------</td>
<td>------------------------------------------------------------------------</td>
<td>------------------------------------------------------------------------</td>
<td>---------</td>
</tr>
<tr>
<td>Z. Li et al., (2015)</td>
<td>(i) ( D_c = 476 ); (ii) ( H_{\text{dynamic}} = 4.76 ); (iii) ( u_g = 12 )</td>
<td>(i) CSA: 5 (ii) Two concentric circular bundles with 16 tubes, Pitch = 0.09 ( d_t = 25 )</td>
<td>Eulerian-Eulerian D:SN, T, (Xiao, Yang, &amp; Li, 2013); L:-0.02; WLF: (Antal, Lahey, &amp; Flaherty, 1991) TD: (Bertodano, 1991) Turbulence: RNG ( k-\varepsilon ); ( d_b = 5 )</td>
</tr>
<tr>
<td>Guan &amp; Yang, (2017)</td>
<td>(i) ( D_c = 476 ); (ii) ( H_{\text{dynamic}} = 4.76 ); (iii) ( u_g = 12 )</td>
<td>(i) CSA: 5 (ii) Two concentric circular bundles with 16 tubes, Pitch = 0.09 ( d_t = 25 )</td>
<td>Eulerian-Eulerian D:SN, T, (Xiao et al., 2013); L:-0.02; WLF: (Antal et al., 1991) TD: (Bertodano, 1991) Turbulence: RNG ( k-\varepsilon ); ( d_b = 5 )</td>
</tr>
<tr>
<td>Guo &amp; Chen, (2017)</td>
<td>(i) ( D_c = 140 ); (ii) ( H_{\text{dynamic}} = 1.56 ); (iii) ( u_g = 3, 45 )</td>
<td>(i) CSA: 5, 25 (ii) Three arrangements: Two Circular with 8 tubes of ( d_t = 12.7 ), 25.6 with one at center; Triangular with 31 tubes of ( d_t = 12.7 )</td>
<td>Eulerian-Eulerian+ PBM D:IZ; L:TL; WLF: (Hosokawa, Tomiyama, Misaki, &amp; Hamada, 2002); BIT:TH; Turbulence: RNG ( k-\varepsilon ); ID-2(11+8); ( d_b = 0.575-29.23 ); (Guo, Zhou, Li, &amp; Chen, 2016a)</td>
</tr>
<tr>
<td>Bhusare, Dhiman, Kalaga, Roy, &amp; Joshi, (2017)</td>
<td>(i) ( D_c = 120 ); (ii) ( H_{\text{dynamic}} = 0.655 ); (iii) ( u_g = 14-132 )</td>
<td>(i) CSA: 0-11.7 (ii) Two configurations, with a central rod of ( d_t = 36 ), with zero and 4 surrounding rods of ( d_t = 12 )</td>
<td>Eulerian-Eulerian - OpenFOAM D:C(_D) chosen based on (Joshi, 2001); L: C(_L) chosen based on (Joshi, 2001)(-0.08, -0.23); TD: C(_TD) chosen based on (Joshi, 2001) (0.008, 0.07); Turbulence: ( k-\varepsilon ) (Mixture); ( d_b = 2.2-2.6 )</td>
</tr>
<tr>
<td>Bhusare, Kalaga, Dhiman, Joshi, &amp; Roy, (2018)</td>
<td>(i) ( D_c = 120 ); (ii) ( H_{\text{dynamic}} = 0.655 ); (iii) ( u_g = 14-221; u_l = 0.5-1.4 )</td>
<td>(i) CSA: 0-11.7 (ii) Two configurations, with a central rod of ( d_t = 36 ), with zero and 4 surrounding rods of ( d_t = 12 )</td>
<td>Eulerian-Eulerian - OpenFOAM D:C(_D) chosen based on (Joshi, 2001); L: C(_L) chosen based on (Joshi, 2001)(-0.08, -0.23); TD: C(_TD) chosen based on (Joshi, 2001) (0.008, 0.07); Turbulence: ( k-\varepsilon ) (Mixture); ( d_b = 2.2-2.6 )</td>
</tr>
</tbody>
</table>

They showed the arrangement and inter-tube distance had a significant effect on liquid circulation and flow pattern. A similar uniform liquid circulation pattern with liquid up-
flow at the core and down-flow near the wall as that in hollow bubble column was observed for uniformly arranged internals. While non-uniform arrangements of internals resulted in more complex flow patterns with even liquid flow in the core region with dense internals in the core region and sparse arrangement near the walls was observed. Further reduction in axial liquid velocity and turbulent kinetic energy was reported in the presence of internals. This was attributed to reduction in hydraulic diameter for eddies due to lower tube pitch of internals.

In their model, Larachi et al. (2006) made assumptions limiting the accuracy and data retrievable from their simulations. Major among them was use of steady drag force as the only interfacial force and a constant bubble size even for simulations in churn-turbulent flow regime. While they presented arguments for the assumptions, the constant bubble size limited the study, since the bubble size distribution and re-distribution as an effect of internals was not simulated.

The effect of bubble size distribution was investigated by Guo and Chen (2017) with inhomogeneous population balance (TFM-PBM) model to study the impact of internals on gas-liquid hydrodynamics. The two-bubble phase inhomogeneous PBM approach was simulated with drag and lateral forces (lift, wall lubrication force) with RNG k-ε turbulence model to accurately study the effect of internal density and configuration on the hydrodynamics. Coalescence and breakup model developed by the authors (Guo et al., 2016) was used to compute the bubble size distribution. The modified drag model given by Ishii & Zuber (1979) used to model the drag based on bubble size and structure. The Tomiyama (1998) lift force and Hosokawa et al. (2002) wall lubrication force models used to simulate the lateral interfacial forces due to bubble shear and wall effects respectively. They simulated the case based on the experimental work of Kagumba & Al-Dahhan (2015) with two tube sizes(0.5 and 1 in) in circular
arrangement covering 25% CSA. Further, they added another internal arrangement with 8 small sized tubes arranged as the large tubes to give total of three arrangements, two circular with 8 tubes of \( d_t = 12.7 \) mm, 25.6 mm with one at center and a triangular with 31 tubes of \( d_t = 12.7 \) mm. The arrangement was made to study the effect of internal tube size and CSA on bubble column hydrodynamics.

A reduction in liquid fluctuations was observed in the presence of internals due to wall resistance with an increase in turbulent dissipation rates in the inter-tube gaps. This increase in dissipation rates give a higher bubble breakup leading to a smaller bubbles in and increased gas holdup in these regions. Further, it was found that with 31 tubes symmetrically placed in a circular pattern, the gas holdup in the core region significantly increased due to restricted bubble motion due to lower inter-tube distance. This also led to a higher axial liquid velocity and an enhanced liquid circulation. In the bubbly flow regime, the dense internals largely controlled the liquid circulations replacing the overall circulation with local vortex flows while at higher superficial gas velocity a number of smaller local circulations were observed in addition to the overall recirculation. With increase in covered CSA, the bubble distribution was largely controlled.

When the internals occupy a smaller fraction of column cross section (~ 10%), the simulation studies generally show a small effect of internals on overall liquid circulation pattern (Bhusare et al., 2017; Laborde-Boutet et al., 2010). Bhusare et al.(2018) simulated a continuous co-current up-flow bubble column of the same geometry used by Bhusare et al. (2017). The reported an increase in eddy diffusivity in the presence of internals attributed to increased turbulence. This led to a better eddy transport in the column and an increase in axial dispersion.
Guan et al. (2017) simulated bubble column with internals studying the single bubble behavior including bubble trajectories, bubble shape, bubble rise velocity, and bubble breakup using VOF method. The model was validated for effect of walls on bubble rise velocity. It was discovered that the bubble paths are rectilinear and bubble is rocking with the amplitude and oscillations increasing with increase in internals covered CSA. This secondary motion was attributed to vortex shedding from bubble wake and bubble induced turbulence. With different pitch type, the triangular pitch was found to give stronger rocking amplitude and frequency than the square pitch owing to its more compact structure which allows a lower hydraulic diameter for the bubble motion. Bubbles were found to undergo axial elongation with the presence of internals with increase in the aspect ratio with internals covered CSA. The effect was more pronounced for larger bubbles than small bubbles. The bubble rise velocity was reported to almost decrease linearly with internals covered CSA while the steepness is higher for larger bubbles which are more sensitive to the presence of internals. While the bubble velocity was found to be smaller for triangular pitch than square pitch owing to its compact structure. Further, an increase in the difference between the velocities for pitch type with internals covered CSA was observed. It was reported that the internal solid walls increase viscous shear and local turbulence and thus augment the bubble breakup rate for smaller bubbles (7 mm), while for larger bubbles (20 mm), the bubble shedding volume indicates breakup which is maximum with a CSA of 10%. While an increase in covered CSA, leads to an increase of viscous shear and decrease in local turbulence causing a decrease in breakup. Thus it was concluded that the bubble lateral size determines the bubble wake behavior and bubble induced turbulence intensity. It was reasoned that for a small bubble, with increase in CSA, the ellipsoidal bubble elongates both laterally and axially, becoming a cap with increase in CSA, while for
large bubbles axial elongation and lateral shortening decreases the bubble wake size weakening bubble induced turbulence. This was also attributed to lower liquid turbulence with the presence of dense internals in heterogeneous regime.

2.8 Discussion on numerical model

Interfacial Forces

The most important distinctive feature of a multiphase system is the existence of an interface. The interaction between the phases are solved by including the correlations for interfacial force terms i.e. drag, lift, turbulent dispersion and mass transfer, in the momentum equation. In a bubble column, the interaction of bubble phase with the liquid phase determines the momentum exchange, and hence the mixing and mass transfer and are dependent on the interfacial area between the phases. This is determined by the bubble size distribution on inclusion of population balance model or is based on gas fraction for constant bubble size. The interfacial force terms i.e. drag, lift, turbulent dispersion and mass transfer, are included in the momentum equation. The effect of interfacial forces have been widely studied and reviewed for hollow bubble column by (Pourtousi, Sahu, & Ganesan, 2014; Tabib, Roy, & Joshi, 2008; Yamoah, Martínez-Cuenca, Monró, Chiva, & Macián-Juan, 2015) among others. While it has been argued that the effect of the interfacial forces remains similar in a column with internals with some of the interfacial forces becoming more dominant due to inclusion of dense internals (Guan & Yang, 2017). The other interfacial forces are dependent on the drag, making it the most essential in terms of required accuracy. This also develops to adverse effect on the numerical accuracy of the model if the drag is not accurately predicted. In comparing the effect of lateral forces (Guan & Yang, 2017) found that, without the lateral force gas holdup tend to increase near the tubes and decrease near the column wall region driven by the just the drag force and no-slip wall conditions pushing the
bubbles closer to the tubes, while on inclusion of lateral forces, the balance of lateral forces drives the large scale circulation and radial profiles.

**2.8.1 Drag Force**

In Eulerian-Eulerian model, the drag force is dominant over other interfacial force terms. Therefore, the drag model used in simulating bubble columns is of prime importance and has been extensively studied in literature for hollow bubble column (Gupta & Roy, 2013; C. Li, Cheung, Yeoh, & Tu, 2009; Rampure, Kulkarni, & Ranade, 2007; Marcela Kotsuka Silva, D'Avila, & Mori, 2012; Soccol, Galliani Pisceke, Noriler, Georg, & Meier, 2015; Tabib et al., 2008) and reviewed by (Pourrousi et al., 2014) recently. Only, (Guan & Yang, 2017) have performed a study on the drag models with internals with correlations from (Tomiyama, 1998), (Schiller & Naumann., 1935) and (Xiao et al., 2013). Among the various models used in literature for both hollow bubble column and those with internals, the drag coefficient based on bubble size structure has been found to be better able to model the effect of different sized bubbles with variation in flow regimes. However, the fact that most of these drag models have been developed considering flow of bubbles in quiescent liquid, and cannot accurately be used to model the drag with motion of continuous phase. Hence, studies to model drag in more realistic conditions is a required for a better numerical accuracy of the model.

**2.8.2 Lift Force**

Among the interfacial forces acting perpendicular to the drag force, the lift force from the Magnus force, as a result of bubble’ rotations, and Saffman force, as a result of shear flow around the dispersed phase (bubbles) has the most impact on flow pattern and bubble size distribution (Kulkarni, 2008). Owing to the instability and to reduce the computational costs, a number of studies have been performed without lift force
(Deckwer, 1992; Dhotre, Deen, Niceno, Khan, & Joshi, 2013; Guan & Yang, 2017; Gupta & Roy, 2013; C. Li et al., 2009; Sokolichin, Eigenberger, & Lapin, 2004). While more recent studies (Dhotre et al., 2013; Díaz et al., 2008; Tabib et al., 2008; D. Zhang, Deen, & Kuipers, 2006), especially those employing a population balance model (M. R. Bhole, Joshi, & Ramkrishna, 2008; Gupta & Roy, 2013; Huang, Yang, Yu, & Mao, 2010; Krepper, Frank, Lucas, Prasser, & Zwart, 2005) have shown that modelling of lift force have impact on radial distribution of bubbles, thus affecting the flow pattern and gas holdup profiles. For a column with internals, Guan & Yang, (2017) reported a flatter profile for gas holdup and axial liquid velocity profiles much like the effect observed in hollow bubble column, however the increase in axial liquid velocity on inclusion of lift force was found to be much higher (138%) with internals than without (20%). While (Larachi et al., 2006) and (Laborde-Boutet et al., 2010) neglected the lift force owing to lower computational cost and lack of information for accurate modelling of lift force coefficient. In their work, (V. H. Bhusare et al., 2017; Vishal H. Bhusare et al., 2018) used chosen values of lift force based on experiments with a hollow bubble column. While this approach may prove to be accurate in their case without a population balance model, a constant value of lift force is over-simplification of its effects. (Guo & Chen, 2017) has used the model given by (Tomiyama, 1998). Basically, the model provides a series of lift force coefficients based on the shape of the bubble by calculating the bubble Eotvos number and bubble Reynolds number with a negative values for smaller bubbles (moving towards the wall region) and a positive values for larger bubbles (movement to the core region). While, movement of bubbles based on shear difference was an addition to accuracy in case of hollow bubble column. In case of dense internals, the effect of lift force becomes more essential, more for geometries where substantial variation in flow patterns are observed as a result of low and high
shear regions. Further studies in the nature of flow for dense internals with small hydraulic diameters can only be reliably performed with accurate modelling of the lift coefficient.

2.8.3 Turbulent Dispersion

The turbulent dispersion force accounts for the effect of liquid eddies on dispersed bubbles while accounting the effects of liquid velocity fluctuations on the gas holdup. The turbulent dispersion models (Burns, Frank, Hamill, & Shi, 2004) and (Bertodano, 1991) have been commonly used for hollow bubble columns (Ekambara, Nandakumar, & Joshi, 2008; Pourtousi et al., 2014; Marcela Kotsuka Silva et al., 2012; Tabib et al., 2008). The turbulent dispersion coefficient was applied by (V. H. Bhusare et al., 2017; Vishal H. Bhusare et al., 2018) to simulate the bubble column with internals. While (Larachi et al., 2006) reasoned that the smoothing effect by the force would affect the abrupt gradients commonly observed in the presence of internals. The presence of internals have direct alters the scale of liquid phase eddies, the sensitivity to turbulent dispersion coefficient with internals varies with the geometry. In their work, (Guan & Yang, 2017) found that the presence of internals varies the sensitivity to turbulent dispersion force. They reported an enhanced the large scale liquid circulation by increasing the gas holdup in the central region instead of the expected flatter profile. Based on their results, it can be argued that the inclusion of turbulent dispersion force is not only responsible for smoothing profiles, but can show other changes based on the geometry.

2.8.4 Turbulence

There are two components of turbulence in a bubbly flow. The inherent liquid turbulence i.e the shear induced turbulence independent of the relative motion of bubbles and the other is the turbulence due to bubble flow in the column called the
bubble induced turbulence. The turbulence model is crucial to capturing the anisotropic nature of turbulence significant at higher velocities and hydrodynamic properties of the bubble column. A review of the recent work on turbulence modelling was included in Pourtousi, Sahu, & Ganesan (2014). Mostly, the k-ε models, RSM and LES have been used in literature (Deen, Solberg, & Hjertager, 2001; Dhotre et al., 2013; Ekambara et al., 2008; Marcela Kotsuka Silva et al., 2012; Tabib et al., 2008). While k-ε models requires lower computational resources, the assumption of isotropic flow limits the model where bubble induced turbulence and anisotropy of turbulence is significant. The RNG k-ε model being able to show the swirling flows and broader scales of turbulence than Standard or Realizable models has been the model of choice in the recent studies. Supporting confirmation has been found in the study of turbulence models examined in detail without the population balance model by (Laborde-Boutet, Larachi, Dromard, Delsart, & Schweich, 2009). Further, the k-ε model was compared with the RSM model in the work of (Tabib et al., 2008). They found the RSM model was better able to predict the turbulent kinetic energy than the k-ε model due to its intrinsic ability in capturing anisotropic energy transfer mechanism. It has been reported that the additional computational cost required for RSM or LES model is not justified by the information gathered (Ekambara et al., 2008; Laborde-Boutet et al., 2009; Tabib et al., 2008).

However, the presence of internals brings asymmetry to the flow creating highly anisotropic flow. The assumption with k-ε model limits the accuracy and physical realization of flow behavior and modelling turbulence with another model would be advisable in this regard.

Most of the studies with bubble column internals have employed k-ε model, with most frequently used RNG k-ε model(Guan & Yang, 2017; Guo & Chen, 2017; Laborde-
Boutet et al., 2010) based on the work of (Laborde-Boutet et al., 2009) has been used with a bubble induced turbulence model.

2.8.5 Population Balance Model (PBM)

The bubble size distribution in a bubble column varies with the operating conditions. The population balance model developed by (Hounslow, Ryall, & Marshall, 1988) is employed to model the coalescence and breakup rates for different bubble size. The population balance equation given by (Kumar & Ramkrishna, 1996) has been frequently used to calculate the distribution of discrete bubble size groups with the breakup and coalescence kernels. It has been discussed in literature that the limitations posed due to assumptions drawn while modelling coalescence and breakup kernels limits the applicability of PBM in heterogeneous flows (Lasheras, Eastwood, Martínez-Bazán, & Montaes, 2002; Martinez-Bazan, Montanes, & Lasheras, 1999; Wang, Wang, & Jin, 2003). The mechanisms for bubble breakup are viscous shear, local turbulence, and interfacial instability. The presence of internals affects the hydrodynamics surrounding the bubbles and therefore, alter the bubble coalescence and breakup phenomena. The effect of internals and the applicability of these kernels in simulating PBM for bubble columns with internals is yet to be tested. While from studies in hollow bubble column it was found that in order to accurately model the coalescence and breakup phenomena, a modification in the kernels or implementation of PBM model is required. (Guan, Li, Wang, et al., 2014) has reported various mechanisms of the effects of internals on bubble breakup.

The presence of internals has been experimentally observed to alter the bubble size distribution in the column. Therefore, in order to study the variation in bubble size distribution and their effects on other parameters including gas phase dispersion and mass transfer, mixing, and flow patterns, the redistribution of bubble size needs to be
taken into consideration as a result of presence of internals. (Guo & Chen, 2017) employed bubble population model with Coalescence and breakup model developed by the authors (Guo et al., 2016b) to compute the bubble size distribution. They reported a variation in bubble size distribution on incorporation of PBM, with higher production of bubbles as means of wall effects and higher turbulence variations near the wall regions affecting the gas holdup and velocity profiles. They were able to report the evolution of bubble size distribution as an effect of internal types.

2.8.6 Wall Lubrication Force

The difference in liquid speed near the wall and away from the wall, creates a force driving the bubble in the region near the wall away called as wall lubrication force (Antal et al., 1991). The effect is only near the wall region. Very highly dense mesh is required near the wall region for accurately modelling wall force. Due to the high density of internal walls, the effect of wall force is higher in bubble column with internals. However, having a dense mesh near the wall region for the complex geometry of the internals has adverse effect on computational cost. Similar reasons were drawn to neglect the effect of wall force in some studies (Laborde-Boutet et al., 2010; Larachi et al., 2006). In their study of the effect of wall lubrication force, (Guan & Yang, 2017) found a magnified effect of wall force for bubble columns with internals. They reported a lower gas holdup close to internals and column wall regions due to wall lubrication force with more than twice the region effected by the wall force in comparison to a hollow bubble column.

(Guo & Chen, 2017) compared effect of free-slip, no-slip boundary conditions for internal walls with wall lubrication force to study the impact of walls on bubble movement. They report a lower gas volume fraction near internals on inclusion of wall lubrication force as opposed to unreasonably high holdup near the tubes due to the
bubbles rising along the wall. However, it is observed that with the present model, the effect is higher, and thus predicts an even lower gas holdup than experimentally observed and the predicted gas holdup profile without wall lubrication force showed a better fit. It was thus concluded that the present models are insufficient to predict

2.9 Summary Comments

CFD simulations can be used to simulate various geometries of internals in a bubble column. However, in order to study various parameters, various modifications are required in the numerical model used in the literature. While developing these modifications require more diverse and accurate experimental studies. While the present status of interfacial forces being used for bubble columns with internals are found to be more sensitive in case of internals especially those dependent on wall surface area. More studies with experimental validation are required to study individual accuracy of these models. Further, while RNG k-ε turbulence model is sufficient to gather information, application of RSM and LES models will be better able to simulate the effect of internals on turbulence parameters as has been reported in experimental studies. Further application of the turbulence model is with the coalescence and breakup kernels. Being dependent on the turbulence model, the accuracy of these kernels increase with that of the turbulence model. However, further work is needed in re-defining the coalescence and breakup models and implementing the PBM model to study the re-distribution of bubble size as a result of dense internals.
References


Chapter 3

3. CFD Modelling of the Hydrodynamic Characteristics of a Bubble Column

3.1 Introduction

Bubble column reactors find applications in chemical and biochemical industries as gas-liquid and gas-liquid-solid contactors due to their advantages of simple design and construction, high mixing effects, mass and heat transfer, and low maintenance costs. Predicting the performance of these reactors requires the knowledge of the hydrodynamics and transport phenomena in the reactor. While several correlations have been developed for predicting these phenomena, these are found to be limited to a set of operating conditions. Therefore, using these correlations for a new set of conditions can lead to a poor design. For a better design, the relationship between the flow pattern and geometry must be established as per the design objective (Joshi, 2001; Joshi & Nandakumar, 2015). Further, the study of the effect of internals with varying geometry proves essential for the reactor design, but it is difficult to predict the performance of reactor using correlations. Computational Fluid Dynamic (CFD) simulations have emerged as a promising tool to study the local characteristics including gas holdup profiles, liquid velocity profiles, mixing time and shear stress profiles of multiphase flow in a bubble column reactor (Jakobsen et al., 2005; Joshi, 2001; Joshi & Nandakumar, 2015).

One of the prominently used approaches for modeling multiphase flows is the Eulerian-Eulerian approach, where both the dispersed and continuous media are treated as interpenetrating continuum. The Eulerian-Lagrangian approach treats the continuous phase the same, while the dispersed phase (discrete bubbles) is tracked using the equations of motion based on the force balance. Those models have been further
discussed in detail in the work of van Wachem & Almstedt (2003). Since, tracking a huge number of bubbles requires a overwhelming amount of computational time, the Eulerian-Eulerian approach is more commonly and used for the type of numerical work conducted in this work. In addition, the high volume fraction of the dispersed phase renders the Lagrangian approach unsuitable for the churn turbulent regime. A two-fluid model based on the Euler-Euler approach treats both the phases as continuum and their mechanics is governed by partial differential equations. The governing equations are solved where variables are ensemble averaged over time and space while calculating the point phase fraction. The conservation equations are solved for each phase together with interphase exchange terms. Various interfacial force correlations are needed in order to solve the transport equations as closures for interactions between the phases. It is assumed that bubble size does not change when calculating the interfacial forces, however in most of cases, the bubble size varies depending upon the gas superficial velocity, pressure, physical properties including density, viscosity, and surface tension of liquid phase etc. Further, most of the industrial columns operate in churn turbulent regime with a distribution of bubble sizes due to coalescence and breakup. This simplification limits the applicability of the model to the homogeneous regime in each set of operating conditions with no pressure variation. It is observed that the flow regime transition into churn turbulent regime affects large bubbles. As the bubbles move from the sparger, they coalesce, break, and change shapes and sizes based on the pressure variations in the column, giving rise to various flow patterns. While the bubble coalescence and breakup are significant in gas-liquid mass transfer, the bubble size directly affects the interfacial forces, which affects the holdup, velocity profiles and circulation patterns in the column. Therefore, the bubble size distribution is required to accurately estimate the flow patterns and profiles. Further, as discussed by Chen,
Sanyal, & Duduković (2005), the gas holdup radial profiles were not accurately predicted based on mean bubble size. Therefore, the bubble size distribution is essential to accurately predict the radial gas holdup profiles since it depends on the lateral interfacial forces such as lift, turbulent dispersion which depend on the bubble size. The importance and advantages of including a bubble size distribution model is drawn in works of Wang (2011) and M. R. Bhole, Joshi, & Ramkrishna (2008).

Application of population balance equation to bubbly flows was first performed in the work by Lo (1996). Further work has been carried out in the recent years to capture the effect of bubble interactions and size distribution with the population balance approach as listed in Table 3.1. Among the models used to predict the bubble size distribution, the population balance model (PBM) for the gas-liquid bubble flow is the most used (Table 3.1), Among the various methods studied for this purpose, the discrete method developed by Kumar & Ramkrishna (1996) has been widely implemented. Here, the bubble size is divided in to a number of intervals, and the PBM equation is integrated over each bubble size interval. The implementation strategy of this approach is discussed in detail in this work. The homogeneous discrete method assumes that bubbles of all size groups travel at the same velocity. While, this assumption reduces the number of equations required to solve where the transport equation is reduced to one, it oversimplifies the situation. This assumption gives the large and small bubbles equal bubble rise velocity, which is contrary to the physical phenomena where the large bubble travel faster than the small sized bubbles (Bhole et al., 2008). This adversely affects the velocity profiles, turbulence and flow pattern prediction accuracy and is the most severe limitation to the PBM discrete model as was evidenced in the work of Ekambara, Nandakumar, & Joshi (2008) especially at higher velocities. To overcome this limitation, two approaches, one based on an algebraic slip model to account for
bubble separation presented by Bhole (2008) while another one with additional momentum equations as used by Krepper (2005) have been proposed in the literature.

The approach implemented by Bhole (2008) was derived by simplifying the momentum equation of the gas phase. Based on the order of magnitude, the inertial, body force and stress terms for the gas phase can be neglected owing to comparably lower density of the gas phase and dominant liquid phase turbulence. This reduces the momentum exchange equation to an algebraic form called the algebraic slip model which states the momentum balance for gas phase is the balance of interphase forces and pressure gradients only. This model allows size specific momentum balance, thus eliminating the assumption of equal velocities for bubbles of different sizes used in the homogeneous discrete PBM. The velocity for bubble phase can now be calculated using the algebraic equation without iterations and thus can solve all discrete gas phase momentum equations with low computational costs. Bhole (2008) showed the applicability of the model at low velocity of 0.02 m/s in the homogeneous regime. However, at higher velocities where gas phase turbulence becomes more significant, neglecting stress terms would be oversimplification and might lead to significant inaccuracy.

The other approach used by Krepper (2005) called the inhomogeneous discrete model, divides the bubble sizes into multiple velocity groups each having a series of bubble sizes. In this model, multiple transport and population balance equations are solved for each discrete velocity group. This model is used in this work and the bimodal bubble size distribution of small and large bubble sizes is based on the experimental observation (unless mentioned otherwise). The small bubble size ranging from 1 mm to 7 mm while the large bubble size from 7mm to 35 mm covering a range of possible bubble sizes. The stability of the model with one, two and three velocity groups was
compared based on the mean Sauter bubble size analysis in both homogeneous and churn turbulent regime. Duan (2011) performed numerical simulations with inhomogeneous discrete and Average Bubble Number Density model to assess their performance for simulations in varied operating conditions in tall pipes. The simulations were performed to study the opposite trends of bubble size evolution and the ability of the models to predict the transition from “wall peak” to “core peak” gas volume fraction profiles. It was reported that both the models were able to predict the trend, while the results with inhomogeneous discrete model were better. This was attributed to the high resolution of results from the inhomogeneous discrete model, however, the coalescence and breakage kernels were regarded as the source of the discrepancies from experimental results. Gupta (2013) did simulations to study the growth of the bubble size using various types of population balance methods namely the Homogeneous Discrete method, Inhomogeneous Discrete method, Quadrature Method of Moments (QMOM) and Direct Quadrature Method of Moments (DQMOM) models for a rectangular bubble column at inlet superficial velocity $U_G = 1.33 \text{ mm/s}$ to ensure lower complexity of flow and interphase interactions. It was concluded that at low superficial velocities i.e. in bubbly flow regime, performing computationally expensive PBM simulations have minor effects on the accuracy of the results. The results show similar profiles from all the models for axial liquid velocity and Sauter-mean diameter. Further, good agreements with experimental results have been reported when including of interfacial forces. Further studies with higher velocities have been suggested to understand the importance of PBM and interfacial forces.

Guo and Chen (2017) used a two-fluid Eulerian-Eulerian model with inhomogeneous population balance (TFM-PBM) model was used for the simulation to study the impacts of internals on gas-liquid hydrodynamics. The two-bubble phase inhomogeneous
approach was used with drag and lateral forces (lift, wall lubrication force) in the simulation to accurately study the effect of internal density and configuration on the hydrodynamics. Coalescence and breakup model developed by Guo, Zhou, Li, & Chen (2016) was used to compute the bubble size distribution. The incorporation of PBM model in resulted in the production of bubbles due to wall effect and higher turbulence variations near the wall regions, which affects other interfacial forces, the holdup and velocity profiles. It was shown that the turbulent dissipation by internals affects the bubble coalescence and breakup thus affecting the bubble size distribution. Other works done with homogeneous and inhomogeneous population balance method (PBM) are given in Table 3.1.

The turbulence model is crucial to capturing the anisotropic nature of turbulence, which is significant at higher velocities and hydrodynamic properties of the bubble column. A review of the recent work on turbulence flow modelling was given by Pourtousi, Sahu, & Ganesan (2014). Mostly, the $k$-$\varepsilon$ models, RSM and LES have been used in literature (Deen et al., 2001; Dhotre et al., 2013; Ekambara et al., 2008; Marcela Kotsuka Silva et al., 2012; Tabib et al., 2008). While the $k$-$\varepsilon$ models requires lower computational resources, the assumption of isotropic flow limits the model where bubble induced turbulence and anisotropy of turbulence is significant. The RNG $k$-$\varepsilon$ model being able to show the swirling flows and broader scales of turbulence than the Standard or Realizable models has been the model of choice in the recent studies. Laborde-Boutet et al. (2009) found similar results by studying different $k$-$\varepsilon$ turbulence models and formulations examined in detail without the population balance model. The LES model was not used in this work for studying multiphase flow due to the high computational requirements. However, a better bubble break up model is desired. Ekambara et al. (2008) examined the population balance model and presented a detailed
study on Sauter mean bubble diameter, local fractional gas holdup, liquid velocity and turbulent parameters at six different heights in the column using RSM-PBM model where the gas inlet superficial velocity is of 2 cm/s. The assumption of same velocity for all bubble sizes in the homogeneous discrete model is the weakness of the model since it provided inaccurate prediction near the sparger and disengagement regions. Other than this limitation, the RSM – PBM model can effectively predict the characteristics of the flows studied. The mechanism of the bubble breakup is due to the turbulent fluctuations i.e. the kinetic energy and dynamics pressure of the eddy. Therefore, a detailed study in the stability of Sauter mean bubble size using the RNG k-ε and RSM was made.

3.2 Objectives of this study

In this work, the 2D transient simulations of the gas-liquid flow in homogeneous and churn-turbulent regime were carried out. Given the high number of simulations, 2D simulations were used during comparisons and model validations, and the selected model was used to perform 3D simulation for the range of velocity from homogeneous to heterogeneous regime. Various formulations of discrete model especially the inhomogeneous discrete models were used. The inlet boundary conditions for homogeneous and churn-turbulent regime were modified, and the results from these simulations were compared with experimental data from Bhole (2006) and Sanyal et al. (1999). The study was performed on the stability of mean bubble size profile along the column using different turbulence models with population balance model to understand the applicability of the model. A comparison of drag models available in literature with the approach used here was made. The proposed model was validated with the experimental data of Xue (2008). Finally, the hollow bubble column and bubble column with internals was simulated. The conversion of concentric type internal to a wall in 2D
with spaces was studied. The results were validated by experimental data from Jhawar & Prakash (2014). Further, the applicability of the proposed approach was shown by comparison with the hollow bubble column. The simulation with internals predicted similar flow patterns as seen experimentally under different superficial air inlet velocities. The comparison with hollow bubble column showed similar effects on bubble groups and liquid velocity due to the presence of internals as have been seen in other works.

3.3 Mathematical Model

3.3.1 Governing Equations

The primary goal of CFD is to capture the physical phenomenon observed. To capture the physics behind the phenomena occurring in bubble columns, a transient two-fluid Eulerian-Eulerian multiphase model is used to simulate the two-phase gas-liquid flow. The volume averaged Eulerian-Eulerian flow equations for continuity and momentum are solved individually for each phase. The governing equations for the multi-phase flow are given as:

Continuity equation for each phase,

$$\frac{\partial}{\partial t} \left( \alpha_k \rho_k \right) + \nabla \cdot \left( \alpha_k \rho_k \bar{u}_k \right) = 0 \quad k = l, g \quad (3.1)$$

Momentum conservation equation for each phase,

$$\frac{\partial \left( \rho_k \alpha_k \bar{U}_k \right)}{\partial t} + \nabla \cdot \left( \rho_k \alpha_k \bar{U}_k \bar{U}_k \right) = -\alpha_k \nabla p + \nabla \cdot \bar{\tau}_k + \rho_k \alpha_k \bar{g} + \sum_{p=1,k \neq p}^{M} \left( R_{pk} + m_{pk} \bar{U}_{pk} \bar{U}_{kp} \right) + (\bar{F}_{lift} + \bar{F}_{TD}) \quad k = l, g \quad (3.2)$$

$$\bar{\tau}_k = \alpha_k \mu_k \left( \nabla \bar{U}_k + \nabla \bar{U}_k^T \right) \alpha_k \left( \lambda_k - \frac{2}{3} \mu_k \right) \left( \nabla \bar{U}_k \bar{I} \right) \quad (3.3)$$
Table 3.1 Summary of previous work on bubble column modelling with PBM (Abbreviations in footnote)

<table>
<thead>
<tr>
<th>Investigators</th>
<th>Column Dimensions &amp; Static Liquid Height (m)</th>
<th>Superficial Inlet gas (U&lt;sub&gt;G&lt;/sub&gt;) &amp; liquid velocity, (m/s)</th>
<th>Interface Closure (D- Drag Force; L- Lift Force; WLF = Wall lubrication force TD = Turbulent Dispersion BIT = Bubble induced Turbulence)</th>
<th>PBM – Bubble Size Groups; Bubble Size Range (mm);</th>
<th>Turbulence Model</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>Krepper et al., (2005)</td>
<td>D&lt;sub&gt;c&lt;/sub&gt; = 0.195; H&lt;sub&gt;L&lt;/sub&gt; = 10.0</td>
<td>U&lt;sub&gt;G&lt;/sub&gt; = 0.0368, U&lt;sub&gt;L&lt;/sub&gt; = 1.017</td>
<td>D:Grace; T; L:TL; WLF: TWLF; TD: Burns; BIT: SBIT</td>
<td>ID-3(7+7+7); dB = 0.01–13;</td>
<td>k-ω SST</td>
<td>1. Reduced the coalescence rates for P&amp;B by 0.25 due to high coalescence levels. 2. Investigation of bubble breakup and coalescence models was suggested. 3. Use of experimental data at different flow conditions was recommended for validation of models.</td>
</tr>
<tr>
<td>Chen, Sanyal, &amp; Dudukovic, (2004)</td>
<td>D&lt;sub&gt;c&lt;/sub&gt; = 0.19, 0.44</td>
<td>U&lt;sub&gt;G&lt;/sub&gt; = 0.12, 0.10</td>
<td>D:SH</td>
<td>HD-1 (9: dB = 1–40, 16: dB = 1–32);</td>
<td>Modified k-ε</td>
<td>1. Bubble population balance equation is implemented using 2D axisymmetric simulations with 9 and 16 classes and 3D with 9 classes. 2. The model predicted coalescence rate was reported to be an order higher than breakup rate. Increased breakup rate by a factor of 10. 3. It was reasoned that the mismatch is due to the inability of k-ε model to provide realistic turbulent energy dissipation. 4. Single modal bubble size distribution was reported for all churn-turbulent flow.</td>
</tr>
<tr>
<td>Chen, Sanyal, et al., (2005)</td>
<td>D&lt;sub&gt;c&lt;/sub&gt; = 0.19, 0.14, 0.44; H&lt;sub&gt;L&lt;/sub&gt; = 1.04, 0.96, 0.98, 1.76</td>
<td>U&lt;sub&gt;G&lt;/sub&gt; = 0.02, 0.12, 0.096, 0.10</td>
<td>D:SH</td>
<td>HD-1(16): dB = 1 – 32 BK:L&amp;S; CK: P&amp;B</td>
<td>Modified k-ε</td>
<td>1. Compared the bubble coalescence and breakup model for different diameter column in bubbly and churn turbulent regime with 2D axisymmetric simulations. 2. Better agreement was reported with population balance model, especially in churn-turbulent regime than with mean diameter. 3. It was illustrated that the population balance model is not needed for bubbly flow regime.</td>
</tr>
<tr>
<td>Author(s)</td>
<td>$D_c$</td>
<td>$H_s$</td>
<td>$U_G$</td>
<td>Model</td>
<td>Notes</td>
<td></td>
</tr>
<tr>
<td>-----------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td>-------</td>
<td></td>
</tr>
<tr>
<td>Chen, Duduković, &amp; Sanyal, (2005)</td>
<td>0.162, 0.44; 1.04, 0.96, 0.98, 1.76</td>
<td>0.30, 0.10</td>
<td>HD-1(9: $d_b = 1 – 40$); BK: L&amp;S; CK: Luo</td>
<td>Modified k-ε</td>
<td>1. The bubble population balance equation is implemented with 3D simulations. 2. Underprediction of breakup rates was reasoned with the underprediction of $\varepsilon$, the energy dissipation rate from the k-ε model, and use of a better turbulence model was suggested.</td>
<td></td>
</tr>
<tr>
<td>Sanyal et al., (2005)</td>
<td>0.145</td>
<td>2</td>
<td>0.02, 0.1</td>
<td>HD-1(6, 12, 18, 24); BK: L&amp;S; CK: Luo</td>
<td>Standard k-ε</td>
<td>1. Classes (CM) and methods of moments (QMOM) methods were compared. 2. A comparison of using different number of classes for discrete model was done at $U_G = 0.02$ m/s showing that with 12 classes and higher, the results are independent of the resolution.</td>
</tr>
<tr>
<td>Ekambara et al., (2008)</td>
<td>0.150</td>
<td>0.9</td>
<td>0.02</td>
<td>HD-1(15: $d_b = 1 – 30$); BK: L&amp;S; CK: P&amp;B</td>
<td>Standard k-ε; RSM</td>
<td>1. Bubbly flow at $U_G = 0.02$ m/s was simulated with homogeneous discrete population balance and RSM turbulence model and compared with experimental data. 2. Model employing RSM and PBM model was reported to have better agreement with the experimental data.</td>
</tr>
<tr>
<td>Silva et al., (2012)</td>
<td>0.162</td>
<td>1.8</td>
<td>0.02, 0.08</td>
<td>HD-1 (3: $d_b = 1 – 5$; 5: $d_b = 1 – 6$; 10: $d_b = 1 – 9.6$); BK: L&amp;S; CK: P&amp;B</td>
<td>Standard k-ε; Reynolds Stress Model (RSM)</td>
<td>1. 3D simulations were performed for heterogeneous flow to study the interfacial forces, turbulence and boundary conditions. 2. 3, 5 and 10 bubble size groups were studied, and the results with 3 bubble sizes was reported to be sufficient to describe the flow. 3. Comparisons for different of drag models, turbulent dispersion models and turbulence models was made. 4. Combinations of drag model with turbulence and boundary conditions was also studied.</td>
</tr>
<tr>
<td>Silva, Mochi, Mori, &amp; D’Ávila, (2014)</td>
<td>0.145</td>
<td>0.7</td>
<td>0.03, 0.05, 0.07</td>
<td>HD-1 (3: $d_b = 1 – 5$); BK: L&amp;S; CK: P&amp;B</td>
<td>Standard k-ε; Reynolds Stress Model (RSM)</td>
<td>1. 3D simulations of laboratory bubble column operating in transition and heterogeneous regime was performed and liquid axial velocity was compared with the experimental results. 2. The drag model by (D. Z. Zhang &amp; VanderHeyden, 2002) was reported to perform better at higher velocities. 3. It was shown that anisotropic consideration of turbulence i.e. using RSM turbulence model instead of standard k-ε in the heterogeneous regime was more appropriate.</td>
</tr>
<tr>
<td>Bhole et al., (2008)</td>
<td>0.15; 0.9</td>
<td>0.02</td>
<td>D:(Tsuchiya, Furumoto, Fan, &amp; Zhang, 1997); HD-1(13); ID-ASM(13)</td>
<td>Standard k-ε</td>
<td>1. Axial liquid velocity, gas holdup, turbulent kinetic energy and bubble diameter were compared with 2D axisymmetric simulations.</td>
<td></td>
</tr>
</tbody>
</table>
Díaz et al., (2008)

<table>
<thead>
<tr>
<th>Height</th>
<th>Velocity</th>
<th>Drag Model</th>
<th>Lift Model</th>
<th>Constant Lift</th>
<th>Remarks</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.80x0.20x 0.04</td>
<td>$U_G = 0.02$ 0.0024; 0.0071; 0.0120; 0.0166;</td>
<td>HD: Homogeneous Discrete PBM model; ID: Inhomogeneous Discrete PBM model; L&amp;S: (Luo &amp; Svendsen, 1996) Breakup Model; P&amp;B: (Prince &amp; Blanch, 1990); Luo (Luo, 1993); SH: (Schiller &amp; Naumann, 1935) drag model; T: (Takamasa &amp; Tomiyama, 1999) drag model; IZ: (Ishii &amp; Zuber, 1979) drag law; ZV: (D. Z. Zhang &amp; VanderHeyden, 2002) drag law; TL: (Tomiyama, 1998) lift model; Burns: (Burns, Frank, Hamill, &amp; Shi, 2004) model, TWLF: (Tomiyama, 1998); LB: (Bertodano, 1991) model; Grace: (J. R. Grace, Waregi, &amp; Nguyen, 1976); SBIT: (Sato &amp; Sekoguchi, 1975); TH: (Trostko &amp; Hassan, 2001)</td>
<td>0.1</td>
<td>$d_b = 1 - 25$; BK: L&amp;S CK: Modified P&amp;B</td>
<td>3. Role of lift force with CFD-PBM in determining the radial profiles was studied. 4. A modification was made for the bubble coalescence rate to the model by (Prince &amp; Blanch, 1990).</td>
</tr>
</tbody>
</table>
Here, \( g \) is the acceleration due to the gravity, \( p \), the pressure shared by all phases, \( \bar{U}_{kp} \), the interphase velocity and \( \bar{t}_k \) is the Reynold Stress tensor significant for turbulent flows. \( \vec{F}_{liift} \) and \( \vec{F}_{td,q} \) are the non-drag interfacial forces acting between the two phases. \( R_{pk} \) is the interaction force between the phases

\[
R_{pk} = K_{pk} (\bar{U}_p - \bar{U}_k) \tag{3.4}
\]

where

\[
K_{pk} = \frac{3\alpha_g \alpha_l \rho_1}{4 d_g} C_D \left| (\bar{U}_g - \bar{U}_l) \right| \tag{3.5}
\]

\( K_{pk} \) is the drag momentum exchange coefficient and \( C_D \) is the single bubble drag coefficient between the phases.

### 3.3.2 Interfacial forces

The drag force arises due to the relative motion of the bubbles with respect to the surrounding liquid. It is the most significant interphase force. As the bubbles of different sizes affect the flow differently, an advantage of performing inhomogenous discrete model simulations is that the effect of the bubbles based on their size is incorporated. The Schiller Naumann drag force correlation (Schiller & Naumann, 1935) and Tomiyama drag force correlation (Takamasa & Tomiyama, 1999) are used for small and large bubble sizes respectively, and suitable drag laws are employed based on the bubble size. Table 3.2 lists all the drag models used in this work. The udf files for Zhang and Vanderheyden and Ishii and Zuber drag models are given in Appendix A.

The interaction among the dispersed and the continuous phases affects the interphase forces (e.g. drag force, lift force and added mass force) and turbulence in the column. Therefore, further work is done in this regards to correctly capture the physics behind.
Several models have been reported and reviewed in the literature (Díaz et al., 2008; Ekambara et al., 2008; Laborde-Boutet et al., 2009; Pourtousi et al., 2014; Rampure et al., 2007; Marcela Kotsuka Silva et al., 2012; Soccol et al., 2015; Tabib et al., 2008; Yamoah et al., 2015; D. Zhang et al., 2006). Further, the effect of addition of lateral forces including the lift and wall lubricating force is studied. In the churn-turbulent regime, the added mass was reported to have negligible effect on the flow dynamics, therefore it is neglected. These interfacial forces are functions of interfacial area. The interfacial area, $A_i$, for bubbly flows as a dispersed gas phase $g$ with volume fraction, $\alpha_g$, is given as:

$$a_i = \alpha_g A_g = \frac{6\alpha_g}{d_{b,s}}$$

(3.6)

where $d_{g,s}$ is the mean sauteur bubble diameter calculated by the discrete bubble size $d_{g,i}$ and fraction $f_i$ as:

$$d_{b,s} = \frac{1}{\Sigma f_i d_{b,i}}$$

(3.7)

The mean bubble diameter and the bubble size distribution are thus essential for correct prediction of the interfacial forces.

Table 3.2 Different drag model equations from literature

<table>
<thead>
<tr>
<th>Drag models</th>
<th>Drag models</th>
</tr>
</thead>
<tbody>
<tr>
<td>(Schiller &amp; Naumann., 1935)</td>
<td>$C_D = \begin{cases} \frac{24(1+0.15Re^{0.687})}{Re} &amp; \text{Re} \leq 1000 \ 0.44 &amp; \text{Re} &gt; 1000 \end{cases}$</td>
</tr>
<tr>
<td>(Takamasa &amp; Tomiyama, 1999)</td>
<td>$C_D = \max \left( \min \left( \frac{24}{Re} (1 + 0.15Re^{0.687}), \frac{72}{Re}, \frac{8}{3Eo+4} \right), \frac{8Eo}{3Eo+4} \right)$</td>
</tr>
<tr>
<td>(D. Z. Zhang &amp; VanderHeyden, 2002)</td>
<td>$C_D = 0.44 + \frac{24}{Re} + \frac{6}{1+\sqrt{Re}}$</td>
</tr>
</tbody>
</table>
(Ishii & Zuber, 1979)

\[
C_D = \begin{cases} 
  \text{Sphere} & \frac{24}{Re_m} \left(1 + 0.15 Re_m^{0.687}\right) \\
  \text{Ellipse} & \left(\frac{1+17.67 f(\alpha_g)^{3/7}}{18.67 f(\alpha_g)}\right)^{2/3} Eo^{1/2} \\
  \text{Cap} & \frac{8}{3} (1 - \alpha_g)^2 
\end{cases}
\]

where \( f(\alpha_g) = \frac{\mu_t}{\mu_m} \left(1 - \alpha_g\right)^{\frac{1}{2}} \);

\[
Re_m = \frac{\rho_l |\vec{U}_g - \vec{U}_l| d_g}{\mu_m},
\]

\[
\mu_m = (1 - \alpha_g)^{-2.5\mu_s} \text{ and } \mu_s = \frac{\mu_g + 0.4\mu_l}{\mu_g + \mu_l}
\]

\( C_D = C_D(\text{Sphere}) \) if \( C_D(\text{Sphere}) \geq C_D(\text{Ellipse}) \)

\( C_D = \min(C_D(\text{Ellipse}), C_D(\text{Cap})) \) if \( C_D(\text{Sphere}) < C_D(\text{Ellipse}) \)

Lift force is the lateral acting interfacial force. Two mechanisms are known for lift force. The Magnus force as a result of bubble’s rotations, and Saffman force as a result of the shear flow around the dispersed phase (bubbles). It depends on the slip velocity and curl of continuous phase velocity:

\[
\vec{F}_{\text{lift}} = -C_L \alpha_b \rho_l (\vec{U}_g - \vec{U}_l) x (\nabla \times \vec{U}_g)
\]  \( (3.9) \)

The Tomiyama lift force coefficient given by (Tomiyama, 1998) varies its sign from negative to positive with increase in size to emulate the physical phenomena of low sized bubbles moving away from the center and large sized bubbles moving towards the center of the column. This lift force is often used in the simulations by the different researchers Bhole et al. (2008), Duan et al. (2011), Ekambara et al. (2008), Guo & Chen, (2017), Gupta & Roy, (2013), Krepper et al. (2005), Silva et al. (2012) and Zhang et al. (2006). The lift force is calculated as a function of Eotvos number with a reversal in sign from particle distortion is given as:
\[ C_L = \begin{cases} 
\min[0.288 \tanh(0.121 Re_g), f(Eo')] & Eo' \leq 4 \\
 f(Eo') & 4 < Eo' \leq 10 \\
 -0.27 & 10 < Eo'
\end{cases} \] \quad (3.10)

Where,
\[ f(Eo') = 0.00105 Eo'^3 - 0.0159 Eo'^2 - 0.0204 Eo' + 0.474 \] \quad (3.11)

and \( Eo' \) is modified Eotvos number given as a function of the deformable bubble size, \( d_b \):

\[ Eo' = \frac{g(\rho_l - \rho_g)d_h^2}{\sigma} \] \quad (3.12)

\[ d_h = d_g(1 + 0.163 Eo^{0.757})^{1/3} \] \quad (3.13)

\[ Eo = \frac{g(\rho_l - \rho_g)d_g^2}{\sigma} \] \quad (3.14)

where \( \sigma \) the surface tension, \( g \) is gravity, and \( d_b \) is the bubble diameter. Gupta & Roy (2013) compared the Tomiyama’s lift force and reported overestimated liquid axial velocity profiles in the central region. Zhang et al. (2006) investigated two rectangular columns: short and tall, and concluded that Tomiyama’s lift force is suitable for tall columns. Bhole et al. (2008) compared Tomiyama’s lift force with \( C_L = 0.0 \) and \( C_L = 0.1 \) and found a radial separation of bubbles using Tomiyama’s lift model. All these studies reported a uniform profile for mean air volume fraction and mean axial liquid velocity if the lift force is included, which affects significantly the prediction of correct radial profiles.

The turbulent dispersion force takes into account for the interphase turbulent momentum transfer, which is a measure of the effect of continuous phase eddies on the dispersed phase (bubbles). The turbulent dispersion force used is given by Simonin and Viollet (1990) as a function of the drift velocity, \( \vec{v}_{dr} \). Here,
\[ \vec{v}_{dr} = -D_{gl} \left( \frac{\nu_{ag}}{a_g} - \frac{\nu_{al}}{a_l} \right) \] (3.15)

and

\[ D_{t,gl} = \frac{1}{3} k_{gl} \tau_{t,gl} \] (3.16)

where, \( D_{t,gl} \) is the fluid-particulate dispersion tensor. The turbulent dispersion force is given by

\[ F_{TD,l} = -F_{TD,g} = C_{TD} k_{gl} \left( \frac{\nu_{ap}}{a_p} - \frac{\nu_{ak}}{a_k} \right) \] (3.17)

Where \( k_{gl} \) is the turbulent kinetic energy of the liquid phase, and \( \nabla \alpha_g \) is the gradient of dispersed phase (gas-phase) volume fraction, while \( C_{TD} \) is a modifiable constant for the turbulent dispersion.

Tabib et al. (2008) found that the value of \( C_{TD} \) is significant at higher velocity using the Lopez de Bertodano turbulent dispersion model (Bertodano, 1991). Among the three values used for \( C_{TD} \), 0, 0.2 and 0.5, 0.2 was found to give the better results. Similarly, Silva et al. (2012) used \( C_{TD} \) of 0.1 and 0.2 with PBM model for bubble sizes and found a lower gas velocity with these values for turbulent dispersion. While Ekambara et al. (2008) reported the value of 0.5 for turbulent dispersion predicted good results.

Drawing on these studies, the value of turbulent dispersion in this study has been varied with inlet superficial velocity with 0.1 for homogeneous regime \( (u_g < 0.05 \text{ m/s}) \), 0.2 for transition regime to churn-turbulent regime \( (0.05 < u_g \text{ (m/s) } < 0.10) \) and 0.3 for higher velocities.

### 3.3.3 Turbulence Equations

Extensive study using the k-\( \varepsilon \) turbulence model for simulating a bubble column has been performed by Boutet et al. (2009). They compared three turbulence models, namely the standard, RNG and realizable k-\( \varepsilon \) turbulence models, with the three
multiphase formulations Dispersed, Dispersed + Bubble Induced Turbulence and Per-Phase. The $k-\varepsilon$ RNG model was found to outperform the other models since it is able to predict the swirling flows and broader scales of turbulence well. It was suggested to use the RNG $k-\varepsilon$ model with the implementation of bubble population balance as it is better able to model the turbulent dissipation rates and turbulent viscosity. Further, the addition of the bubble induced turbulence for lower velocities gave a better prediction for the turbulent quantities and was thus suggested for flows in churn-turbulent regime. Further, the $k-\varepsilon$ model was compared with the RSM model in the work of Tabib et al. (2008). They found the RSM model was able to predict the turbulent kinetic energy better than the $k-\varepsilon$ model due to its intrinsic ability in capturing anisotropic energy transfer mechanism. Since, the population balance models are dependent on the energy of eddies, this factor is investigated in this work. Therefore, two turbulence models have been used namely the $k-\varepsilon$ RNG model and RSM model with dispersed phase formulation. Further, bubble induced turbulence has been added since it is significant in the churn turbulent regime.

### 3.3.3.1 RNG $k-\varepsilon$ Turbulence Model

The closure relations for the Reynolds stress tensor are required for the renormalized group (RNG) $k-\varepsilon$ model(Yakhot et al., 2016).

The turbulent eddy viscosity is formulated as:

$$\mu_t = \rho_t C_\mu \frac{k^2}{\varepsilon} \tag{3.18}$$

The transport equations of the turbulent kinetic energy and turbulent dissipation rate for the liquid phase are given as:
\[
\frac{\partial}{\partial t} (\alpha_l \rho_l k) + \nabla \cdot (\alpha_l \rho_l U_l k) = \nabla \cdot \left( \alpha_l \left( \mu_l + \rho_l C_\mu \frac{k^2}{\varepsilon k} \right) \nabla k \right) + \\
\alpha_l \left( G_{k,l} + G_{k,g} \right) - \alpha_l \rho_l \varepsilon + \alpha_l \rho_l \Pi_{k,l}
\]

(3.19)

\[
\frac{\partial}{\partial t} (\alpha_l \rho_l k \varepsilon) + \nabla \cdot (\alpha_l \rho_l U_l \varepsilon) = \nabla \cdot \left( \alpha_l \left( \mu_l + \rho_l C_\mu \frac{k^2}{\varepsilon k} \right) \nabla \varepsilon \right) + \\
C_{1\varepsilon} \left( G_{k,l} + C_{3\varepsilon} G_{k,g} \right) \frac{\alpha_l \rho_l \varepsilon}{k} - C_{2\varepsilon} \frac{\alpha_l \rho_l \varepsilon^2}{k} + R_\varepsilon + \alpha_l \rho_l \Pi_{\varepsilon,l}
\]

(3.20)

where, \( R_\varepsilon \) is the strain rate specific to RNG (zero in the Standard and Realizable formulations). \( G_{k,l} \) and \( G_{k,g} \) are the turbulent kinetic energy generation due to viscous and buoyancy forces. \( \Pi_{k,l} \) and \( \Pi_{\varepsilon,l} \) are source terms for bubble induced turbulence (BIT). For gas superficial velocity in the range of churn turbulent regime, the gas turbulence affects the hydrodynamics significantly. In this work, the Troshko Hassan model (Troshko & Hassan, 2001) as suggested by Zhang et al. (2008) was used to model the bubble induced turbulence. For the dispersed phase turbulence model, it is defined as:

\[
\Pi_{k,l} = C_{ke} \sum_{p=1}^{M} \frac{K_{gl}}{\alpha_{l} \rho_l} \left| \overrightarrow{U}_g - \overrightarrow{U}_l \right|^2
\]

(3.21)

and

\[
\Pi_{\varepsilon,l} = C_{td} \frac{1}{\tau_l} \Pi_{k,l}
\]

(3.22)

Where the modifiable constants used in equations 18-22 are given in Table 3.3.

Table 3.3 List of constants and their values for the two turbulence models

| Constants | \( C_\mu \) | \( C_{1\varepsilon} \) | \( C_{2\varepsilon} \) | \( C_{3\varepsilon} \) | \( \sigma_k \) | \( \sigma_\varepsilon \) | \( C_{ke} \) | \( C_{td} \) |
### 3.3.3.2 RSM Turbulence Model

The Reynolds stress terms are individually calculated through the differential transport equations, abandoning the isotropy of eddy-viscosity assumption. Hence, solving additional five transport equations. The exact form of transport equations for the transport of Reynolds stresses, $\rho_l u'_i u'_j$, is as follows:

$$\frac{\partial}{\partial t} (\rho_l u'_i u'_j) + C_{ij} = -D_{T,ij} + D_{L,ij} - P_{ij} + \varphi_{ij} - \varepsilon_{ij} - F_{ij} \quad (3.23)$$

where, $C_{ij}$ is the convection term, and $D_{T,ij}$, $D_{L,ij}$, $P_{ij}$, $\varphi_{ij}$, $\varepsilon_{ij}$ are respectively terms for turbulent diffusion, molecular diffusion, stress production, pressure strain, dissipation terms given as:

$$C_{ij} = \frac{\partial}{\partial x_k} (\rho_l u_k u'_i u'_j) \quad (3.24)$$

$$D_{T,ij} = \frac{\partial}{\partial x_k} \left[ \rho_l u'_i u'_j u'_k + p' (\delta_{kj} u'_i + \delta_{ik} u'_j) \right] \quad (3.25)$$

$$P_{ij} = \rho_l \left( u'_i u_k \frac{\partial u'_j}{\partial x_k} + u'_j u_k \frac{\partial u'_i}{\partial x_k} \right) \quad (3.26)$$

$$\varphi_{ij} = p' \left( \frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \quad (3.27)$$

$$\varepsilon_{ij} = 2\mu_L \frac{\partial u'_i}{\partial x_k} \frac{\partial u'_j}{\partial x_k} \quad (3.28)$$

RSM accounts for the effects of various turbulent phenomena in a more rigorous manner than the two-equation model therefore, it produces more accurate predictions for complex flows.
3.3.4 Population Balance model

The population balance model is employed to model the coalescence and breakup rates for different bubble sizes and it takes the kinetic energy dissipation rate and calculates the bubble size distribution, which is used in calculation of interphase forces. However, the homogeneous discrete population balance model assumes equal velocity for all bubble size groups to reduce the computation cost. This allows for only one gas phase momentum equations as in the case of single bubble size model. However, this simplification is against the experimentally observed phenomenon. Instead two bubble populations have been observed and reported for churn turbulent flow in literatures (Jhawar & Prakash, 2014; R. Krishna, Urseanu, van Baten, & Ellenberger, 1999; R. Krishna & Van Baten, 2001). Earlier, the three-bubble population with coalescence and breakup using the population balance approach based on the work of Marcela et al., (2012) was used and it was found to give good agreement even with homogenous discrete method developed by Hounslow, Ryall, & Marshall (1988). Further improving the model, 12 bubble sizes were used for a distribution of bubble as 12 bins in the range of 1 mm to 35 mm bubble sizes. However, the results showed lower centerline water velocity as compared to the experimental values. This was attributed to the assumption of equal velocity for all bin sizes. To further enhance the model, in this work we have assumed N (N>1) bubble phase each having a different velocity. This approach is based on the inhomogeneous discrete population balance model used by Krepper et al. (2005). Each bubble phase is sub-divided into M groups representing M bubble classes. This allows for individual velocity for each bubble phase with a distribution of bubble size. Therefore, the inhomogeneous approach is used here to model the bubble flow in the churn turbulent regime.
The population balance model is employed to model the coalescence and breakup rates for different bubble size. The population balance equation can be written as (Kumar & Ramkrishna, 1996):

$$\frac{\partial n(v, t)}{\partial t} + \nabla \cdot (U_g n(v, t)) = B_b + B_c - D_b - D_c$$  \hspace{1cm} (3.29)

where, the left hand side are time variation and convection terms while on the right hand side, $B_b, B_c, D_b, D_c$ are, respectively, the production and death rates due to coalescence and breakup as given in Table 3.4. Equation (3.29) is an integrodifferential equation, which is a proposed approach by Kumar & Ramkrishna (1996) has been widely used in literature.

The pivot size method developed divides the bubble sizes into a number of intervals, each with a pivot size $x_i$ and equation (3.29) is integrated over each interval and redistributed for each size $x_i$.

Table 3.4 Population balance aggregation and breakage kernels

<table>
<thead>
<tr>
<th>Phenomena</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Birth due to coalescence</td>
<td>$B_c = 0.5 \int_0^v c(v - v', v)n(v - v')n(v')dv''$ (3.29a)</td>
</tr>
<tr>
<td>Death due to coalescence</td>
<td>$D_c = \int_0^\infty c(v, v')n(v)n(v')dv''$ (3.29b)</td>
</tr>
<tr>
<td>Birth due to breakup</td>
<td>$B_b = \int_v^\infty b(v')\beta(v, v')n(v')dv'$ (3.29c)</td>
</tr>
<tr>
<td>Death due to breakup</td>
<td>$D_b = b(v)n(v)$ (3.29d)</td>
</tr>
</tbody>
</table>

Thus, the number density of the $i^{th}$ class $n_i$ is then related to the gas hold-up, $\alpha_g$ by

$$n_i v_i = \alpha_g f_i$$  \hspace{1cm} (3.30)

where $f_i$ represents the volume fraction of the bubbles of group $i$ and $v_i$ is the corresponding volume of bubble of group $i$. The bubble coalescence $c(v, v')$, bubble
breakup $b(v)$ and the daughter size distribution $\beta(v, v')$ terms in Table 3.4 are calculated from the coalescence and breakup kernels described below.

3.3.4.1 Breakup Model

The breakup model given by (Luo & Svendsen, 1996) which accounts for the binary breakup of bubbles from turbulent fluctuation and collision is used for predicting the bubble breakup. This model calculates breakup with turbulent fluctuation and collision among the four mechanisms – viscous shear stress; shearing-off process; interfacial instability; since compared to turbulent fluctuation, the influence of the other mechanisms in a turbulent flow is usually neglected. Lashers et al. (2002) and Liao et al. (Liao & Lucas, 2009) have reviewed in detail the turbulent characteristics required for breakup. Luo & Svendsen (1996) breakup model is a theoretical model based on the kinetic gas theory for drop and bubble breakup in turbulent flows. The bubbles size distribution model depends on the turbulent kinetic energy of the hitting eddy greater than a critical value. This critical value corresponds to the increase in the surface energy before and after breakup is different from the model by Prince & Blanch (1990) bubble breakup model. This model shows the required characteristics of a suitable bubble breakup model as suggested by Wang (2003) and further compared in Wang (2011). These characteristics include local nonzero minimum probability at the center, for equal sized daughter bubbles, since more energy is required for equal-sized breakup than unequal sized breakup. Furthermore, the breakup is a result of the capillary pressure of the mother bubble and the turbulence kinetic energy of the eddy. Therefore, the daughter bubble size distribution is dependent on the diameter of the mother bubble and the turbulent kinetic energy. For the case of binary breakup, $f_{BV}$ is given as the dimensionless fraction describing the daughter bubbles is defined as
\[ f_{BV} = \frac{v_i}{v} = \frac{d_i^3}{d^3} = \frac{d_i^3}{d_i^3 + d_j^3} \]  

(3.31)

where \( d_i \) and \( d_j \) are diameters of daughter bubbles on binary breakage of parent bubble of volume \( v \) and diameter \( d \). \( f_{BV} \) lies between 0 and 1, with 0.5 for equal binary breakage and 0 and 1 for no breakage of the parent bubble.

The breakup rate of bubbles of size \( v_i \) or \( d_i \) into particles sizes of \( v_i f_{BV} \) and \( v_i (1 - f_{BV}) \) is expressed as

\[
\Omega(v_i; v_i f_{BV}) = 0.923(1 - \alpha_g)n_i \left( \frac{\varepsilon}{d_i^2} \right)^{\frac{1}{2}} \int_{\xi_{min}}^{1} \frac{(1+\xi)^{\frac{5}{2}}}{\xi^{\frac{11}{2}}} \exp \left( -\frac{12c_f \sigma}{2 \rho \varepsilon^{\frac{3}{2}} d_i^5} \right) d\xi
\]

(3.32)

where \( \xi = \frac{\lambda}{d_i} \) is the size ratio between the eddy and a particle in the inertial subrange and \( c_f \) is the increase coefficient of surface area given by

\[
c_f = \left[ f_{BV}^2 + (1 - f_{BV})^2 - 1 \right] \quad (3.32b)
\]

The total breakage rate of particle of size \( v_i \) or \( d_i \) for death/birth rate of group \( i \) bubbles is then expressed as:

\[
b(v_i) = \frac{1}{2} \int_{0}^{1} \Omega(v_i; v_i f_{BV}) d f_{BV}
\]

(3.33)

while the daughter bubble fraction for birth due to breakup is expressed as:

\[
\beta(v_i) = \frac{\Omega(v_i; v_i f_{BV})}{b(v_i)}
\]

(3.34)

The model provides the “partial” breakage frequency to derive the daughter size distribution \( \beta \) directly. However, the model is dependent on the discretization of bubble size, and has no limits on the lower breakup bubble fraction (Wang et al., 2003). The daughter bubble size distribution is a “U-shaped” curve with the minimum at the center depicting the lowest probability of equal bubble distribution.
The rate defining factor for breakup is thus derived from the bubble-eddy collision frequency and kinetic energy of the eddy (Kumar & Ramkrishna, 1996), which is obtained using the turbulence model. Therefore, in order to suitably model the breakup rate, the choice of turbulence model is vital. Also, the factors affecting the energy dissipation rates also affect the bubble breakup and hence the gas holdup rates. Among others, the presence of internals and thus ensuing tunneling effect from their presence plays a major role in energy dissipation among eddies and therefore the bubble size distribution in the column.

3.3.4.2 Coalescence Model

Binary bubble coalescence in a turbulent flow is a three-step process. First the bubbles collide trapping a small amount of liquid between them. This liquid then drains out until the liquid film separating the bubbles reaches a critical thickness, at which point the film ruptures resulting in coalescence. Here, coalescence happens only when two bubbles collide and keep in contact for a time. Thus the process can be analyzed as a function of collision frequency ($\omega_c$) and the probability ($P_c$) of collision resulting in coalescence. This is expressed for coalescence between bubbles $i$ and $j$, with diameters $d_i$ and $d_j$ as a closure for equation (3.29 a, b) as (Luo, 1993):

$$c(d_i, d_j) = \omega_c(d_i, d_j)P_c(d_i, d_j)$$  \hspace{1cm} (3.35)

While the coalescence frequency is a function of bubble number density and flow structure of the liquid phase, the coalescence efficiency depends on the forces acting between the colliding bubbles.

Three mechanisms for bubble coalescence have proposed by Prince & Blanch, (1990). These are, due to turbulent eddies, different rise velocities and shear stress. However, the model used in this study only accounts for the coalescence due to turbulent eddies.
The mean bubble approaching velocity is calculated through the velocity of turbulent eddies of same size. This is because the small eddies having low energy are unable to cause bubble motion, while the larger eddies have no effect on the motion of bubbles. Turbulent collisions of bubbles occur due to the random motion of these turbulent eddies. For an assumption of isotropic turbulence, for bubbles in the inertial subrange of turbulence, the fluctuating bubble velocity, $u_{g,i}$ for bubble diameter, $d_i$ is expressed as:

$$u_{g,i} = 1.414\varepsilon^{1/3}d_i^{1/3} \quad (3.36)$$

where $\varepsilon$ is the turbulent energy dissipation rate in liquid. Thus for statistically independent velocities, the bubble mean approaching velocity is given as RMS velocity of the two bubbles of diameter $d_i$ and $d_j$ with equation (3.35) as:

$$u_{g,ij} = (u_{g,i}^2 + u_{g,j}^2) = 1.414\varepsilon^{1/3}(1 + \zeta_{ij}^{-2/3})^{1/2} \quad (3.37)$$

where $\zeta_{ij} = \frac{d_i}{d_j}$. Thus the collision frequency is expressed as:

$$\omega_c = \frac{\pi}{4}(d_i + d_j)^2u_{g,ij} \quad (3.38)$$

As the bubbles collide, the coalescence occurs if the interaction time, $t_i$, of the bubbles exceeds the coalescence time, $t_c$, required for the drainage of the liquid film between the bubbles to critical rupture thickness. Thus, the coalescence probability is given as a function of their ratio, $t_c/t_i$, with the coalescence probability tending to zero for large values of the ratio and unity for a low values. This is thus expressed as:

$$P_c = exp\left(-\frac{t_c}{t_i}\right) \quad (3.39)$$

The values of $t_c$ is given by Chesters (1991) for partial-fully mobile interfaces as:
\[ t_c = 0.5 \frac{\rho_{g,ij} d_i^2}{(1+\zeta_{ij})^2 \sigma} \]  

(3.40)

while \( t_I \) for two equal and unequal sized fluid particles given by Luo (1993) as:

\[ t_I = (1 + \zeta_{ij}) \sqrt{\frac{\rho_g (\rho_i + 0.5)}{3(1+\zeta_{ij})^2(1+\zeta_{ij}^3)}} \frac{\rho_i d_i^3}{\sigma} \]  

(3.41)

Substituting equations 39 and 40 in equation 38, the coalescence probability can be expressed as:

\[ P_c = \exp \left\{ \frac{0.75(1+\zeta_{ij}^2)(1+\zeta_{ij}^3)}{(\rho_g/\rho_i + 0.5)^{1/2}(1+\zeta_{ij})^3} We_{ij}^{1/2} \right\} \]  

(3.42)

where \( We_{ij} \), the Weber number is defined as

\[ We_{ij} = \frac{\rho_i d_i u_{g,ij}^2}{\sigma} \]  

(3.43)

The assumption of significant coalescence frequency through only the turbulent eddies, leads to a lower predicted rate of coalescence at higher superficial velocities where the collisions due to other mechanisms of different bubble rise and shear forces become significant, especially with different bubble rise velocities and bubble size.

### 3.4 Numerical Method

The simulations were carried using the commercial CFD software package ANSYS – Fluent of version 16.0. A pressure based finite volume method was used to solve the discretized equations. Air-water system was used for the simulations at ambient temperature and pressure was simulated. Table 3.5 shows the numerical models and parameters used in this work for all of the simulations as well as the boundary conditions. The settings for turbulent quantities is still an open problem due to lack of experimental data and complexity of multiphase flow. In the present work, based on the its application in literature, the default parameter of unity for turbulent kinetic...
energy and dissipation at inlet was used. The numerical methods have been kept consistent throughout this work as given in Table 3.5.

The Green-Gauss Cell based method was used to calculate scalar gradients. Gupta & Roy (2013) found that all discretization schemes including QUICK, MUSCL and 2nd order upwind were of comparable accuracy with minimum numerical diffusion. Laborde-Boutet et al., (2009) compared the first order upwind, second order upwind and third order MUSCL schemes. For the simulations in this work, the QUICK scheme was used to solve the momentum and volume fraction equations while the second order upward scheme was used for turbulence terms and bin fractions to ensure lower numerical diffusion. The convergence was assumed for residuals below $10^{-3}$ for each time step or a maximum number of iterations of 200 for the case of no-convergence. The simulation was assumed to reach a pseudo-steady state at 20 seconds after which the simulations results were averaged for 200 seconds. Furthermore, a step wise increase in time step was implemented. The simulations were performed on SHARCNET server employing multi-processors with 8 cores and 8 GB RAM. The geometry and operating conditions for various simulations performed are given in Table 3.6. The grid sizes used are also listed in Table 3.6, which are based on the previous works in the literatures, except for the Case JH (both 2D and 3D), where the grid independent test was conducted in this work.

Table 3.5 Numerical model used in the present work

<table>
<thead>
<tr>
<th>Scheme</th>
<th>Phase Coupled SIMPLE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temporal Discretization</td>
<td>Bounded Second Order Implicit</td>
</tr>
<tr>
<td>Volume Fraction Formulation</td>
<td>Implicit</td>
</tr>
<tr>
<td>Spatial Discretization: Gradient</td>
<td>Green-Gauss Cell Based</td>
</tr>
<tr>
<td>Spatial Discretization: Momentum</td>
<td>QUICK</td>
</tr>
<tr>
<td>Spatial Discretization: Volume Fraction</td>
<td>QUICK</td>
</tr>
<tr>
<td>Spatial Discretization: Turbulent Terms</td>
<td>Second Order Upwind</td>
</tr>
<tr>
<td>---------------------------------------</td>
<td>---------------------</td>
</tr>
<tr>
<td>Spatial Discretization: Reynolds Stress (In case of RSM)</td>
<td>Second Order Upwind</td>
</tr>
<tr>
<td>Spatial Discretization: Air Bin Fractions (PBM)</td>
<td>Second Order Upwind</td>
</tr>
<tr>
<td>Time Step</td>
<td>(0.0001 \times 500 + 0.0005 \times 100 + 0.001) (220 Seconds)</td>
</tr>
<tr>
<td>Quasi-Steady State</td>
<td>20 seconds (20500 time steps)</td>
</tr>
<tr>
<td>Averaging</td>
<td>&gt;200 seconds (200,000 time steps)</td>
</tr>
<tr>
<td>Under-Relaxation Factors</td>
<td>Pressure: 0.3; Momentum: 0.4, Volume Fraction: 0.4, Turbulence Terms: 0.8; Air Bin Fractions: 0.5</td>
</tr>
<tr>
<td>Boundary Conditions: Inlet</td>
<td>Velocity specified Population balance variables specified for mom-dispersed bubbles of 5 mm at the inlet Turbulent kinetic energy specified as unity Turbulent kinetic energy dissipation specified as unity</td>
</tr>
<tr>
<td>Outlet</td>
<td>Outflow</td>
</tr>
<tr>
<td>Walls (Column and internal walls)</td>
<td>No-slip</td>
</tr>
<tr>
<td>Static liquid height</td>
<td>1.4 m (Case JH, Case 15T)</td>
</tr>
<tr>
<td>Setup for homogeneous discrete model</td>
<td>2PH</td>
</tr>
<tr>
<td>Number of Bins</td>
<td>12</td>
</tr>
<tr>
<td>Geometric ratio exponent</td>
<td>1.4 (ratio consecutive bubble diameters)</td>
</tr>
<tr>
<td>Bubble Diameter range</td>
<td>1 mm – 35 mm</td>
</tr>
<tr>
<td>Setup for Inhomogeneous Discrete model</td>
<td>3PIH, 4PIH</td>
</tr>
<tr>
<td>Number of secondary phases</td>
<td>2 (3PIH), 3 (4PIH)</td>
</tr>
<tr>
<td>Number of bins per phase</td>
<td>(6+7), (4+3+4)</td>
</tr>
<tr>
<td>Bin diameters and ratio</td>
<td>Same as that for homogeneous discrete model</td>
</tr>
</tbody>
</table>

### 3.5 Results and Discussions

In the present work, the numerical simulations of the gas-liquid two-phase flow in a bubble column were carried out using the discrete bubble population balance method with one bubble phase, i.e. one bubble size at the inlet (homogenous) and two and three bubble phases, i.e. two and three bubble sizes at the inlet (inhomogeneous), which are
abbreviated as 2PH, 3PIH and 4PIH, respectively. The numerical results were compared with the experimental data for homogeneous flow regime (Bhole et al., 2006) at $U_g = 2 \text{ cm/s}$ and churn-turbulent regime (Sanyal et al., 1999) with $U_g = 12 \text{ cm/s}$ to examine the accuracy of these models in the churn turbulent regime. Furthermore, the simulations were also conducted using different turbulence models and drag correlations and the results were compared with the experimental data to investigate the accuracy of those models. The result from the RSM turbulence model was compared with that from the RNG $k-\varepsilon$ model to study the effect of those two models on the bubble size distribution and the liquid axial velocity. The result using the Ishii-Zuber drag correlation was compared with that using the approach to model the drag of individual bubble phases. In the drag correlation for modeling individual bubble phases, The Schiller-Naumann drag correlation was used for small bubbles and Tomiyama drag correlation was used for larger bubble with different sizes. The structure of the simulations performed to select the most accurate model is shown in Figure 1. The most accurate model was then used for Case JH, which has a range of superficial inlet gas velocities from 0.02 m/s to 0.147 m/s. The radial profiles were validated against experimental data from Xue et al., (2008) for radial profiles of gas volume fraction and velocity. Furthermore, a 3D simulation is carried out and the results are compared with the experimental data from the work of Rampure et al. (2007) and with the results from 2D simulations for the range of velocities from bubbly to churn turbulent regimes. The results are then compared to those for the hollow bubble column to study the effect of internals on hydrodynamics along the column. The evolution of the bubble size class with velocity is studied for three velocities at 0.042 m/s, 0.097 m/s and 0.147 m/s. Table 6 lists the various experimental data taken from literatures, which are used to validate the numerical results.
### Table 3.6 Experimental data used to validate the numerical results

<table>
<thead>
<tr>
<th>Investigators</th>
<th>Object for selection</th>
<th>Superficial Velocity (m/s)</th>
<th>Dimensions</th>
<th>Technique</th>
<th>Experimental values Used for comparison</th>
<th>Grid size used</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Case B</strong></td>
<td>(Bhole et al., 2006)</td>
<td>$U_g = 0.02$ m/s</td>
<td>Diameter: 0.15 m</td>
<td>Laser Doppler Anemometry</td>
<td>Radial profiles at Z = 2, 3 and 4: Bubble Diameter (m)</td>
<td>(Bhole et al., 2008) $\Delta r = 0.0025$ m $\Delta z = 0.006$ m</td>
</tr>
<tr>
<td></td>
<td>Coalescence and breakup equilibrium and bubble size distribution</td>
<td>Static liquid height: 0.9 m</td>
<td></td>
<td></td>
<td>Gas Holdup</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Laser Doppler Anemometry</td>
<td></td>
<td></td>
<td>Axial Liquid Velocity (m/s)</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Laser Doppler Anemometry</td>
<td></td>
<td></td>
<td>Turbulent Kinetic Energy ($m^2/s^2$)</td>
<td></td>
</tr>
<tr>
<td><strong>Case S</strong></td>
<td>(Sanyal et al., 1999)</td>
<td>$U_g = 0.12$ m/s</td>
<td>Diameter 0.19 m</td>
<td>Computed Tomography (CT) for gas holdup and liquid axial velocity using CARPT</td>
<td>Radial Profiles at 0.53 m: Gas Holdup Axial Liquid Velocity (m/s) Turbulent Kinetic Energy ($m^2/s^2$)</td>
<td>(Sanyal et al., 1999) $\Delta r = 0.005$ m $\Delta z = 0.006667$ m</td>
</tr>
<tr>
<td></td>
<td>Significance of interfacial forces in churn turbulent regime.</td>
<td>Static liquid height: 1.0 m</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Laser Doppler Anemometry</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Case X</strong></td>
<td>(Xue et al., 2008)</td>
<td>$U_g = 0.02$, 0.08 and 0.14 m/s</td>
<td>Diameter = 0.1626 m</td>
<td>Gas holdup and mean bubble velocity using Four-Point Optical probe</td>
<td>Radial Profiles at $z/D = 5$: Gas Holdup Axial Liquid Velocity (m/s)</td>
<td>Compared with simulations at $U_g = 0.02$, 0.097 and 0.147 m/s for the Case JH</td>
</tr>
<tr>
<td></td>
<td>Test of the model for a series of gas inlet velocities ranging from homogeneous to churn turbulent regime.</td>
<td>Dynamic liquid height: 1.8 m</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Laser Doppler Anemometry</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Case JH</strong></td>
<td>(Jhawar &amp; Prakash, 2011)</td>
<td>$U_g = 0.042$ to 0.147 m/s</td>
<td>Diameter 0.15 m</td>
<td>Gas Holdup: Pair of pressure transducers Liquid Velocity: Micro-foil heat flux sensor</td>
<td>Overall Gas Holdup Centerline Liquid Velocity ($r/R=0$) (m/s)</td>
<td>Grid Test performed $\Delta r = 0.005$ m $\Delta z = 0.006667$ m Tested (0.005 m – 0.007575 m)</td>
</tr>
<tr>
<td></td>
<td>Validate the selected model for a range of velocities</td>
<td>Static liquid height: 1.4 m</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Figure 3.1 Flow of simulations performed (abbreviations taken from the Table 3.1)
Table 3.7 List of bubble sizes for PBM model

(a)

<table>
<thead>
<tr>
<th>Bin Number</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Size (m)</td>
<td>0.001</td>
<td>0.00138</td>
<td>0.00191</td>
<td>0.00264</td>
<td>0.00364</td>
<td>0.00504</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bin Number</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
<th>11</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Size (m)</td>
<td>0.00696</td>
<td>0.00962</td>
<td>0.0133</td>
<td>0.01838</td>
<td>0.02539</td>
<td>0.03509</td>
</tr>
</tbody>
</table>

(b)

<table>
<thead>
<tr>
<th>Bin (Phase 1)</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Size (m)</td>
<td>0.001</td>
<td>0.00138</td>
<td>0.00191</td>
<td>0.00264</td>
<td>0.00364</td>
<td>0.00504</td>
<td>0.00696</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bin (Phase 2)</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Size (m)</td>
<td>0.007</td>
<td>0.00967</td>
<td>0.01336</td>
<td>0.01847</td>
<td>0.02552</td>
<td>0.03528</td>
</tr>
</tbody>
</table>

(c)

<table>
<thead>
<tr>
<th>Bin (Phase 1)</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Size (m)</td>
<td>0.001</td>
<td>0.00138</td>
<td>0.00191</td>
<td>0.00264</td>
<td>0.00364</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bin (Phase 2)</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Size (m)</td>
<td>0.0037</td>
<td>0.00511</td>
<td>0.00706</td>
<td>0.00976</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Bin (Phase 3)</th>
<th>0</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bubble Size (m)</td>
<td>0.01</td>
<td>0.0138</td>
<td>0.01909</td>
<td>0.02639</td>
<td>0.03647</td>
</tr>
</tbody>
</table>

The interfacial interactions of various bubble sizes, when divided into separate velocity groups, have been found to be different, i.e. the interaction in the bubbly regime is very different from that in the churn-turbulent regime. Thus, it is vital to understand these underlying interactions in order to model such flows accurately. A set of simulations using the homogeneous discrete model and the inhomogeneous discrete model with two and three bubble phases are performed in order to understand the bubble distribution in both homogeneous and churn turbulent regimes as well as the number of velocity groups.
required to correctly model these flows. Furthermore, to study the significance of the turbulence model used, simulations with both RNG k-\(\varepsilon\) and RSM turbulence model have been used in the two-velocity group model. Case B02 is for homogeneous regime with the inlet gas superficial velocity of 0.02 m/s and Case S12 is for the churn turbulent regime with the gas superficial inlet velocity of 0.12 m/s. The inlet bubble size is defined as 5 mm and no other interfacial force than drag force is implemented unless otherwise mentioned. Table 3.7 gives the list of bubble sizes used in the simulations. The geometric ratio exponent of 1.4 is used to calculate the successive bubble sizes. Since there was no clear directive in literatures for the division of bubble sizes among each phase for the distribution of gas superficial velocity at the inlet, a gas inlet size of 5 mm is used. This will be modified later based on the observations from this test and the data from literatures for similar cases.

Two bubble phases are selected based on the studies on the bimodal bubble size in churn turbulent regime by Krishna et al. (1999) and Jhawar & Prakash (2014). At the inlet, different volume fractions for small and large bubble phase were used based on the work of Krishna et al. (1999). The major application of this approach is for gas superficial inlet velocities in churn turbulent regime (\(U_G>0.045\) m/s). Based on the model of Krishna & Ellenberger, (1996), it is assumed that in the churn turbulent regime the share of superficial gas velocity as small bubbles is limited to that at \(U_{\text{trans}} = 0.034\) m/s, regarded as the transition point. Based on this assumption the fraction of gas flow going in as small bubbles was calculated as \(U_{\text{trans}} / U_G\) while the large bubbles constitute a fraction \((U_G-U_{\text{trans}}) / U_G\) at the inlet. This is used as the modified inlet boundary condition (3PIHM) for flow in churn turbulent regime while the original inlet condition of only 5 mm diameter is maintained for bubbly flow. The volume fractions of small and large bubbles at the inlet used in the two-
bubble phase model are given in Table 3.8 for the different cases simulated in this work. The Case S12 with inhomogeneous discrete model with two bubble phases was simulated using this modified inlet formulation (3PIHM). The inlet gas superficial velocity is limited to the small bubble phase as per the assumption from Krishna et al. (1999).

Table 3.8 Division of gas inlet volume fractions of two-bubble phases at the inlet for different cases

<table>
<thead>
<tr>
<th>Case/Geometry + U_G</th>
<th>Small Bubble Fraction</th>
<th>Large Bubble Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case S-12</td>
<td>0.2833</td>
<td>0.7166</td>
</tr>
<tr>
<td>Case JH11-097</td>
<td>0.3505</td>
<td>0.6495</td>
</tr>
<tr>
<td>Case JH11-147</td>
<td>0.2313</td>
<td>0.7687</td>
</tr>
<tr>
<td>Case JH11-198</td>
<td>0.1717</td>
<td>0.8282</td>
</tr>
</tbody>
</table>

For the bubbly flow regime, a comparable bubble size distribution was predicted with both homogeneous and inhomogeneous discrete PBM's. Therefore, either of the three models were found suitable to simulate the bubbly flow regime. However, due to lower complexity and computational time, discrete single bubble phase model will be used to simulate bubbly flow. Figure 3.2 shows the evolution of mean bubble diameter along the centerline (r/R=0) for the case of churn-turbulent regime i.e. “Case S12”. The mean bubble diameter should ideally increase till the coalescence and breakup reaches an equilibrium, and the mean bubble size becomes constant. The ability of the model to predict this phenomena of equilibrium with constant bubble size is used as the selection criteria. The model with discrete homogenous (2PH) PBM is sufficient at low velocity, however in churn turbulent regime, it predicts an unstable growth of bubble size along the column height. Therefore, it is rejected for simulations in churn-turbulent flow regime. The other three models i.e.,
3PIH, 3PIHM and 4PH show a considerably stable profile and represent the stability in bubble growth with increase in column height. To further select the most accurate model, the mean and maximum bubble size from experimental work of Xue at al. (2008) is plotted as straight lines. The profiles closest to mean bubble size and within the limits of maximum bubble size represents the phenomena most accurately. The models with two bubble phases (3PIH and 3PIHM) lie within these limits. The model with modified inlet (3PIHM) is comparatively closer to the experimental mean bubble size while that with three velocity groups (4PIH) predicts a higher average bubble size than the maximum bubble size.

Figure 3.3 shows the distribution of number fraction of different bubble sizes in the gas phase for “Case B02” and “Case S12”. All the models simulated for “Case B02” give a good description of bubble size distribution with high fraction of small sized bubbles. In the distribution for “Case S12”, the number of large sized bubbles is higher in the churn-turbulent regime in comparison with those in bubbly flow regime as predicted by the models. This is due to enhanced coalescence observed in this flow regime. Figure 3.3 (c) compares the bubble number density with the inhomogeneous models (3PIH, 3PIHM and 4PH) for “Case S12” in churn-turbulent regime with the bubble number density predicted by inhomogeneous (3PIH) model for “Case B02” in bubbly flow regime. As observed in Figure 3.3 (b), at higher velocity, the bubble size distribution shifts towards higher bubble sizes. The size distribution for “Case 12” using 3PIH and 4PIH models show a decrease in small bubbles. A higher fraction of large bubbles should physically accompany an increase in smaller sized bubbles formed as a result of higher bubble breakups with increase in turbulence. This is most accurately shown by 3PIHM model. It can be argued that this is because, a higher inlet fraction of large bubbles, allows higher breakup rates producing
much higher number of smaller bubbles. The profile shows a much higher number of bubbles in the column for “Case S12” in comparison to that in “Case B02” as can be expected with rise of inlet superficial gas velocity. Thus, the 3PIHM model with modified inlet gives a more accurate description of bubble size fraction and number density in comparison to the other models.

Based on the above discussions, the discrete homogenous model with single bubble inlet is sufficient for homogenous regimes with RSM turbulence model while a modified inlet two-bubble phase PBM model with RSM turbulence model was found more accurate for simulating churn-turbulent regimes.

Furthermore, the air volume fraction and axial liquid velocity for using different models discussed earlier are compared with the experimental data in Figure 3.4 (a) and (b). The 2PH model with discrete homogeneous model i.e. one velocity group also shows gives comparable accuracy a better agreement with the experimental data than other models for Case B03, which is in the homogenous regime. In the homogeneous regime, the flow is mostly influenced by small bubbles, which have similar almost uniform velocities, while that of the effect of large bubbles on the flow is insignificant.
Figure 3.2 Instantaneous bubble diameter along the centerline at $U_g = 0.12$ m/s (Case S12)

(a) Bubble size distribution in the column at $U_g = 0.02$ m/s (for Case B02)
(b) Bubble size distribution in the column at \( U_g = 0.12 \) m/s (for Case S12)

(c) Comparison of bubble size distributions in the column at \( U_g = 0.12 \) m/s and \( U_g = 0.02 \) m/s (for Case B02 and Case S12)

Figure 3.3 Comparison of the bubble size distributions using different models
Hence, the assumption of equal uniform velocity with used in the homogenous discrete PBM model holds is reasonable for flow in the homogeneous regime. So, the 2PH model give better result than those from two and three bubble phase models as shown in Figure 3.4(a). The profiles with two and three gas velocity groups lack in comparison. The axial liquid velocity profiles predicted by the RNG model for 2PH, 3PIH and 4PIH have a similar trend, but, the one predicted by the RSM model (3PIH_RSM) is different from other three as shown in Figure 3.4 (b). Figure 3.4 (b) also shows that the numerical results from the homogeneous discrete model (2PH) and inhomogeneous discrete model with three bubble velocity groups (4PH) agree better with the experimental data than those from the two-bubble velocity groups model (3PIH). Due to the lower computational cost of the homogeneous discrete PBM model (2PH) and the better accuracy in predicting the axial gas volume fraction, 2PH model will be used to simulate flows in the bubbly flow regime.

The distributions of the axial liquid velocity and gas volume fraction using the models with the modified inlet boundary condition (3PIHM) and without the modified inlet boundary condition (2PH, 3PIH and 4PIH) are compared with the experimental data as shown in the Figures 3.5. It can be seen that the difference of the axial velocities predicted by different models is big at the centerline of the column. The two-bubble phase model without the modified inlet boundary condition (3PIH) gives the best result for the axial liquid velocity distribution compared with the experimental data as shown in Figure 5 (b). The two-bubble phase model with the modified inlet boundary condition (3PIHM) slightly over-predicts the axial liquid velocity in the centerline region, but, it gives a much better prediction for the axial volume fraction distribution than other three models without the modified inlet boundary condition (2PH, 3PIH and 4PIH) as shown in Figure 5 (a). The discrete
homogenous model (2PH) gives much higher gas volume fraction and much lower axial liquid velocity compared with the experimental data. So, it is the least accurate model compared with the other three inhomogeneous models for the flow in the churn-turbulent regime. This is because the influence of large bubbles, which play a significant role for the flow in the churn turbulent regime, is taken into account in the inhomogeneous model. Also, the modified boundary condition represents the physical phenomena at the inlet more accurately. So, it can predict the high central peak profile for the gas volume fraction while other three models without using the modified inlet boundary condition give flatter profiles for the air volume fraction as seen in Figure 3.5(a).

Therefore, the modified inlet boundary condition for flows in the churn- turbulent regime was will be adopted in the subsequent simulations. Also, the RSM turbulence model, which predicts a more stable bubble size distribution, will be included used instead of RNG k-ε turbulence model.

![Figure 3.5(a)](image)

(a) Time averaged radial profiles of the air volume fraction at z/D = 3 at U_g = 0.02 m/s (for Case B02)
(b) Time averaged radial profiles of the axial liquid velocity at $z/D = 3$ at $U_g = 0.02$ m/s
(for Case B02)

Figure 3.4 Comparison of the predicted time averaged radial profiles of air volume fraction and liquid velocity using different models with the experimental data from Bhole et al. (2008)

(a) Time averaged radial profiles of the air volume fraction at $z = 0.53$ m at $U_g = 0.12$ m/s
(for Case S12)
(b) Time averaged radial profiles of the axial liquid velocity at \( z = 0.53 \) m at \( U_g = 0.12 \) m/s (for Case S12)

Figure 3.5 Comparison of the predicted time averaged radial profiles of air volume fraction and axial liquid velocity using different models with the experimental data from Sanyal et al. (1999) at \( U_g = 0.12 \) m/s

The most significant interfacial force in a bubble column is the drag force. Several correlations have been proposed for modelling the drag force in gas-liquid flows (Díaz et al., 2008; Gupta & Roy, 2013; Marcela Kotsuka Silva et al., 2012; Tabib et al., 2008; Yamoah et al., 2015; D. Zhang et al., 2006). However, most of those correlations are for flows in the homogeneous regime or with only one bubble size. Therefore, to develop accurate models to simulate the flows in both the homogeneous and churn-turbulent regimes, different drag correlations listed in Table 3.2 will be tested in this study based on the experimental data from Case S12. Tabib et al. (2008) tested the four drag correlations listed in Table 3.2 using one bubble size. In this work, the simulations were performed using these models with multiple bubble sizes for flows in both bubbly and churn-turbulent regimes.
regimes. Furthermore, a combination of Schiller Naumann (Schiller & Naumann, 1935) and Tomiyama (Takamasa & Tomiyama, 1999) drag correlations was used to simulate the flow with spherical bubbles in which the small diameter bubbles were modeled using the Schiller-Naumann drag correlation (Schiller & Naumann, 1935) while different sized large diameter bubbles were modeled using the Tomiyama drag correlation (Takamasa & Tomiyama, 1999). So, in this approach, small bubbles were modeled by the drag correlation for uniform bubble size (Schiller-Naumann correlation) and large bubbles were modeled by the drag correlation considering bubble size difference (Tomiyama correlation).

Since Figure 3.4 shows that the 2PH model is the best for Case B02, which is in the homogenous regime, compared with the inhomogeneous models, 2PH model with Tomiyama drag correlation will be used for flows in homogeneous regime.

For heterogeneous flows, the simulations were performed using different drag correlations and inhomogeneous two-bubble phase model with modified inlet boundary condition with RSM turbulence model (3PIHM-RSM). Figures 3.6 (a) and (b) shows the comparison of the gas holdup and axial liquid velocity distributions for Case S12 using various drag correlations with lift force. Among other models, the Ishii-Zuber (IZ) gives the best agreement with the experimental data. However, with lift force, it over-predicts the axial liquid velocity. The combination of Schiller-Naumann and Tomiyama drag correlation (SNT) without lift force give results comparable with experimental data (average less than 5%), but it over-predicts the axial liquid velocity if the lift force is included for Case S12. However, this model predicted the most accurate results in comparison with experimental
results. Hence, this model will be included as the part of the model to calculate interfacial forces for the rest of the simulations.

In addition, the turbulent dispersion model given by Simonin & Viollet (1990) was incorporated with a $C_{TD}$ of 0.3 for churn turbulent regime and 0.2 for homogeneous regime was added to the model. This model is used to in the later sections to simulate flow in bubbly and churn-turbulent regime in the bubble column.

(a) Time averaged radial profiles of air volume fraction at $z = 53$ cm at $U_g = 0.12$ m/s (for Case S12)
(b) Time averaged radial profiles of liquid axial velocity at $z = 53$ cm at $U_g = 0.12$ m/s
(for Case S12)

Figure 3.6 Comparison of the time averaged radial profiles of gas volume fraction and axial liquid velocity using different drag correlations with experimental results from Sanyal et al. (1999) at $U_g = 0.12$ m/s

Another set of the experimental data for a range of inlet superficial velocities in the churn-turbulent regime from Jhawar & Prakash (2011) were selected to validate the numerical results from using the proposed model. The geometry and operating conditions of the hollow bubble column from Jhawar & Prakash (2011) are given in Table 3.6. A grid independence test was performed for the case of hollow bubble column from Jhawar et al., (2011) (Case JH). Two grid sizes were used for the grid independent tests. The coarse grid mesh has the grid size of 5 mm in the horizontal direction and 7.575 mm in the vertical direction, and the dense one has the grid size of 5 mm in the horizontal direction and 6.667 mm in the vertical direction. The number of cells are 11250 and 10170 for the dense and coarse grids, respectively. The simulations were conducted for 220 seconds and the
predicted axial liquid velocity and gas holdup distributions using both grids as shown in the Figure 3.7. It can be seen the difference between the results from those two grids is very small. Therefore, the dense grid, which is shown in Figure 3.8 (a) was chosen to perform further simulations.

(a) Gas Volume Fraction

(ii) Axial liquid velocity
Figure 3.7 Grid independent test: Time averaged radial profiles of air volume fraction and axial liquid velocity

(a) 2D Mesh (Dense mesh)

(b) 3D mesh (iii) Longitudinal View

Figure 3.8 Mesh
The bubble column with geometry from Jhawar & Prakash (2011) i.e. “Case JH” was simulated at air superficial inlet velocities 0.020 m/s, 0.042 m/s, 0.097 m/s and 0.147 m/s. The results from these simulations were compared to the experimental data from Xue et al. (2008) for $U_g = 0.02$, 0.08 and 0.14 m/s. The comparison for gas volume fraction and gas phase velocity is shown in Figure 3.9. It is observed that the predicted results for gas volume fraction and gas velocity profile is comparably accurate in bubbly and churn turbulent regime. However, there is some deviation when using the 3PIHM model in transition regime at 0.97 m/s.

Based on these results, it can be concluded that the variation in model based on the initial study proves accurate for both the regime, however, further work is required for developing a similar understanding of flow and bubble distribution in transition regime.

(a) Gas volume fraction
Further, application of the model on a 3D geometry for the geometry from Jhawar et al. (2011) similar to “Case JH” was performed. Two mesh with 72760 and 91200 cells as shown in Figure 3.8 (b) were simulated to perform grid independence test for gas volume fraction with only drag force as the interfacial force. Further, the 3D geometry was simulated with the above defined model for gas inlet superficial velocities of 0.042 m/s, 0.097 m/s and 0.147 m/s. Figure 3.10 shows the comparison between the results from 2D and 3D geometries. The 3D geometry predicted similar results as 2D geometry for flow in bubbly regime, while slightly higher results were predicted for flow in churn turbulent
regimes in the core region. Hence, the model was found to give more accurate results with 3D geometry for gas volume fraction and can be used to simulate other geometries with both 2D and 3D geometries.

Figure 3.10 Comparison between gas volume fraction results from 2D and 3D geometry from Jhawar et al (2011) (for case JH).

3.6 Conclusions

Developed a CFD model suitable for simulating multiphase gas liquid flow in the bubble column for a range of velocities from homogeneous to churn turbulent regime. Bubble population model has been incorporated in its modified form to capture effects of bubble breakup and coalescence in different flow regimes. The inhomogeneous population balance model with 2 and 3 bubble phases (phases) was compared with discrete model for both homogeneous and heterogeneous regime. Stable rate of breakup and coalescence was
observed on using RSM turbulence model which is better able to capture the anisotropic
nature of the flow than RNG k-ε model. Discrete homogeneous method was found to be
comparable with homogeneous regime, however, its accuracy in heterogeneous was lower
than the inhomogeneous methods. Further, work regarding application of the method to a
range of velocities from homogeneous to churn turbulent regime was developed based on
series of experimental observations in literature. This was seen to increase the accuracy of
the predicted results. Four drag models from literature were compared to evaluate the
accuracy, other than Schiller-Naumann, which is made for small spherical shaped bubbles
only, other models gave similar predictions. Different models were selected to model the
drag for small and large bubbles. Finally, the selected model was used to simulate a 2D
and 3D geometry of hollow bubble column for a range of velocities. The results with both
the 2D and 3D geometries were in good agreement with the experimental results at similar
operating conditions from literature studies.
References


Dhotre, M. T., Deen, N. G., Niceno, B., Khan, Z., & Joshi, J. B. (2013). Large eddy


Chapter 4

Numerical Studies on Effects of Geometrical Parameters of Internals on Bubble Column Hydrodynamics

4.1 Introduction

Bubble column reactors find applications in chemical and biochemical industries as gas-liquid and gas-liquid-solid contactors for its advantages of simple design and construction, high mixing effects, mass and heat transfer, and low maintenance costs. Many industrial applications include exothermic reactions that require heat removal for maintaining equilibrium. To facilitate heat exchange in such cases longitudinal tube bundle type internals inserted directly into the reactor provide a practical means for heat removal eliminating the need for external heat exchangers and pumps. Based on their geometry, configuration and density, the presence of these internals affect the hydrodynamics of the column, thus varying the performance of the reactors. Majorly two such internal configurations have been studied in relation to bubble column with internals, i.e. for the methanol synthesis and Fischer Tropsch (FT) synthesis with 5 and 25% of cross sectional area covered by the internals (Krishna et al., 2000; Youssef et al., 2009).

The gas holdup, flow pattern, interfacial area and bubble distribution are essential parameters to study the performance of a bubble column reactor. While these factors accentuate the performance other factors including liquid back-mixing and slug-flow formations are counter-productive. The understanding of effects of various geometrical modifications on the above factors thus becomes essential in designing internals.
Some studies on the influence of internals reported that the overall gas holdup increased with increase in CSA (Berg et al. 1994; Möller et al., 2018; Pradhan, Parichha, & De, 1993; Jhawar et al., 2014; Yamashita, 1987; Youssef et al., 2009). However, further studies with superficial inlet gas velocity based on free and total CSA revealed that the increase in overall gas holdup is majorly due to a decrease in area for bubble flow (Al Mesfer et al., 2018).

It has been shown that local gas holdup profile is strongly affected by configuration and occluded CSA of the internals. At higher densities (22%), the local gas holdup profiles were found to have peaks at the center with lower gas holdup near the walls. Youssef & Al-Dahhan (2009) and Youssef et al. (2013) studied effect of increase of occluded CSA from 5% to 20% and reported an increase in gas holdup profiles and interfacial area with occluded CSA. Kagumba et al., (2015) studied effect of different tube diameters (12.7 and 25.4 mm) covering 25% CSA with the superficial inlet gas velocity based on free CSA and found a slight increase in local gas holdup profiles with both configurations. Further, they reported a higher interfacial area with lower sized tubes. Based on their results, they reasoned the increase in gas holdup profiles to a higher bubble breakup resulting in an increased number of bubbles (Jasim, 2016; Kagumba et al., 2015; Youssef, 2010). However, it was not clarified if the observed effects were due to change in tube-to-tube distance or the density of internals in the column. Al-Mesfer et al. (2016a) and Sultan et al. (2018) compared the gas holdup profiles for 25 % CSA with that of hollow bubble column and found only a slight increase in the gas holdup peak in the presence of internals with superficial inlet gas velocity based on free CSA. However, the internal configuration used by the authors did not include a circular configuration with an empty core area.
Jasim (2016) studied the circular and hexagonal configurations and found that the circular arrangements showed a significant increase in gas holdup in the core region in churn turbulent regime. Further, an increase in bubble chord length and bubble velocity with a lower interfacial area was reported for the circular configuration with an empty core area while the presence of hexagonal internal arrangement showed a decrease in bubble chord length. Jhawar et al. (2014) reported an increase in overall gas holdup with a concentric tube bundle. These effects were attributed to an enhanced coalescence resulting in large bubbles in the core region as reported by Youssef et al. (2013). However, the complete reasoning of increase in gas holdup and bubble chord length at the core region has not been discussed. Further, the influence of tube-to-tube distance on gas phase distribution has not been studied in literature.

Bernemann, 1989 found the liquid axial velocity was higher in the presence of internals for all gas inlet velocities while the liquid phase flow profile was maintained. He also reported an increase in liquid recirculation with internals as well as a higher axial liquid velocity at the center. The values reported were higher for column with no tubes in the central region as compared to one with a distributed arrangement. He reasoned that this was due to the geometry of internals and their effect in bubble rising motion. Chen et al. (1999) studied the effect of internals covering 5% CSA in a 0.44 m diameter column with a viscous Drake oil-air system on gas holdup, liquid recirculation, turbulent stresses and eddy diffusivities. Lower turbulent stresses and eddy diffusivities in radial direction were reported in the presence of internals owing to the reduction in turbulence length scales. However, no significant effect on liquid axial velocity and gas holdup was found at low occluded CSA of 5%. Forret et al. (2003) reported an increase in axial liquid velocity at
the core while the radial profile remains the same. Also, an enhanced large scale recirculation in a large column with internals was observed, due to lower liquid velocity fluctuations with internals in agreement with observations of (J. Chen et al., 1999). George et al. (2017) and Jhawar et al. (2014) studied the liquid velocity profile with a circular tube bundle and found an enhanced liquid centerline velocity with the presence of concentric bundle of internals with 15 tubes due to the funneling effect of this type of geometry. Further, they observed alterations in flow pattern and a reduced backmixing when a baffle type internal was included above the distributor region. The effect of varying the number of tubes (and tube-to-tube distance) or the height of internals from gas distributor was not investigated in their work.

Al Mesfer et al., (2017) reported an increase in the liquid centerline velocity in the presence of internals using Radioactive Particle Tracking technique to study the liquid velocity field in a bubble column of 0.14 m diameter with dense internals covering 25% CSA. Further, they reported a sharp decrease turbulent parameters including normal and shear liquid stresses, eddy diffusivity and liquid turbulent kinetic energy profiles. With the same experimental method, Kalaga et al. (2017) studied the effect of internals in a 0.12 m diameter bubble column with internals covering 0-11.7% over a wide range of superficial inlet air velocities (1.4-26.4 cm/s). They reported a significant effect of internals on liquid axial velocities in the presence of internals with increased fluctuations in axial direction.

The studies point to an overall reduction in radial fluctuations and turbulence parameters with an increase in liquid recirculation with symmetrical internals. However, a systematic study of the effects of tube-to-tube distance and its significance in internal design has not been performed. Knowledge of the underlying effects of varying tube-to-tube distance on
the column hydrodynamics and flow field will assist in elucidating the effects of other geometrical variations like tube size, and configuration which are essentially varying the tube-to-tube distance. In this perspective, Computational Fluid Dynamic (CFD) simulations have been used to gain an understanding of the complex two-phase flow through studying flow patterns, momentum transfer and turbulence parameters. While a number of experimental studies have been performed on bubble columns with internals, these studies are limited by the experimental setup and technique used. On the other hand, through CFD simulations, a complete set of detailed effects can be studied for varying geometries and operating conditions. Further, a detailed understanding can be drawn from the results to devise the mechanism of these effects to develop a more optimized reactor design.

In literature, a few authors have studied the effects of internals in a bubble column using CFD simulations. Guan et al. (2017) studied the importance of including interfacial forces in simulating flow in bubble column. They reported that, while using lateral forces for may be optional for the simulating flow in hollow bubble columns, they are required in the presence of internals to accurately predict flow characteristics. In literature, Laborde-Boutet et al. (2010) and Larachi et al. (2006) have used a constant bubble size without any lateral forces in their model and found a decrease in liquid fluctuations and turbulence in the presence of internals. Laborde-Boutet et al. (2010) reported an increase in gas volume fraction near the internal walls. Guan et al. (2014) studied the influence of internals on single bubble flow using VOF simulations. They found a longitudinal increase in bubble shape as a result of lateral stress due to the presence of internals. They related this to increase in gas phase velocity for small and large bubbles. Guo et al. (2017) simulated a
two-fluid PBM model to study the effect of three arrangement of internals. They reported a higher liquid velocity and gas holdup in regions away from the internal walls. While Larachi et al. (2006) studied different configurations of internal geometry and Guo et al. (2017) studied effect of different size internals, the effect of tube-to-tube distance on liquid flow field, air volume fraction and bubble size distribution has not been investigated. Hence, in this work, we have systematically studied the effect of tube-to-tube distance using a two-fluid model with population balance.

The longitudinal variation in the internal positions from the gas distributor is expected to affect the liquid flow pattern and bubble size distribution in the column. The height of internal from the gas distributor defines the type of interaction between internals and the flow field. When the internals are placed close to gas distributor in the distributor region, it is expected to guide the flow pattern. This type of interaction is expected to give a uniform axial profile for gas volume fraction and liquid axial velocity. However, if it is placed at a higher height from the gas distributor, the interactions occur after the flow is already developed, and the internals act as restriction or disturbance to the flow field. This can lead to a higher turbulence dissipation close to the lower tip of internal causing higher bubble breakup giving a non-uniform axial profile for gas holdup and liquid axial velocity. To understand these effects, we have studied the effect of internals positioned at heights of 2D, 3.33D and 4.66D. The objective was to study the effect on gas holdup and liquid flow pattern as the internals positioned at different heights from the distributor region.

Additionally, the effect of the total height of the internal in the column has been studied. Decreasing the height of internal to below dynamic liquid height allows for lower
restrictions in near top of flow region. This has been investigated to observe the effect on flow pattern and gas holdup.

4.2 Numerical Method

A CFD model for flow regimes from the bubbly to churn turbulent regimes was developed and validated in previous work (chapter 3). In this work, the studies were carried out to investigate the effect of three geometrical parameters of the circular tube bundle type internals used in a bubble column on the hydrodynamics of the column. The three geometrical parameters are 1) the tube-to-tube gap, 2) the height of internals from the distributor and 3) the total vertical height of the internal. The objective was to optimize the configuration of the internals.

Air-water system was used for the simulations at ambient temperature and pressure was simulated. The convergence was assumed for residuals below $10^{-3}$ for each time step or a maximum number of iterations of 200 for the case of no-convergence with a time step of 0.001. The simulation was assumed to reach a pseudo-steady state at 20 seconds after which the simulations results were averaged for 200 seconds.

4.3 Results and Discussions

The simulation was first conducted for the bubble column with a diameter of 15 cm, height of 2.5 m and the concentric tube bundle internal with 15 tubes of diameter 0.0095 m, which was the same as that used in the experimental work of George et al. (2017) and Jhawar and Prakash (2014). The configuration of the column was shown in Figure 4.1. The case for the column with 15 tube internals was referred as Case 15T and the case for the hollow bubble column without the internals was named as Case JH, and the experimental data for
both cases are from Jhawar et al. (2014). The 2D geometry was used in the simulations. The geometry of internals was represented by replacing the position of internals on the central plane of 3D geometry with two perforated internal walls with the size of perforation holes equal to the tube-to-tube space (0.0044 m). Furthermore, the fraction of the internal wall was made equal to the fraction of the total free surface area available in the 3D tube-bundle geometry (31%). The calculations of the fraction and number of perforations for Case 15T is given in Appendix B. The height of the vertical internal walls was kept equal to that of the internals (1.5 m) spanning from 0.5 m to 2 m in the column and the distance of the internal walls from center is given by the radius of the tube-bundle (0.03385 m). Figure 4.2 (b) shows the dimensions of the converted parameters for Case 15T. The 2D simulations were carried out, instead of 3D simulations, to reduce the computational cost and the 2D simulations results were validated by the experimental data.

A grid independence test and model validation for Case JH has been presented in the previous work (Chapter 3). The simulations for both Cases 15T and Case JH were conducted with the same inlet superficial gas velocity in the range of 0.02 m/s to 0.147 m/s to cover from the bubbly regime to the churn turbulent regime. The results for the predicted overall gas volume fraction and centerline liquid axial velocity were validated with the experimental results from Jhawar et al. (2014) as shown in Figure 4.3. The predicted centerline axial liquid velocity at z/D =5 was compared with the experimental data. The overall gas holdup is the average of the gas volume fraction in the column from z=0.5 m – 1.4 m height. This method gives more consistent results in calculating the average gas volume fraction than extrapolating the dynamic height as mentioned by McKeen & Pugsley (2003) and Peirano, Delloume, & Leckner (2001). It is because the mean pressure
or volume fraction used to extrapolate the final bed height does not have a linear profile near the surface of the bed. The numerical results were in good agreement with the experimental data over the velocity range with a slight difference in the transition regime at $U_G = 0.097$ m/s. A slight difference was observed in the case of bubble column with internals for the gas holdup profiles. This is because Jhawar & Prakash (2014) considered the total surface area while calculating the inlet superficial velocity, while the area for flow was 10.75%
lower due to the CSA covered by the internals. The numerical results shows the increase in the axial liquid velocity for the column with internals as observed in experiments. However, there was no significant difference between the predicted gas holdup for the columns with and without internals.

(a) Case 12T with tube-to-tube spacing of 8.2 mm

(b) Case 15T with tube-to-tube spacing of 4.4 mm
(c) Case 18T with tube-to-tube distance of 2.3 mm.

(d) Columns with different internal heights from the gas distributor

Figure 4.2 Geometries of different tube-to-tube spacing and height of the internal from the gas distributor
At position $z/D = 4$ (0.6 m), the effect of the internal was clearly seen as peaks and troughs in the overall gas fraction. However, it can be observed that the overall gas holdup remains the same for columns with and without internals.

(a) Overall gas holdup

(b) Centerline liquid axial velocity at $z/D = 5$
Figure 4.3 Comparison between the numerical results and the experimental data from Jhawar et al. (2014) of the time averaged overall gas holdup and centerline liquid axial velocity (for Cases JH and 15T).

The effect of this type of internals (15 tubes) on the gas holdup and hydrodynamics can be seen by comparing with the flow field in the hollow bubble column. The dimensions and grid resolutions Cases 15T and JH are given in Table 4.1.

Table 4.1 Dimensions and grid resolutions for each case used in the simulations

<table>
<thead>
<tr>
<th>Case (Figure)</th>
<th>Internal Geometry</th>
<th>Tube-to-tube Space (mm)</th>
<th>Fraction of total empty surface area</th>
<th>Maximum grid distances/Mesh cells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case JH</td>
<td>Hollow (Jhawar et al., 2011)</td>
<td>-</td>
<td>-</td>
<td>Grid Test performed for $\Delta r = 0.005$ m $\Delta z = 0.006667$ m Tested ($\Delta z = 6.67–7.5$ mm) Cells: 11250</td>
</tr>
<tr>
<td>Case 15T (Figures 4.1 and 4.2 (b))</td>
<td>Concentric bundle of 15 Tubes (Jhawar et al., 2014)</td>
<td>4.4</td>
<td>0.31</td>
<td>Maximum Values $\Delta r = 0.005$ m $\Delta z = 0.006667$ m Cells: 15360</td>
</tr>
<tr>
<td>Case 12T (Figure 4.2 (a))</td>
<td>Concentric bundle of 12 Tubes</td>
<td>8.2</td>
<td>0.46</td>
<td>Maximum Values $\Delta r = 0.005$ m $\Delta z = 0.006667$ m Cells: 16736</td>
</tr>
<tr>
<td>Case 18T (Figure 4.2 (a))</td>
<td>Concentric bundle of 18 Tubes</td>
<td>2.3</td>
<td>0.19</td>
<td>Maximum Values $\Delta r = 0.005$ m $\Delta z = 0.006667$ m Cells: 17056</td>
</tr>
</tbody>
</table>
Figure 4.4 shows a comparison of the radial profiles of the gas volume fraction at velocities $U_g = 0.042 \text{ m/s}$, $0.097 \text{ m/s}$ and $0.0147 \text{ m/s}$ at $z/D = 4$ ($0.6 \text{ m}$) for the columns with and without internals. The effect of internals was clearly seen as a sudden increase and decrease in the gas volume fraction, which has been observed in both experimental and CFD studies in literatures (Guo & Chen, 2017; Jhawar & Prakash, 2014; Kagumba & Al-Dahhan, 2015; Youssef & Al-Dahhan, 2009; Youssef et al., 2013). Further, the variation in gas volume fraction as contributions from the bubble phases used was studied. The volume fraction profiles of the small bubbles ($\leq 7 \text{ mm}$) and large bubbles at $U_g=0.042 \text{ m/s}$ and $0.147 \text{ m/s}$ are presented in Figures 4.5.

Figure 4.4 Comparison of the time averaged radial profiles of the gas holdup with the inlet gas velocity for the columns with and without internals based on setup from Jhawar et al. (2014) (Cases 15T and JH)
Similar to Figure 4.4, the distributions of the small and large bubble volume fractions are different for columns with and without internals. The profile of the gas volume fraction in the column internals has several peaks and troughs due to the presence of the internals. The small bubble fraction increases near the internal walls. This is attributed to a higher turbulent energy dissipation near the wall regions and hence higher breakup phenomena occurring near the wall. The large bubble fraction, however, has a peak at the center of core and the annular regions. While the large bubbles breakup into smaller bubbles near the walls, they get entrained in the liquid flow with a higher velocity (upward and downward flow in core and annular region), resulting in a higher holdup in the center of these regions.

(a) Small bubbles fraction
(b) Large bubbles fraction

Figure 4.5 Comparison of the time averaged radial distributions of small and large gas bubble fractions for the columns with and without internals (Cases JH and 15T) at $z/D = 4$ for $U_g = 0.042$ m/s and $U_g = 0.147$ m/s

Figure 4.6 shows the liquid axial velocity contour lines and vectors for Cases JH and 15T in the bubbly and churn-turbulent regimes. It was clear that the liquid velocities in both upward and downward flow in the bubble column with internals are higher than those in the column without internals. This is due to the funneling effect due to the presence of internals which enhances the recirculation resulting in an increased axial liquid velocity. Also, this leads to a higher number of contours, i.e. a steeper change in the axial velocity in the presence of internals. In the figure, the regions with very small velocity vectors ascertain to a velocity of zero. It was observed that the position where the flow change the direction was different in the presence of internals compared with that without internals. In the case with the internals, the core region becomes smaller, resulting in a higher number
of small scale circulations in the annular regions. The scale and number of these circulations increases with the increase in the inlet gas velocity. These results are similar to that observed for symmetrically arranged internals by Al Mesfer et al. (2017) based on the free CSA. Similar flow patterns due to the internals were also observed from the simulations at low and high superficial inlet gas velocities, which were observed experimentally by George et al. (2017) for the same geometry.

More detailed comparison has been made in this work for the axial and radial fluctuations in the liquid velocity, turbulent kinetic energy and turbulent Reynolds number. Here, the turbulent Reynolds number is a non-dimensional quantity defined as the Reynolds number at the energy containing scale \( (k)^{3/2} \). It is given as

\[
Re_y = \frac{\rho d_{wall}^3}{\mu_{lam}} \sqrt{k}
\]  

(4.1)

where \( k \) is the turbulent kinetic energy, \( d_{wall} \) the distance from nearest wall, and \( \mu_{lam} \) is the laminar viscosity. Hence, a better understanding of the effect of internals on turbulence in a bubble column can be obtained. The time averaged liquid velocity fluctuations and instantaneous turbulent parameters were compared for Cases JH and 15T. The plots at \( z/D = 5 \) for the liquid RMSE velocities in the axial and radial directions are shown in the Figure 4.7. A sharp reduction in the radial RMSE velocity in the presence of the internals implying a lower radial fluctuations and dispersion was observed. Whereas the axial liquid RMSE velocity distribution showed an increase in the region near the internal walls.

The turbulent parameters including the turbulent kinetic energy and turbulent Reynolds number are shown in Figure 4.8. The profiles for both the parameters show a reduction in the presence of internals. The decrease in turbulent kinetic energy and turbulent Reynolds
number was attributed to a lower length scale available for eddy formation. This results in the observed reduction in radial fluctuations in liquid velocity. Similar effects due to presence of internals have been observed in literature (Al Mesfer et al., 2017; Chen et al., 1999; George et al., 2017; Kalaga et al., 2017; Larachi et al., 2006). The contour plots for these profiles are given in Appendix B. Using 2D simulations in this work, were able to represent the experimentally observed trends from literature.

This validated their applicability in studying the effects of internals on flow pattern and gas holdup in a bubble column with internals. The methodology applied for “Case 15T” was further implemented for a case with 12 tubes and a case with 18 tubes with tube-to-tube space of 8.2 mm and 2.3 mm respectively to study the effect of variation in tube-to-tube distance on bubble column hydrodynamics.

The study was also carried out for different geometrical parameters of the internals. The perforation sizes of 2.3 mm and 8.2 mm corresponding to the open surface area of 54% and 81%, the 12-tube bundle internal and 18-tube bundle internal, respectively, were used.

The dimensions for these two cases, named as Case 12T and Case 18T, are given in Figure 4.2 (a) and (c), respectively, and the grid information is given in Table 4.1. The geometries with three different tube-to-tube distances were simulated at superficial inlet gas velocity, $U_g = 0.042, 0.097$ and $0.147$ m/s to study the effects in both bubbly and churn-turbulent regime. Figures 4.9 and 4.10 show the variation in the gas volume fraction and liquid axial velocity at $z/D = 5$, for the three configurations at superficial inlet gas velocity of 0.042 and $0.147$ m/s.

A slight variation between the profiles for gas volume fraction was observed in the bubbly flow regime implying no variation in gas holdup in bubbly flow regime in the core region.
A small increase in gas volume fraction in the annular region was observed for “Case 18T” as the low tube-to-tube space inhibits the radial movement of the bubbles. In the churn-turbulent regime, an increase in gas volume fraction was observed for the “Case 12T”. Due to low restrictions, more liquid flows radially in, towards the core of the column. This movement creates a low-pressure region in the core region, creating a pull for gas phase resulting in a higher flow of gas phase towards the center resulting in an increase in gas volume fraction for the case with large tube-to-tube distance.

The axial liquid velocity profiles at both velocities showed an increasing trend with increase in tube-to-tube space. The difference in axial velocity peak values was higher at higher superficial inlet gas velocity. Another observation from this study was for a
Figure 4.6 Comparison of the liquid velocity contours and velocity vectors for the columns with and without internals (Cases JH and 15T) (a) $U_g = 0.020$ m/s (b) $U_g = 0.147$ m/s
(a) RMSE radial velocity

(b) RMSE axial velocity

Figure 4.7 Comparison of the RMSE radial and axial velocities for Cases JH and 15T at $U_g = 0.042 \text{ m/s}$ and $U_g = 0.147 \text{ m/s}$
(a) Turbulent Kinetic Energy

(b) Turbulent Reynolds number

Figure 4.8 Comparison of turbulent kinetic energy and turbulent Reynolds number for Case JH and Case 15T at $U_g = 0.042$ m/s and $U_g = 0.147$ m/s
(a) Radial gas volume fraction at $U_g = 0.042 \text{ m/s}$

(b) Radial gas volume fraction at $U_g = 0.147 \text{ m/s}$

Figure 4.9 Comparison of gas volume fraction for Case 12T, Case 15T and Case 18T at $U_g = 0.042 \text{ m/s}$ and $U_g = 0.147 \text{ m/s}$

126
Figure 4.10 (a) Axial liquid velocity at $U_g = 0.042 \text{ m/s}$

Figure 4.10 (b) Axial liquid velocity $U_g = 0.147 \text{ m/s}$

Figure 4.10 Comparison of axial liquid velocity for Case 12T, Case 15T and Case 18” at $U_g = 0.042 \text{ m/s}$ and $U_g = 0.147 \text{ m/s}$
decreasing tube-to-tube space in the churn turbulent regime, the steepness in axial liquid velocity profile was observed to decrease. To further study the variation of effect of tube-to-tube distances in bubble and churn-turbulent flow regimes, the liquid velocity vectors and axial liquid velocity contours in bubbly flow \( (U_g = 0.042 \text{ m/s}) \) and churn-turbulent regime \( (U_g = 0.097 \text{ and } 0.147 \text{ m/s}) \) are shown in Figure 4.11 (i), (ii) and (iii) respectively. The density of contour lines shown in Figure 4.11 show the same trend i.e. an increase density of contour lines with increasing tube-to-tube space. This increase in axial liquid velocity with increasing tube-to-tube size can be attributed to the reduction in restriction in flow from annular region to core region.

Same can observed following the liquid velocity vectors shown in these plots. The number and size of liquid velocity vectors pointing radially inwards reduces with decrease in tube-to-tube spacing. It was observed that given a low restriction flow i.e. for “Case 12T”, the liquid preferred maintaining the same recirculation observed for hollow bubble column. However, the funneling effect due to presence of internals increases the magnitude of the velocity vectors as observed in comparison to hollow bubble column in the previous work.

Another observation made at for flow in churn-turbulent regime the increase in low velocity region (area near zero axial velocity contour line or low scale vectors on contour plots) with decreasing tube-to-tube space. The radial flow towards the center reduces with decrease in tube-to-tube space as shown in Figure 4.11 (iv). This reduction in radial flow, lowers the intensity of overall recirculation that was observed with higher tube-to-tube space (Case 12). Instead higher number of low scale recirculation are observed in these regions. The increase in small-scale re-circulation regions in the presence of dense internals with low tube-to-tube distance has been experimentally shown by Möller et al. (2018).
Further, George et al. (2017) was able to identify these regions in their work through tracer particles as regions of high mixing.

Figure 4.11 (iv) shows the velocity vectors for liquid flow for three cases under investigation. The major patterns in flow has been outlined using blue stripes. The size of the blue stripe is proportionate to the intensity of overall recirculation. Two major observations were made through these patterns. First, the intensity of overall recirculation decreases with decrease in tube-to-tube space. Second, the scale or length of the overall recirculation increased with decrease in tube-to-tube spacing. The decrease in intensity was explained as a result of higher restrictions to flow with decrease in tube-to-tube space while the increase in scale of recirculation was reasoned as the mechanism to maintain the flow and compensate for lower intensity of radial flow observed with decrease in tube-to-tube space.

For all the three cases with internals, the flow through the core region was higher than that in a hollow bubble column owing to the funneling effect discussed earlier. However, with decrease in tube-to-tube space, more radial flow was observed towards the annular region from the core region as shown in Figure 4.11 (iv) using small blue stripes. This was because the high velocity in the core region (larger velocity vectors) and low velocity in the annular region (very small velocity vectors) create a low-pressure region near the walls in the annular region. Further, the low pressure in the annular region also creates small scale local recirculation patterns. The number of these small-scale recirculation increase with the superficial gas inlet velocity, due to a higher-pressure difference created between liquid flow in core and annular region. These observations imply towards lower radial mixing for low tube-to-tube space. Similar observations were made in the work of George (2015).
through mixing studies using buoyant particles. A higher residence time of these particles were reported in the annular regions at similar operating conditions.

Based on these observations, it is concluded that the backmixing which is reduced with decreasing tube-to-tube diameter. While the centerline axial velocity increases with increase in tube-to-tube diameter. It has been shown by Krishna et al. (2000) that the axial dispersion coefficient increases with increase in axial dispersion coefficient for the liquid phase in the column. Therefore, an optimization is required between these two phenomena to maintain a higher axial dispersion and decrease backmixing. Another, strategy as explained by Jhawar et al. (2014) and George et al. (2017) is through use of a baffle, which reduces the backmixing.

Further, it is observed that a lower tube-to-tube size is results in a lower axial dispersion coefficients and therefore, is preferential for reaction-containing system to reduce dilution and maintain reactant concentration gradient along the column.

The effect of internal height from the gas distributor was studied for three heights of 0.3 m (2D), 0.5 m (3.33D) and 0.7 m (4.67D). The variation in gas holdup and liquid velocity axially in bubbly and churn flow regimes have been studied. Figure 4.12 shows the gas volume fraction profile for bubbly (0.042 m/s) and churn-turbulent (0.147 m/s) flow regimes at z/D = 5.5. In the bubbly flow, a uniform gas volume fraction profile was observed when the height of internal was at z/D = 2 (0.3 m) with sharper profiles for internals positioned at higher heights.

Figure 4.13 (a) shows the gas volume fraction along the centerline (r/R=0) till the height of 1 m for bubbly flow regime (0.042 m/s). No variation in gas holdup profile near the tip
of internal at height of 0.3 m (2D) was observed. The internal at height 0.3 m interacts close to distributor region and thus guides the flow and thus the axial profile stays uniform near the internal. On the other hand, for the internals at higher positions of 0.5 m and 0.7 m create a disturbance in already developed flow causing an increase in turbulent kinetic energy and bubble breakup which results in a slight increase in gas volume fraction as observed in the axial profiles near 0.5 m and 0.7 m respectively. This increase in gas volume fraction was evident in both the radial and axial profiles shown in Figure 4.11 (a) and 4.13 (a). Further evidence can be seen in the turbulent kinetic energy profile at $z/D = 5$ (0.75 m) i.e. above the tip of internal at 0.7 m height from the gas distributor.

The observed increase in turbulent kinetic energy corresponds to the disturbance caused by internal at height of 0.7 m in the flow. However, no effect of changing internal height was seen in the churn-turbulent regime owing to vigorous mixing and high turbulence at this flow regime.

Figure 4.9 (b) shows the axial profile for liquid axial velocity along the centerline ($r/R = 0$) till the height of 1 m at $U_g = 0.042$ m/s. A steep increment in liquid velocity before the tip of the internal was consistently observed for each case. This implies the presence of an upward pull experienced near the circular internals by the liquid phase due to their presence.
(i) Comparison of liquid axial velocity contours and velocity vector for (a) Case 12T, (b) Case 15T and (c) Case 18T at $U_g = 0.042$ m/s
(ii) Comparison of liquid axial velocity contours and velocity vector for (a) Case 12T, (b) Case 15T and (c) Case 18T at $U_g = 0.097 \text{ m/s}$
(iii) Comparison of liquid axial velocity contours and velocity vector comparison for (a) Case 12T, (b) Case 15T and (c) Case 18T at $U_g = 0.147$ m/s
(iv) Comparison of velocity vectors for (a) Case 12T, (b) Case 15T and (c) Case 18T at $U_g = 0.147 \text{ m/s}$ with flow pattern marked
Figure 4.11 Comparison of liquid axial velocity contours and velocity vector for Case 12T, Case 15T and Case 18T at $U_g = 0.042$ m/s, 0.097 m/s and 0.147 m/s

(a) Comparison of radial profiles of gas volume fraction at $U_g = 0.042$ m/s at $z/D = 5$

(b) Comparison of radial profile of gas volume fraction comparison at $U_g = 0.147$ m/s at $z/D = 5$
Figure 4.12 Comparison of radial profiles of gas volume fraction for internal at 0.3 m, 0.5 m and 0.7 m from the gas distributor at \( U_g = 0.042 \text{ m/s} \) and \( U_g = 0.147 \text{ m/s} \) at \( z/D = 5 \)

(a) Comparison of axial profile for gas volume fraction at \( U_g = 0.042 \text{ m/s} \)

(b) Comparison of axial profile for liquid axial velocity at \( U_g = 0.042 \text{ m/s} \)
Figure 4.13 Comparison of axial profiles of gas volume fraction and axial liquid velocity for internal at 0.3 m, 0.5 m and 0.7 m from the gas distributor.

![Figure 4.13](image)

Figure 4.14 Comparison of radial profiles of turbulent kinetic energy at $U_g = 0.042 \text{ m/s}$ at $z/D = 5 \ (0.75 \text{ m})$ for internal at 0.3 m, 0.5 m and 0.7 m from the gas distributor.

In the presence of internals, the height of denser contours which represent regions of higher liquid axial velocity, was defined by the height of internals. A lower height of internals thus guides the flow to have a longer and enhanced circulation pattern in comparison to internals at a higher height from the gas distributor. At higher superficial gas inlet velocity, the same effects were not clearly visible. This was because the effect of internal height was diminished by the increase in turbulence at higher velocity.
(a) Comparison of radial profiles of axial liquid velocity at $U_g = 0.042 \text{ m/s}$ at $z/D = 5$

(b) Comparison of radial profiles of axial liquid velocity at $U_g = 0.147 \text{ m/s}$ at $z/D = 5$

Figure 4.15 Comparisons of radial profiles of axial liquid velocity at $U_g = 0.042 \text{ m/s}$ and $U_g = 0.147 \text{ m/s}$ at $z/D = 5$ for internal at 0.3 m, 0.5 m and 0.7 m from the gas distributor.

The effect of reducing the final height of internal to height below the dynamic liquid height
was studied in comparison to internal with higher height than liquid dynamic height. Simulation results for height of internals at 2 m i.e. “Case 15T” and with height of internals at 0.9 m i.e. the final height at 1.4 m which is the static liquid bed height were compared in bubbly and churn turbulent regime at $U_g = 0.042$ and $0.147$ m/s. Figure 4.17 (a) and (b) shows the comparison between the gas volume fraction profiles for both the cases at $z/D = 8$. A higher gas holdup for the case of lower internal height was observed in the annular region. This was attributed to the flow of entrained bubbles flowing unrestricted above the height of the internals. A higher liquid axial velocity and negative axial liquid velocity was observed in the case of lowered internals. This was attributed to the un-restricted backflow of liquid as well as the effect of an enhanced liquid recirculation due to higher holdup at the core region. However, no significant effect on liquid axial velocity profile can be observed in Figure 4.18. Further, it was to be noted, that the accuracy of simulations was not established for this region of flow field. Therefore, further comparisons at higher $z/D$ was not performed while no significant effect was observed due to the variation at a lower $z/D$. 
Figure 4.16. Comparison of liquid axial velocity contours and velocity vectors for internals at (a) 0.3 m, (b) 0.5 m and (c) 0.7 m from the gas distributor at $U_g = 0.042$ m/s
Figure 4.17 Comparison of radial profiles of gas volume fraction for internal height of 0.9 and 1.5 m at $U_g = 0.042$ m/s and $U_g = 0.147$ m/s at $z/D = 8$

(a) Comparison of radial profiles of gas volume fraction at $U_g = 0.042$ m/s at $z/D = 8$

(b) Comparison of radial profile of gas volume fraction at $U_g = 0.147$ m/s at $z/D = 8$
4.4 Conclusions

CFD simulations were performed to study the effect of concentric tube bundle type internal on bubble column hydrodynamics. The effect of internals on hydrodynamics was shown. A reduction in radial fluctuations, turbulent kinetic energy and turbulent Reynolds number was observed in the presence of internals. The presence of circular internals give rise to a funnealing affect which results in an increased liquid axial velocity and gas holdup.

Figure 4.18 Comparison of axial liquid velocity contours and velocity vectors for different total height of internals (a) Total height = 0.9 m; (b) Total height = 1.4 m
The variation in tube-to-tube distance significantly effects the liquid axial velocity and circulation patterns. The decrease in tube-to-tube distance decreases the axial liquid velocity in the core region and results in formation of low liquid velocity regions of small scale circulations in the annular region churn-turbulent regime. It was observed that the back-mixing and axial dispersion coefficient can be controlled by varying tube-to-tube distance. Further, the effects of height of internals from gas distributor and the overall height of the internal was studied.
References


Chapter 5
5. Conclusions and Recommendations

This chapter presents a number of detailed summary of the major findings from the present work on the study of the effects of the geometry of internals on bubble columns hydrodynamics based on Computational Fluid Dynamics (CFD) simulations.

5.1 Conclusions

The main objective of the thesis was to better understand the effect of vertical tube bundle internals on the hydrodynamics in a bubble column. The study was carried out in two parts. First a numerical approach was developed to accurately predict the gas-liquid two-phase flow in the bubbly and churn-turbulent regimes. This model was then applied to simulate the flows in three bubble columns with different tube-bundle type internals used in the columns to study effects of different configurations on the bubble column hydrodynamics. The major findings from the present study are as follows:

- Comparison of results using homogeneous and inhomogeneous (with multiple bubble phases) discrete population balance model for both bubbly and churn-turbulent flow was performed for the first time.

- Based on the comparison between the inhomogeneous discrete population balance model with 2 and 3 bubble velocity groups (phases) and discrete homogeneous model for both homogeneous and heterogeneous regimes, it was found that the inhomogeneous discrete population balance model gives a better prediction for the mean bubble size growth in churn-turbulent regime.

- A stable rate of breakup and coalescence were observed using the RSM turbulence model which is able to capture the anisotropic nature of the flow than the RNG k-ε model.
- The discrete homogeneous PBM method was found accurate in the homogeneous regime, however, its accuracy in the heterogeneous regime was lower than the inhomogeneous discrete PBM models.

- The higher coalescence rate was found without modifying inlet boundary condition.

- Based on the bimodal bubble size distribution observed in the experiments, the inhomogeneous population balance model with 2 bubble phases and the modified inlet boundary condition was proposed and it gives a more physically-realizable bubble size distribution and better agreement with the experimental data profile.

- Based on the comparison of the simulation results using four different drag models, the Ishii-Zuber drag model and a combination of the Schiller-Naumann drag model for small bubbles and the Tomiyama drag model for large bubbles was found suitable to simulate the gas-liquid flow in the churn-turbulent regime. It was also found that the combination of the Schiller-Naumann lift force for the small bubble phase and the Tomiyama drag force and Tomiyama lift force for the large-bubble phase gives the most accurate (average less than 5%) results for the gas-liquid flow in the churn-turbulent regime.

- The selected model was validated for different flow regimes using 2D and 3D geometries and comparable accuracy was observed with both.

- The selected model was used to simulate a hollow bubble column and a similar column with 15 tube bundle internals. The results with both the hollow bubble column and bubble column with internals were in good agreement with the experimental results from literature studies.

- The effects of three geometrical parameters namely the tube-to-tube space, the height of the tube from the gas distributor and the height of the tube from the dynamic liquid
level on the hydrodynamics of the column have been studied for a 15 cm diameter bubble column with the superficial gas velocity in the range of 20-147 mm/s.

- The effect of tube-to-tube distance was directly studied for the first time. It has a significant impact on the liquid axial velocity and circulations. With the decrease in the tube-to-tube space, the scale of overall liquid circulation increases as well as more small-scale circulations are observed in the churn-turbulent flow regime. From the results, it was concluded that the back-mixing and axial dispersion can be controlled by modifying tube-to-tube diameter, however an optimization is required to maintain a balance between them as per requirement.

- Effect of varying total heights and internal height from gas distributor from bubbly to churn-turbulent regime was uniquely studied. The height of the internals from the gas distributor was found to alter the liquid flow pattern in bubbly flow regime. At higher velocities, the effect of the height of the internals is diminished due to higher turbulence and vigorous mixing.

- Changing the top height of the internals from above the liquid dynamic height to below the liquid dynamic height has no effect on the liquid axial velocity or circulation. An increase in the gas holdup was observed near the top of the internals with the top height of internals below the dynamic liquid height as a result of entrained bubbles moving without restrictions.

5.2 Recommendations

Based on the analysis of results from the present study, the following recommendations for future work can be made:

- The modified inlet boundary condition-based model with the inhomogeneous discrete population balance is less accurate in the transition regime between the bubbly and
churn-turbulent regimes. In the present study, the superficial gas inlet velocity of 0.034 m/s was taken as the velocity for the transition from homogeneous to heterogeneous flow regimes in the bubble column. A better estimate of the transition velocity would provide higher accuracy for simulations with superficial inlet gas velocities in close range to the transition regime.

- The turbulence parameters at the inlet boundary was used based on literature study. Performing a sensitivity analysis for different values to use the same values or using a calculated value is recommended.

- 3D simulations to validate the applicability of 2D simulations for the study of the effect of internals as was demonstrated with hollow bubble column.

- In the present work, the internal geometry covered only 10% CSA of the bubble column, while higher occluded CSA is required for some processes, like Fischer Tropsch synthesis. These geometries have multiple concentric tube bundles arranged in different configurations. The studies for single tube bundle can be expanded for multiple tube bundles.

- Analysis for columns with highly dense internals (occluded CSA > 20%) needs to be conducted.
Appendix A

A UDF for drag laws

A.1 Zhang and Vanderheyden (Zhang & Vanderheyden, 2002) drag law

```c
#include "udf.h"
#define GRA 9.81
#define ST 0.072

DEFINE_EXCHANGE_PROPERTY(ZhangVanderheyden, c, mix_thread, s_col, f_col)
{
    Thread *thread_l, *thread_g;

double C_D, bs, drho, frd, eotvos, mustar, mumix, rd, remix,slipx,
        slipy,uslip, cds, cdcap = 1e-7, cdel, kpq, taup, mu_l, rho_l;

    thread_l = THREAD_SUB_THREAD(mix_thread, s_col); /* continuous */
    thread_g = THREAD_SUB_THREAD(mix_thread, f_col); /* discontinuous */
    bs = C_PHASE_DIAMETER(c, thread_g);
    rd = C_VOF(c, thread_g);

    /* calculate slip velocity */
    slipx = C_U(c, thread_g) - C_U(c, thread_l);
    slipy = C_V(c, thread_g) - C_V(c, thread_l);
    uslip = sqrt((slipx*slipx) + (slipy*slipy));

    /* calculate mixture viscosity and Reynolds, and Eotvos number */
    mustar = (C_MU_L(c, thread_g) + 0.4*C_MU_L(c, thread_l))/(C_MU_L(c, thread_g) +
                C_MU_L(c, thread_l));
    mumix = C_MU_L(c, thread_l)*(pow((1.-rd),(-2.5*mustar)));

    remix = bs*uslip/mumix;
    drho = (C_R(c, thread_l) - C_R(c, thread_g));
```

eotvos = (drho*bs*bs* GRA)/ST;
rho_l = C_R(c,thread_l);
mu_l = C_MU_L(c, thread_l);
C_D = 0.44 + 24/remix + 6/(1+sqrt(remix));
kpq = 3*C_D*rd*rho_l*uslip/(4.*bs);
return kpq;
}

A.2 Ishii Zuber (Ishii & Zuber, 1979) drag law
#include "udf.h"
#define GRA 9.81
#define ST 0.072
DEFINE_EXCHANGE_PROPERTY(ishiizuber,c,mix_thread,s_col,f_col)
{
Thread *thread_l, *thread_g;
real C_D, bs, drho, frd, eotvos, mustar, mumix, rd, remix,slipx,
slipy,uslip, cds, cdcap = 1e-7, cdel, kpq, taup, mu_l, rho_l;
thread_l = THREAD_SUB_THREAD(mix_thread, s_col); /* continuous */
thread_g = THREAD_SUB_THREAD(mix_thread, f_col); /* discontinuo */
bs = C_PHASE_DIAMETER(c,thread_g);
rd = C_VOF(c,thread_g);
/* calculate slip velocity */
slipx = C_U(c, thread_g) - C_U(c, thread_l);
slipy = C_V(c, thread_g) - C_V(c, thread_l);
uslip = sqrt((slipx*slipx) + (slipy*slipy));
/* calculate mixture viscosity and reynolds, and eotvos number */
mustar = (C_MU_L(c,thread_g) + 0.4*C_MU_L(c,thread_l))/(C_MU_L(c,thread_g) + C_MU_L(c,thread_l));
mumix = C_MU_L(c,thread_l)*(pow((1.-rd),(-2.5*mustar)));
remix = ((C_R(c,thread_l)*bs)/mumix)*uslip;
frd = (C_R(c,thread_l) - C_R(c,thread_g));
eotvos = (frd*bs*bs* GRA)/ST;
\[
\rho_l = C_R(c,\text{thread}_l);
\mu_l = C_{MU_L}(c, \text{thread}_l);
\]

/*Cd for spherical bubbles*/
\[
cds = (24./\text{remix})*(1. + (0.15*\text{pow(remix,0.687)}));
\]

/*cd for elliptical bubbles*/
\[
frd = (C_{MU_L}(c,\text{thread}_l)/\text{mumix}) * \text{pow}((1.-\text{rd}),0.5);
\]
\[
cdel = (\text{pow}(((1. + 17.67*\text{pow(frd,(6./7.))})/(18.67*\text{frd})), 2.)) *( (2./3.) * (\text{pow(eotvos,0.5)}));
\]

/*cd for the cap regime*/
if (!(1.-\text{rd}=0))
{
    cdcap = (8./3.)*(1.-\text{rd})*(1.-\text{rd});
}

/*determine which coefficient to use*/
if(cdel < cdcap)
{
    C_D = cdel;
}
else
{
    C_D = cdcap;
}
if (cds > C_D)
{
    C_D = cds;
}
kpq = 3*C_D*rd*\rho_l*uslip/(4.*bs);
return kpq;
}
References


Appendix B

B.1 Calculation of perforation fraction

\[ \text{Radius of Inner Circle} = 0.0291 + \frac{0.0095}{2} = 0.03385 \, m \]

\[ \text{Diameter} = 0.0677 \, m \]

\[ \text{Circumference} = 0.212686 \, m \]

Total Surface Area of the cylinder with height as shown in the Figure 2.

\[ \text{TSA} = \pi \times \text{Diameter} \times \text{Height} = 0.319029 \]

Space area calculated as rectangles with space length 0.0044 is given as:

\[ \text{SpA} = 15 \times \text{Space Length} \times \text{Height of Tubes} = 0.099 \]

\[ \text{Space Fraction} = \frac{\text{Space Area(SpA)}}{\text{Total Surface Area (TSA)}} = 0.31 \]

For the case of 15 tubes we have,

\[ \text{Total Length} = 1.5 \, m \]

\[ \text{Length covered with Perforation holes} \]

\[ = \text{Space Fraction} \times \text{Total Length} = 0.464 \, m \]

Hence, the number of equally spaced perforations span over the length of the bundle with space length of 0.0044 m for the case of 15 tubes. The final geometry and mesh are shown in the figure below.
B2. Contour plots for comparing Hollow bubble column, “Case JH” and bubble column with internals, “Case 15T”

(i) gas volume fraction at $U_g = 0.042$ m/s

(ii) small and large bubble fractions at $U_g = 0.147$ m/s
Figure B.1 Contour plots for Case JH and Case 15T

(i) (a) Radial liquid fluctuation, (b) Turbulent Kinetic Energy, (c) Reynolds Stress, and (d) Turbulent Reynolds number, $Re_y$ at $U_g = 0.042$ m/s

(ii) (a) Radial liquid fluctuation, (b) Turbulent Kinetic Energy, (c) Reynolds Stress, and (d) Turbulent Reynolds number, $Re_y$ at $U_g = 0.147$ m/s

Figure B.2 Contour plots for Case JH and Case 15T
Figure B3. Liquid axial velocity contour and vector plots for different heights of internals (a) 0.3 m, (b) 0.5 m, (c) 0.7 m at $U_g = 0.147$ m/s
Curriculum Vitae

Name: Tuntun Gaurav

Post-secondary Education and Degrees:

Birla Institute of Technology (BIT), Mesra, Ranchi, India
2011-2015
Bachelor of Engineering (Chemical Engineering)

The University of Western Ontario
London, Ontario, Canada
2016-Present
Master of Engineering Science (Chemical and Biochemical Engineering with Scientific Computing)

Honours and Awards:

Western Engineering Scholarship
2016-2018

Industrial Problem Solving Week, Runners up
Feb – 2017

Related Work Experience

Graduate Engineering Trainee,
Reliance Industries Limited, Jamnagar
2015-2016

Teaching Assistant
The University of Western Ontario
2017-2018

Research Assistant
The University of Western Ontario
2017-2018

Conference Proceedings: