Simulations of Two-phase Flows Using Interfacial Area Transport Equation

DISSERTATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of The Ohio State University

By

Xia Wang

Graduate Program in Nuclear Engineering

The Ohio State University

2010

Dissertation Committee:

Dr. Xiaodong Sun (Advisor)

Dr. Tunc Aldemir

Dr. Richard Christensen

Dr. Richard Denning
Abstract

The current study focuses on providing a reliable computational fluid dynamics (CFD) tool for two-phase flow simulations, which is capable of capturing dynamic changes of interfacial structures and achieving accurate predictions of flow behaviors. A set of interfacial area transport equations (IATEs), which dynamically evaluates the interfacial area concentration, was successfully implemented into a CFD software package, namely, Fluent. The interfacial area concentration is a key parameter in modeling the interfacial transfer terms in the two-fluid model due to mechanical and thermal non-equilibrium between the two phases. Given the various flow regimes in two-phase flows, one-group IATE and two-group IATE developed in the literature were separately incorporated into the two-fluid model and subsequently validated under different flow conditions: liquid-liquid two-component bubbly; air-water bubbly, cap-bubbly, and churn-turbulent flows. Numerical results obtained from the two-fluid model incorporated with the IATE models were generally in good agreement with the experimental data. A set of adjustable model coefficients was also established for three-dimensional simulations when the influence of the lateral phase distribution in a circular flow channel on the one-group IATE model was considered.

In addition, contributions of the bubble interaction mechanisms and interfacial forces to the phase distributions of two-phase flow were numerically investigated. It was observed that the lift force was significant for the phase distributions in gas-liquid two-
phase flows; however it might cause convergence issues when large bubbles exist in the
flow field of interest.

Furthermore, a mathematical property, i.e., the well-posedness of the proposed
one-dimensional three-field model with the two-group IATE model, was studied. The
necessary condition to ensure well-posedness was obtained using characteristic analysis.
The momentum flux parameters were introduced to help stabilize the proposed model.
Dedication

This document is dedicated to my family.
Acknowledgments

The author would like to express her deep appreciation to her advisor, Dr. Xiaodong Sun for his intellectual guidance and continuous support for this research. The author would also like to thank her committee members: Prof. Tunc Aldemir, Prof. Richard Christensen, and Prof. Richard Denning for their encouragement, patience as well as constructive comments on this work.

Furthermore, the author is grateful to the computing resources and support provided by the Ohio Supercomputer Center.

The author also wishes to thank all the professors, staff, and students in Nuclear Engineering Program at The Ohio State University for their support, especially to Jonathan Kulisek for his discussions regarding the writing of this dissertation.

Finally, the author expresses her sincere gratitude to her parents and husband for their love, understanding, and support over the years.
Vita

2005..........................................................B.S. Mechanical Engineering, University of Science and Technology of China, Hefei, China

2007..........................................................M.S. Nuclear Engineering, The Ohio State University

2005 to present ..............................................Graduate Research Associate, Nuclear Engineering Program, Department of Mechanical Engineering, The Ohio State University

Publications


Fields of Study

Major Field: Nuclear Engineering
<table>
<thead>
<tr>
<th>Table of Contents</th>
</tr>
</thead>
<tbody>
<tr>
<td>Abstract .................................................................................................................. ii</td>
</tr>
<tr>
<td>Dedication ................................................................................................................ iv</td>
</tr>
<tr>
<td>Acknowledgments ....................................................................................................... v</td>
</tr>
<tr>
<td>Vita ........................................................................................................................... vi</td>
</tr>
<tr>
<td>List of Tables ........................................................................................................... xii</td>
</tr>
<tr>
<td>List of Figures ......................................................................................................... xiii</td>
</tr>
<tr>
<td>Nomenclature ........................................................................................................... xxi</td>
</tr>
<tr>
<td>Chapter 1. Introduction ............................................................................................. 1</td>
</tr>
<tr>
<td>1.1. Research background .......................................................................................... 1</td>
</tr>
<tr>
<td>1.2. Computational fluid dynamics codes and simulation scales .............................. 5</td>
</tr>
<tr>
<td>1.3. Brief introduction to Fluent ............................................................................. 6</td>
</tr>
<tr>
<td>1.4. Two-fluid model .................................................................................................. 7</td>
</tr>
<tr>
<td>1.5. Statement of the problem .................................................................................. 11</td>
</tr>
<tr>
<td>1.6. Objectives ......................................................................................................... 12</td>
</tr>
<tr>
<td>1.7. Dissertation outline .......................................................................................... 13</td>
</tr>
<tr>
<td>Chapter 2. Interfacial Area Transport Equations .................................................... 16</td>
</tr>
</tbody>
</table>
2.1. Background ........................................................................................................ 16

2.2. Interfacial area transport equation................................................................. 21

2.3. One-group IATE ................................................................................................. 23

2.4. Two-group IATE ................................................................................................. 26

Chapter 3. Technical Approach................................................................................ 35

3.1. Implementation of IATE into Fluent ................................................................. 35

3.2. Continuity equations of three-field two-fluid model ......................................... 39

3.3. Momentum equations of three-field two-fluid model ....................................... 41

3.3.1. Governing equations ................................................................................... 41

3.3.2. Discussion on drag force ............................................................................. 43

3.3.3. Discussion on lift force ............................................................................... 46

3.3.4. Discussion on wall lubrication (wall lift) force ........................................... 48

3.3.5. Discussion on turbulent dispersion force .................................................... 50

3.3.6. Discussion on transient forces .................................................................... 51

3.4. Enthalpy equations of three-field two-fluid model ........................................... 52

3.5. Discussion on bubble velocity.......................................................................... 53

Chapter 4. $k - \varepsilon$ Turbulence Model................................................................. 58

4.1. Governing equations of $k - \varepsilon$ turbulence model ....................................... 58

4.2. Standard $k - \varepsilon$ turbulence model ............................................................. 61
4.2.1. Dispersed model ................................................................. 61
4.2.2. Per-phase model ............................................................... 65
4.3. RNG $k - \varepsilon$ turbulence model .......................................... 66

Chapter 5. Model Validation of One-group IATE .................................. 68

5.1. PC-SIMPLE algorithm .......................................................... 68
5.2. Mesh generation ................................................................. 69
5.3. Boundary conditions and convergence criteria .......................... 70
5.4. Model validation: air-water bubbly flows in a circular pipe ............ 70
  5.4.1. Flow conditions ............................................................ 70
  5.4.2. Simulations with model coefficients from Ishii et al. (2002) ........ 73
  5.4.3. Discussion on the three-dimensional model ......................... 75
  5.4.4. Testing on model coefficients with one-dimensional simulation .... 77
  5.4.5. Suggestions on model coefficients for three-dimensional IATE model... 78
  5.4.6. Study on the lift force .................................................... 81
  5.4.7. Comparisons of results .................................................. 83
5.5. Model validation: air-water bubbly flows in a duct ....................... 88
  5.5.1. Description of experiments .............................................. 88
  5.5.2. Numerical model and flow conditions ............................... 89
  5.5.3. Comparison of results .................................................... 90
5.6. Model validation: liquid-liquid two-component flows in a pipe
5.6.1. Background
5.6.2. Description of experiments
5.6.3. Numerical model and flow conditions
5.6.4. Comparison of results
5.7. Conclusions

Chapter 6. Well-posedness Study of Three-field Two-fluid Model
6.1. Background
6.2. Governing equations
6.3. Characteristic analysis
6.4. Results and discussions: a case study
6.5. Conclusions

Chapter 7. Simulations Using Three-field Two-fluid Model
7.1. Definition of error
7.2. Description of experiments
7.3. Numerical model
7.4. Assumptions and coefficients in two-group IATE model
7.5. Discussion on interfacial forces
7.6. Numerical scheme
7.7. Mesh sensitivity ................................................................. 147
7.8. Test on boundary conditions ........................................ 148
7.9. Test on turbulence models ............................................. 152
7.10. Test on interfacial forces ............................................. 152
7.11. Model validation: cap-bubbly flows ......................... 154
7.12. Model validation: churn-turbulent flows .................... 176
  7.12.1. Study on unsteady solver ..................................... 176
  7.12.2. Comparison of results ......................................... 179
7.13. Test on inlet effect ....................................................... 182

Chapter 8. Conclusions and Future Work .......................... 184
  8.1. Conclusions .............................................................. 184
  8.2. Future work ............................................................. 185

References .................................................................................. 187
List of Tables

Table 2.1 Summary of source and sink of the interfacial area concentration in the two-group IATE (Sun, 2001) ............................................................ 31

Table 5.1 Flow conditions at $z / D = 5$ ................................................................. 72

Table 5.2 Measurements at location $z/D_H = 34.8$ in a rectangular duct ............... 89

Table 5.3 Measurements at the location of $z / D = 30$ for liquid-liquid flows (Vasavada et al., 2007) ........................................................................... 98

Table 5.4 Comparisons of computed mass outflow rates to the inflow rates .......... 99

Table 6.1 Area-averaged data for Runs 13-29 at $z / D = 13$ (Vasavada, 2008) .... 118

Table 7.1 Flow conditions for model validation (Sun, 2001; Sun et al., 2004b; Sun et al., 2005) ...................................................................................... 141

Table 7.2 Coefficients of interfacial forces ............................................................... 145

Table 7.3 Relative errors of the interfacial area concentration for Test 1 .......... 166
List of Figures

Figure 2.1. Flow regime map proposed by Mishima and Ishii (1984) .............................. 17

Figure 3.1. A cap bubble rising in an infinite liquid ......................................................... 54

Figure 5.1. Flow conditions in the flow regime map (Mishima and Ishii, 1984) ............ 72

Figure 5.2. Relative error of the interfacial area concentration using model coefficients from Ishii et al. (2002) ........................................................................................................ 74

Figure 5.3. Bubble velocity profiles from experiments and simulations: (a) Run 5, (b) Run 6, (c) Run 10, and (d) Run 16 .................................................................................................. 76

Figure 5.4. Lateral distributions in Run 10 from simulations and experiments at the location $z/D = 55$: (a) the interfacial area concentration, (b) the void fraction, and (c) counter of the void fraction from Fluent code with one-group IATE model ...................... 78

Figure 5.5. Relative errors of interfacial area concentration using the suggested model coefficients.......................................................................................................................... 80

Figure 5.6. Comparisons of interfacial area concentration using different coefficients with experiments at the location $z/D = 55$: (a) Run 5 and (b) Run 6 ........................................ 81

Figure 5.7. Simulations of the void fraction in comparison to experimental data at $z/D = 55$: (a) Run 2 and (b) Run 5 ................................................................................................................ 82

Figure 5.8. Predictions of void fraction with comparison to experimental data at $z/D = 55$: (a) Run 3, (b) Run 5, (c) Run 6, (d) Run 10, (e) Run 16, and (f) Run 17 .... 85
Figure 5.9. Predictions of interfacial area concentration with comparison to experimental data at $z / D = 55$: (a) Run 3, (b) Run 5, (c) Run 6, (d) Run 10, (e) Run 16, and (f) Run 17. 

Figure 5.10. Predictions of gas velocity with comparison to experimental data at $z / D = 55$: (a) Run 3, (b) Run 5, (c) Run 6, (d) Run 10, (e) Run 16, and (f) Run 17.

Figure 5.11. Comparisons of numerical results with the experimental data (Kim, 1999) at $z/D_h = 88.2$ for Run R-1: (a) void fraction, (b) interfacial area concentration, and (c) bubble Sauter mean diameter.

Figure 5.12. Comparisons of numerical results with the experimental data (Kim, 1999) at $z/D_h = 141.7$ for Run R-2: (a) void fraction, (b) interfacial area concentration, and (c) bubble Sauter mean diameter.

Figure 5.13. Evaluation of the individual bubble interaction contributions at $z/D_h = 141.7$ for Run R-2.

Figure 5.14. Comparisons of the radial void fraction distributions using different lift force coefficients for Run L-3 at $z / D = 58$.

Figure 5.15. Numerical predictions of radial profiles of the axial velocities of water and Therminol 59® for Run L-3 at $z / D = 58$: (a) $C_i = 0$ and (b) $C_i = 0.5$.

Figure 5.16. Radial profiles of local flow parameters at $z / D = 58$: (a) void fraction for Run L-1, (b) interfacial area concentration for Run L-1, (c) void fraction for Run L-2, and (d) interfacial area concentration for Run L-2.
Figure 5.17. Radial profiles of local flow parameters at $z / D = 58$: (a) void fraction for Run L-3, (b) void fraction for Run L-5, (c) void fraction for Run L-7, and (d) velocity of Therminol 59® for Run L-7 .................................................................................................................. 104

Figure 5.18. Radial profiles of local flow parameters at $z / D = 58$: (a) void fraction for Run L-6, (b) interfacial area concentration for Run L-6, (c) void fraction for Run L-8, and (d) interfacial area concentration for Run L-8 ........................................................................................................ 106

Figure 5.19. Radial profiles of the void fraction at $z / D = 58$ for Run L-4 ................ 107

Figure 6.1. $C_{\nu,k}$ vs. the total void (drop) fraction $\alpha$: (a) $C_{\nu,1}$, (b) $C_{\nu,2}$, and (c) $C_{\nu,3}$ .... 119

Figure 6.2. $g(w)$ for Runs 13, 17, and 18 over: (a) a wide range of $w$ from 0 to 4 and (b) a narrower range of $w$ ..................................................................................................................................... 123

Figure 6.3. $g(w)$ for Runs 14, 15, and 19 over: (a) a wide range of $w$ from 0 to 3 and (b) a narrower range of $w$ ..................................................................................................................................... 124

Figure 6.4. $g(w)$ for Runs 16, 21, and 29 over: (a) a wide range of $w$ from 0 to 6 and (b) a narrower range of $w$ ..................................................................................................................................... 125

Figure 6.5. $g(w)$ for Runs 20 and 27 over: (a) a wide range of $w$ from 0 to 10 and (b) a narrower range of $w$ ..................................................................................................................................... 126

Figure 6.6. $g(w)$ for Runs 22 and 26 over: (a) a wide range of $w$ from 0 to 6 and (b) a narrower range of $w$ ..................................................................................................................................... 127

Figure 6.7. $g(w)$ for Run 23 over: (a) a wide range of $w$ from 0 to 3.5 and (b) a narrower range of $w$ ..................................................................................................................................... 128
Figure 6.8. $g(w)$ for Runs 24, 25, and 28 over: (a) a wide range of $w$ from 0 to 8 and (b) a narrower range of $w$ .......................................................................................................................... 129

Figure 6.9. $U_r$ vs. $\alpha$ for the distorted and slug drops.................................................. 131

Figure 6.10. Stability criteria of the one-dimensional two-fluid-IATE model with momentum flux parameters ........................................................................................................... 133

Figure 6.11. Stability criteria of the one-dimensional two-fluid-IATE model with momentum flux parameters for (a) $S_1$ and (b) $S_2$ ........................................................... 134

Figure 7.1. Experimental facility (Sun, 2001; Sun et al., 2004b; Sun et al., 2005)........ 139

Figure 7.2. Two-phase mixture injection unit (Sun, 2001; Sun et al., 2004b; Sun et al., 2005)............................................................................................................................... 140

Figure 7.3. Numerical results of Group-1 bubbles using different schemes at the location of $z / D_h = 141.7$ in Test 1: (a) gas velocity and (b) void fraction................................. 146

Figure 7.4. Predicted void fractions at the location of $z / D_h = 141.7$ using different meshes in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles ......................... 147

Figure 7.5. Void fractions in Run 17 for: (a) Group-1 and Group 2 bubbles at $z / D_h = 34.8$ (measured), (b) Group-1 bubbles at $z / D_h = 141.7$, and (c) Group-2 bubbles at $z / D_h = 141.7$ .......................................................................................................................... 149

Figure 7.6. Profiles of Test 1 at the location of $z / D_h = 34.8$ for: (a) interfacial area concentration for Group-1 bubbles, (b) void fraction of Group-1 bubbles, (c) interfacial area concentration for Group-2 bubbles, and (d) void fraction of Group-2 bubbles ...... 150
Figure 7.7. Profiles of Test 2 at the location of \( z / D_h = 34.8 \) for: (a) interfacial area concentration for Group-1 bubbles, (b) void fraction of Group-1 bubbles, (c) interfacial area concentration for Group-2 bubbles, and (d) void fraction of Group-2 bubbles...... 151

Figure 7.8. Void fraction at \( z / D_h = 88.2 \) in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 154

Figure 7.9. Velocity at \( z / D_h = 141.7 \) in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 155

Figure 7.10. Void fraction at \( z / D_h = 141.7 \) in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 156

Figure 7.11. Contours of the void fraction in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 157

Figure 7.12. Interfacial area concentration at \( z / D_h = 141.7 \) in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 159

Figure 7.13. Contours of the interfacial area concentration in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 160

Figure 7.14. Velocity at \( z / D_h = 141.7 \) in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 161

Figure 7.15. Void fraction at \( z / D_h = 141.7 \) in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 162

Figure 7.16. Contours of the void fraction in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles.............................................................................................................. 163
Figure 7.17. Interfacial area concentration at $z / D_h = 141.7$ in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 164

Figure 7.18. Contours of the interfacial area concentration in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 165

Figure 7.19. Velocity at $z / D_h = 88.2$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 167

Figure 7.20. Void fraction at $z / D_h = 88.2$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 168

Figure 7.21. Interfacial area concentration at $z / D_h = 88.2$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 169

Figure 7.22. Velocity at $z / D_h = 141.7$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 169

Figure 7.23. Void fraction at $z / D_h = 141.7$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 170

Figure 7.24. Interfacial area concentration at $z / D_h = 141.7$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 171

Figure 7.25. Contours of the void fraction in Test 1 from experimental observations (left), predicted Group-1 bubbles (middle), and predicted Group-2 bubbles (right).............. 171

Figure 7.26. Bubble velocity at $z / D_h = 141.7$ in Test-2 for: (a) Group-1 bubbles and (b) Group-2 bubbles......................................................................................................................... 173
Figure 7.27. Void fraction at $z/D_h = 141.7$ in Test 2 for: (a) Group-1 bubbles and (b) Group-2 bubbles............................................................ 173

Figure 7.28. Interfacial area concentration at $z/D_h = 141.7$ in Test 2 for: (a) Group-1 bubbles and (b) Group-2 bubbles............................................................ 174

Figure 7.29. Drag force coefficient in different flow regimes........................................ 174

Figure 7.30. Contours of the void fraction in Test 2 from experimental observations (left), predicted Group-1 bubbles (middle), and predicted Group-2 bubbles (right)........... 175

Figure 7.31. Void fraction at $z/D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles............................................................ 177

Figure 7.32. Bubble velocity at $z/D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles............................................................ 177

Figure 7.33. Void fraction at $z/D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles............................................................ 178

Figure 7.34. Velocity at $z/D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles............................................................ 178

Figure 7.35. Void fraction at $z/D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles............................................................ 179

Figure 7.36. Bubble velocity at $z/D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles............................................................ 180
Figure 7.37. Void fraction at $z / D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.38. Interfacial area concentration at $z / D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.39. Bubble velocity at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.40. Void fraction at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.41. Interfacial area concentration at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.42. Contours of the void fraction of Group-2 bubbles at center-plane in Run 17 for: (a) short section and (b) long section
# Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>cross-sectional area of flow channel, m²</td>
</tr>
<tr>
<td>$A_d$</td>
<td>projected area of a typical fluid particle, m²</td>
</tr>
<tr>
<td>$A_i$</td>
<td>average surface area of fluid particles of volume $V$, m²</td>
</tr>
<tr>
<td>$a$</td>
<td>half width of the base line of a cap bubble, m</td>
</tr>
<tr>
<td>$a_i$</td>
<td>interfacial area concentration, m⁻¹</td>
</tr>
<tr>
<td>$B_d$</td>
<td>volume of a typical fluid particle, m³</td>
</tr>
<tr>
<td>$C$</td>
<td>adjustable coefficient</td>
</tr>
<tr>
<td>$C_o$</td>
<td>distribution parameter in the drift flux model</td>
</tr>
<tr>
<td>$C_D$</td>
<td>drag coefficient</td>
</tr>
<tr>
<td>$C_d$</td>
<td>coefficient for the diameter of small bubbles from shearing-off mechanism</td>
</tr>
<tr>
<td>$C_l$</td>
<td>lift coefficient</td>
</tr>
<tr>
<td>$C_T$</td>
<td>turbulent dispersion coefficient</td>
</tr>
<tr>
<td>$C_w$</td>
<td>wall lubrication coefficient</td>
</tr>
<tr>
<td>$C_v$</td>
<td>momentum flux parameter</td>
</tr>
<tr>
<td>$D$</td>
<td>length scale or diameter, m, or diffusivity, m²s⁻¹</td>
</tr>
<tr>
<td>$D_{avg}$</td>
<td>average bubble diameter, m</td>
</tr>
<tr>
<td>$D_{c1}$</td>
<td>volume-equivalent diameter of a particle with the critical volume, m</td>
</tr>
<tr>
<td>$D_{c1}^{*}$</td>
<td>ratio of $D_{c1}$ to $D_{sm,1}$</td>
</tr>
</tbody>
</table>
$D_{c,\text{max}}$ maximum stable cap bubble limit, m

$D_d$ bubble drag diameter, m

$D_{dc}$ critical bubble diameter in phase change, m

$D_{d,\text{max}}$ maximum distorted bubble limit, m

$D_{ds}$ spherical bubble limit, m

$D_e$ volume-equivalent diameter, m

$D_H$ maximum horizontal dimension of a bubble, m

$D_s$ surface-equivalent diameter, m

$D_{sm}$ bubble Sauter mean diameter, m

$d_w$ distance between the bubble and the wall, m

$E_0$ Eotvos number

$\bar{F}$ force vector, kgms$^{-2}$

$f$ fluid particle number density distribution function per unit volume, m$^{-6}$, or drag function in drag coefficient model

$G$ gap of the flow duct, m, or production of turbulence kinetic energy per unit volume, kgm$^{-1}$s$^{-3}$

$\bar{g}$ gravitational acceleration constant, ms$^{-2}$

$H$ enthalpy per unit mass, m$^2$s$^{-2}$

$I$ turbulent intensity

$j$ superficial velocity, ms$^{-1}$

$k$ turbulence kinetic energy per unit mass or covariance of the velocities, m$^2$s$^{-2}$

$L_c$ critical distance, m
$M_i^*$ general interfacial force, kgms$^{-2}$

$\Delta \dot{m}_{12}$ net inter-group mass transfer rate from Group-1 to Group-2 bubbles due to bubble interactions and pressure effect, kgm$^{-3}$s$^{-1}$

$N_d$ number density of the gas (dispersed) phase, m$^{-3}$

$N_\mu$ viscous number

$n$ bubble number density, m$^{-3}$

$\vec{n}_w$ unit outward normal vector of the wall surface

$p$ pressure, kgm$^{-1}$s$^{-2}$

$\bar{\vec{q}}$ heat flux, kgs$^{-3}$

$R$ number source/sink rate per unit volume, m$^{-3}$s$^{-1}$, or radius of a pipe, m

$R_c^*$ dimensionless radius of curvature of a cap bubbles

$\text{RE}$ relative error, %

$Re$ Reynolds number

$R_{m2}$ radius of curvature of the maximum bubble in the system, m

$r$ radial position or apparent radius of curvature of a cap bubble, m

$S$ source term of a user-defined scalar (UDS), or slip ratio

$t$ time, s

$V$ fluid particle volume, m$^3$

$\vec{V}$ drift velocity, ms$^{-1}$

$\vec{v}$ velocity vector, ms$^{-1}$

$\vec{v}_r$ relative velocity, ms$^{-1}$

xxiii
\( \bar{v}_i \)  
- turbulent fluctuating velocity or root mean square of velocity fluctuations, 
\( \text{ms}^{-1} \)

\( W \)  
- width of the flow duct, m

\( We \)  
- Weber number

\( W_{em,2} \)  
- Weber number for maximum Group-2 bubbles

\( x \)  
- coordinate in width direction of the test section, m, or a vector

\( Y_M \)  
- contribution of the fluctuating dilatation to the dissipation rate, \( \text{kgm}^{-1}\text{s}^{-3} \)

\( y \)  
- coordinate in gap direction of the test section, m

\( z \)  
- coordinate along flow direction, m

**Greek symbols**

\( \alpha \)  
- void fraction

\( \Gamma \)  
- mass generation rate per unit volume, \( \text{kgm}^{-3}\text{s}^{-1} \), or diffusion coefficient of a UDS

\( \varepsilon \)  
- turbulent kinetic energy dissipation rate per unit mass, \( \text{m}^2\text{s}^{-3} \)

\( \eta \)  
- constant, or void fraction source/sink rate, \( \text{s}^{-1} \)

\( \theta \)  
- coefficient in turbulence model, or angle between the mean particle velocity and the mean relative velocity, or angle

\( \mu \)  
- dynamic viscosity, \( \text{kgm}^{-1}\text{s}^{-1} \)

\( \xi \)  
- modification factor

\( \rho \)  
- density, \( \text{kgm}^{-3} \)

\( \Delta \rho \)  
- density difference between two phases, \( \text{kgm}^{-3} \)
\( \sigma \) surface tension, kgs\(^{-2}\), or effective Prandtl number

\( \tau \) time constant

\( \mathbf{\tau} \) shear stress tensor, kgm\(^{-1}\)s\(^{-2}\)

\( \Phi \) interfacial area concentration source/sink rate, m\(^{-1}\)s\(^{-1}\), or a user-defined scalar, or source terms of \( k \) or \( \varepsilon \)

\( \phi \) energy dissipation per unit volume, kgm\(^{-1}\)s\(^{-3}\)

\( \chi \) coefficient that takes into account the inter-group void transport at the group boundary

\( \psi \) bubble shape factor

**Subscripts**

1 Group-1 bubbles

2 Group-2 bubbles

\( B \) Bassett

\( b \) bubble, or buoyancy

\( c \) critical, or boundary between Groups 1 and 2, or continuous phase

\( cr \) critical

\( d \) drag, or bubble, or dispersed phase

\( dr \) drift

\( EXP \) experimental

\( f \) liquid phase

\( g \) gas phase
\( h \)  
hydrodynamic

\( i \)  
interface between the phases

\( j \)  
index

\( k \)  
\( k^{th} \) phase, or turbulence kinetic energy

\( l \)  
lift, or liquid

**Model**  
numerical

\( \text{max} \)  
maximum

\( \text{min} \)  
minimum

\( n \)  
Group-\( n \)

\( p \)  
phase-\( p \)

\( \text{ph} \)  
phase change due to nucleation/condensation

\( \text{RC} \)  
random collision

\( SI \)  
surface instability

\( SO \)  
shearing-off

\( TD \)  
turbulent dispersion

\( TI \)  
turbulent impact

\( t \)  
total or turbulence

\( \text{vm} \)  
virtual mass

\( W \)  
wall lubrication

\( WE \)  
wake entrainment

\( x \)  
\( x \)-direction

\( y \)  
\( y \)-direction
$z$  \hspace{1cm} z-direction

$\varepsilon$  \hspace{1cm} turbulent kinetic energy dissipation rate

$\parallel$  \hspace{1cm} parallel

$\perp$  \hspace{1cm} perpendicular

**Superscripts**

(1) interactions with Group-1 bubbles

(11,2) coalescence of a Group-1 bubble with another Group-1 bubble to generate a Group-2 bubble

(12,2) coalescence of a Group-1 bubble with a Group-2 bubble to generate a Group-2 bubble

(2) interactions within Group-2 bubbles

(2,11) breakup of a Group-2 bubble to generate two Group-1 bubbles

(2,12) breakup of a Group-2 bubble to generate a (or multiple) Group-1 bubble(s) and a Group-2 bubble

$\text{exp}$  \hspace{1cm} experimental

$num$  \hspace{1cm} numerical

$T$  \hspace{1cm} turbulence

$\mu$  \hspace{1cm} viscous

**Mathematical symbols**

$<>$  \hspace{1cm} area averaging
void-weighted area averaging
Chapter 1. Introduction

1.1. Research background

Multiphase flow plays an important role in most industrial applications, such as power generation, energy conversion and safety technology in power plants, paper manufacturing, food processing, medical applications, as well as processes in the automobile, aeronautical and space industries. Multiphase flow is considered as a heterogeneous mixture of multiple fluids or phases, which are not homogeneously mixed at a molecular level but can be identified as macroscopic structures, such as solid particles, droplets, and bubbles, in a certain region. The variety of the types of multiphase flows is illustrated, of which two-phase flow is of particular significance. Depending on the constituents of the flow, Ishii (1975) suggested that two-phase flow was classified into four groups: solid-gas flow, gas-liquid flow, solid-liquid flow, and liquid-liquid flow consisting of two immiscible fluids.

Gas-liquid two-phase flow is not only crucial to many industrial problems but also important in some natural processes, as in the ocean-atmosphere interactions. Typical gas-liquid two-phase flow problems consist of void and pressure wave propagation, bubble-driven circulation systems, as well as some well-known thermal-hydraulic and safety problems in nuclear reactor systems. Issues relevant to nuclear reactor systems include critical heat flux (CHF) problems, direct contact condensation from emergency core cooling system (ECCS) injection, flow oscillations in boiling water reactors...
(BWRs), and heat transfer through boiling. Knowledge of two-phase flow is essential when we deal with economical and technological constraints, as well as safety and environmental issues involving two-phase flow. However, many important fluid dynamic and thermal aspects of the prevailing gas-liquid two-phase flows are still poorly understood.

The main difficulty in the physico-mathematical description of two-phase flow arises from the unknown interfaces separating the two phases of the mixture (Ishii, 1975). The physical difficulty lies in the modeling of fluid particle interactions and interfacial structures between the two phases, while the mathematical difficulty lies in the formulation of the two-phase flow as two separated single phases coupled with moving boundaries that could deform over time. The interfaces and discontinuities in fluid properties result in a singular-like behavior in Navier-Stokes equations. In particular, the large magnitude of the step change in the fluid density occurs at the interface as far as gas-liquid two-phase flow is concerned. Surface tension and the change in the thermal conductivity at the interface are equally important in the studies of the heat transfer and bubble dynamics.

Though two-phase flow usually exists in an unsteady manner, considerable effort has been made on the development of models that use macroscopic cells with averaged parameters, which eliminate the details of the local instantaneous values. To provide a macroscopic description of the flow parameters, an understanding of the fundamental mechanisms of local transfers and dynamics of fluid particles is required. In the past,
three main approaches have been used to develop a two-phase flow model (Ishii and Kocamustafaogullari, 1982):

(1) Interacting Continua Assumption -> Diffusion Model,

(2) Control Volume -> Postulated Balance Equations, and

(3) Averaging Method -> Averaged Balance Equations.

The developments of the first and second approaches are based primarily on the hypothesis that a two-phase flow system shares similarity with a single phase flow system.

In the first approach, it is assumed that the two phases exist simultaneously in the mixture. The mixture properties depend on the properties of each phase and its concentration in the mixture. The balances of the mixture are developed along with the transfers between phases or components, i.e., inter-diffusion of phases or components. In addition, interfacial transfer is lumped into a single term in the governing equations, which brings difficulties in understanding the interfacial transfers and developing the corresponding physical correlations. Furthermore, the conceptual difficulty of this method over the continuum assumption limits its applications in highly dispersed flows.

The second approach is to use a one-dimensional or quasi-one-dimensional model in a control volume where two separated phases flow in parallel with an interface. The balance equations for mass, momentum, and energy can be given either for a mixture as a whole or for individual phases. This model is capable of predicting separated two-phase flow such as annular flow under normal conditions, but it fails to predict the flow where transverse distribution is significant or under transient conditions.
The third method is more mathematically rigorous. High frequency signals from local instant fluctuations of a variable are eliminated in the averaging process, analogous to a low pass filter. The information of the statistical fluctuations, which may affect the macroscopic field, is reintroduced in the form of appropriate closure laws in the governing equations. The modeling of constitutive relations is usually very complicated and heavily dependent on empirical data. It may become even more complicated if phase change processes and/or chemical reactions are involved, which may result in an order of magnitude change in some flow properties and the mass, momentum and heat transfer between different phases across the interface boundary.

As far as a two-phase flow system is concerned, averaging procedures are categorized into Boltzmann averaging, Lagrangian averaging, and Eulerian averaging, of which the last one is widely used and focused on in the current work. The Eulerian averaging can be further classified into spatial averaging, temporal averaging, and ensemble averaging. The spatial averaging is performed around a fixed point at a certain time; whereas, the time averaging is performed at a fixed point over a time interval. The ensemble averaging is the statistical averaging procedure for a parameter at a fixed point and time over a large number of experiments with the same initial and boundary conditions. The ensemble averaging has necessitated the introduction of the ensemble averaged parameter such as void fraction as a pseudo-dependent parameter in the governing equations of two-phase flow models. The averaging method is limited when a high-resolution solution is required.
1.2. *Computational fluid dynamics codes and simulation scales*

High cost and restricted conditions of either full-size or scaled-down experimental facilities, as well as a rapid increase in computer technology, make computational fluid dynamics (CFD) a potentially promising method to understand two-phase flows. CFD simulations can be virtually performed with any configuration, providing qualitative and/or quantitative predictions.

A CFD package is usually written in either a procedural language or an object-oriented language, which are different in terms of data management and architecture. Both “in house” and “commercial” softwares have been developed in the literature. In order to produce trustworthy numerical solutions, intensive work on the robustness, accuracy and efficiency of CFD codes has to be performed with a wide set of validation tests in their reliability domains.

One difficulty in modeling and analyzing the thermal-hydraulics behavior of two-phase flow is the various hydrodynamic phenomena associated with their corresponding length scales, which typically range from several meters down to the Kolmogorov scales of turbulence. They are categorized as:

1. System scale, which is used to describe the whole system. It is useful in the accidental transient simulations for safety analysis, operation studies and real-time simulators.

2. Macro-scale, which is also called the component scale. This scale is useful in the design, safety and operation studies. The minimum spatial resolution is usually fixed by the sub-channel size, i.e., 1 cm.
(3) Meso-scale, which is dedicated to the scale of mm or less. This scale is associated with a turbulence model, such as RANS or LES. It is especially useful for local analysis of flows.

(4) Micro-scale, which denotes a characteristic length less than a micrometer. It allows simulations focusing on very small domains through Direct Numerical Simulation (DNS) such that the local flow phenomena can be understood. It is essential to develop closure relations for more macroscopic models.

In view of this, a “hierarchy of model” generally enables us to obtain valuable information on physical phenomena at a low cost and is appropriate for us to study the dynamic behavior of two-phase flow systems. In the current work, Fluent, a CFD code released by ANSYS, Inc., is considered to have a reasonable degree of maturity and reliability. Therefore, we chose the Fluent code as the simulation tool for two-phase flows.

1.3. Brief introduction to Fluent

Fluent is a control-volume-based CFD code written in the C++ language for multiple mesh types, such as structured hexahedral, unstructured tetrahedral, and hybrid meshes (Fluent 6.3 User’s Guide, 2006). In Fluent code, two fundamental approaches are available for multiphase modeling, i.e., Euler-Lagrange method and Euler-Euler method.

In the Euler-Lagrange approach, the Navier-Stokes equation is solved for the continuous phase while the trajectories of the individual dispersed phase are tracked in a Lagrangian frame of reference. This approach provides a detailed description of individual bubble motion and has greater generality and flexibility with respect to the
incorporation of the microscopic transport phenomena. For example, a bubble diameter
distribution can be easily incorporated and hydrodynamic interaction between
neighboring bubbles can be taken into account. However, this approach requires an
intensive computational load especially when the dispersed phase is not sufficiently
dilute.

On the other hand, the Euler-Euler approach is more efficient and effective to
model a wider range of multiphase flows with today’s computer capacity. For instance, in
one type of Euler-Euler model, namely, the Eulerian model, all of the different phases are
treated as interpenetrating continua governed by the conservation equation of mass,
momentum, and energy. In addition, the probability of occurrence of an individual phase
at one special location is specified by the instantaneous volume fraction of that phase at
that point. It is noteworthy that the Euler-Lagrange model can, to a certain extent, assess
the validity of the closure laws used in the Eulerian model. This Eulerian model is
essentially the two-fluid model, which will be discussed in the next section. The Eulerian
multiphase model is adopted in the present numerical studies.

1.4.  Two-fluid model

The two-fluid model was first proposed back in the late 1960s and early 1970s
(Ishii, 1975). The basic approach of the two-fluid model is to formulate the conservation
equations of mass, momentum and energy for a fixed control volume where both phases
co-exist with the assumption of interpenetrating continua or fluids. This balance must be
satisfied at any point in space and at any time, and thus requires two types of local
equations: 1) local instantaneous governing equations for each phase and 2) local instantaneous jump conditions, i.e., the interactions between the phases at the interface.

In the two-fluid model, each phase is represented by a local volume fraction (or void fraction if gas-liquid two-phase flow is considered) where the summation of volume fractions over all phases is unity at each location in the physical space and at each moment in time. The two separate sets of governing equations that represent the balance of mass, momentum, and energy for each phase are formulated according to Eqs. (1.1)-(1.3) (Ishii, 1975; Ishii and Mishima, 1984):

Continuity equation:

\[
\frac{\partial (\alpha_k \rho_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \bar{v}_k) = \Gamma_k, \tag{1.1}
\]

Momentum equation:

\[
\frac{\partial (\alpha_k \rho_k \bar{v}_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \bar{v}_k \bar{v}_k) = -\nabla(\alpha_k \rho_k) + \nabla \cdot \left[ \alpha_k \left( \bar{\tau}^\mu_k + \bar{\tau}^r_k \right) \right] + \alpha_k \bar{g} \\
+ \Gamma_k \bar{v}_{i,k} + p_{i,k} \nabla \alpha_k - \nabla \alpha_k \cdot \bar{\tau}^i_{i,k} + \bar{F}_{i,k}, \tag{1.2}
\]

Enthalpy equation:

\[
\frac{\partial (\alpha_k \rho_k \bar{H}_k)}{\partial t} + \nabla \cdot (\alpha_k \rho_k \bar{v}_k \bar{H}_k) = -\nabla \cdot \left( \alpha_k \left( \bar{q}_k + \bar{q}^r_k \right) \right) + \frac{D_k \left( \alpha_k \rho_k \right)}{Dt} + \Gamma_k \bar{H}_{i,k} \\
+ a_{i,k} \bar{q}''_{i,k} - p_{i,k} \frac{D_k \alpha_k}{Dt} + \phi_k. \tag{1.3}
\]

Here, the subscripts \( k \) and \( i \) stand for the \( k^{th} \) phase and the interface between the phases, respectively. \( \alpha, \rho, \bar{v}, \) and \( \bar{H} \) are the local time-averaged void fraction, density, velocity, and enthalpy, respectively. \( \bar{\tau}^\mu_k, \bar{\tau}^r_k, \bar{q}_k, \) and \( \bar{q}^r_k \) are the average viscous stress...
tenser, average turbulent stress tensor, conduction heat flux, and turbulent heat flux, respectively. As the void fraction alone is not enough to describe the spatial topological structure between the phases, the flow regime cannot be determined from Eqs. (1.1)-(1.3) alone.

Equations (1.1)-(1.3) contain unknown terms representing the coupled effects of one phase with the other. As aforementioned, the averaging in a two-phase flow model is more complex than that in a single-phase flow model. Physical and mathematical difficulties lie in the existence of the discontinuities in the properties across the phase interfaces, in addition to the mechanical and thermal non-equilibrium between different phases that result in the interfacial transfer terms in Eqs. (1.1)-(1.3). These transfer terms are $\Gamma_k$, $\vec{F}_{i,k}$, $\vec{F}_{i,k}$, and $q''_{i,k}$, which stand for the mass generation, generalized interfacial force, interfacial shear stress, and interfacial heat flux, respectively. These interfacial transfer terms follow the balance laws at the interface, resulting in the local jump conditions given by Eqs. (1.4)-(1.6):

$$\sum_k \Gamma_k = 0, \quad (1.4)$$

$$\sum_k \vec{F}_{i,k} = 0, \quad (1.5)$$

$$\sum_k \left( \Gamma_k H_{i,k} + a_i q''_{i,k} \right) = 0. \quad (1.6)$$

A comprehensive understanding and reliable modeling of these terms are indispensable to the overall accuracy of the two-fluid model. As discussed by Ishii and Mishima (1984), these terms are proportional to a geometric parameter, namely, the
interfacial area concentration, \( a_i \), defined as the total interfacial area per unit mixture volume. Mathematically, given the fluid particle number density distribution function, \( f(x,V,t) \), the interfacial area concentration can be calculated as

\[
a_i(x,t) = \int_{V_{\text{min}}}^{V_{\text{max}}} f(x,V,t) A_i(V) \, dV,
\]

where \( V_{\text{min}} \) and \( V_{\text{max}} \) are respectively the minimum and maximum volumes of all the fluid particles. \( A_i(V) \) is the averaged interfacial area of fluid particles having a volume of \( V \). A closure is needed to provide an accurate value for the interfacial area concentration.

In the literature, there are two popular approaches to evaluate the interfacial area concentration: the flow regime-dependent empirical correlations along with the flow regime transition criteria and the interfacial area transport equation. As pointed out by Hibiki and Ishii (2000b), this flow regime-based method cannot represent gradual transition of flow regimes, i.e., it provides instantaneous transitions of flow regimes, and may introduce non-physical oscillations. Other disadvantages of this method are its strong dependence on the geometry and dimensions of the system, as well as its inability to account for the boundary conditions and entrance effects. Therefore, a dynamic approach, namely, the interfacial area transport equation (IATE), has been developed to capture the changes of interfacial structure (Ishii, 1975). A detailed discussion of the IATE is provided in Chapter 2.
1.5. *Statement of the problem*

Some current CFD codes, such as CFX and Fluent, and some reactor system safety analysis codes, such as RELAP5, TRACE, and CATHARE, simulate gas-liquid two-phase flows using the two-fluid model, in which the static empirical correlations are typically applied for the coupled phasic transfer terms between different phases. For instance, in the Fluent 6.3.33 code, the evolution of the interfacial structure is not dynamically modeled and the bubble-bubble and bubble-eddy interactions are not taken into account. Instead, a constant-bubble-size assumption or a user-specified bubble size is usually applied in the code, which generally results in inaccurate predictions and non-physical oscillations in the code calculations. In some cases, the overall results may be acceptable, but are the results of incorrect physics.

To deal with these issues, the interfacial area transport equation, which has the potential to dynamically model the interfacial transfer terms, has been suggested and developed within the framework of the two-fluid model (Ishii, 1975; Kocamustafaogullari and Ishii, 1995; Millies et al., 1996; Wu et al., 1998a, 1998b; Kim, 1999; Morel et al., 1999; Hibiki and Ishii, 2000a, 2000b; Fu, 2001; Sun, 2001; Smith, 2002; Fu and Ishii, 2003a; Kim et al., 2003; Sun et al, 2004a; Vasavada, 2008; Vasavada et al., 2009).

Recently, the capabilities of CFD codes together with the IATE model for two-phase flow simulations have been examined. Graf and Papadimitriou (2007) demonstrated that the interfacial area concentration could be reasonably captured by the FLUBOX code equipped with the IATE model in upward vertical pipe flows. Bae et al.
developed a CFD code based on the finite volume method using the simplified marker and cell algorithm, and systematically coupled the two-fluid model and the one-group IATE. In addition, Wang (2007), Wang and Sun (2007, 2008, 2009), and Sari et al. (2009) implemented the one-group IATE into the Fluent code and conducted three-dimensional simulations for bubbly flows, both in a rectangular duct and a circular pipe. It was shown that the implementation of the one-group IATE into the Fluent code improved the predictions of the lateral phase distributions appreciably in some cases of bubbly flows in a pipe; though there existed some discrepancies between the simulations and experimental data for some flow conditions (Wang and Sun, 2007, 2008, 2009). This disagreement is possibly caused by the adjustable model coefficients of the one-group IATE model that were obtained from the one-dimensional model benchmark exercises (Kim, 1999; Ishii et al., 2002) but used for three-dimensional simulations. Thus, making a CFD model applicable to general three-dimensional two-phase flow conditions is still an unresolved issue.

1.6. Objectives

As aforementioned, when the two-fluid model with the one-group IATE model is applied, some disagreement still exists between code predictions and experiments in certain bubbly flow conditions. The first objective of the present study is to test the applicability of the coefficients derived by Ishii et al. (2002) to a three-dimensional simulation under pipe bubbly flow conditions by investigating the contributions of non-uniform lateral phase distributions to the source/sink terms of the one-group IATE model. A slightly different set of adjustable coefficients in the one-group IATE model are
suggested for the three-dimensional simulations and validated in air-water bubbly flow conditions in a circular pipe. The Fluent code with the one-group IATE model is further examined for air-water bubbly flows in a confined rectangular duct and two-component flows consisting of two immiscible liquids in a circular pipe.

Secondly, the present study aims at developing an approach to implement the two-group IATE model into the two-fluid model in the Fluent and accurately modeling two-phase flows in a wide range of flow conditions, including cap-bubbly and churn-turbulent flows. The issue of well-posedness of the proposed numerical model is carefully considered before model validation. The study on hyperbolic characteristics of the one-dimensional model is performed employing the momentum flux parameters. The proposed model is finally validated with experiments under different flow conditions.

1.7. *Dissertation outline*

In summary, the following main contributions of the present study are made:

1. Development of a set of coefficients in the one-group IATE model for a three-dimensional simulation

2. Validations of the two-fluid model with one-group IATE model in different bubbly flow conditions

3. Development of a methodology of implementing the two-group IATE model into the two-fluid model into the Fluent code

4. Investigations of the hyperbolicity of the one-dimensional two-fluid model with two-group IATE
(5) Validations of the two-fluid model with two-group IATE model in different flow conditions

(6) Investigations of the effects of the interfacial forces on the phase distributions in two-phase flows

Chapter 2 provides an introduction to the interfacial area transport equation (IATE), the development of one-group IATE and two-group IATE, as well as a discussion on the important bubble interaction mechanisms, which contribute to the source or sink terms in the IATE model.

In Chapter 3, the technical approach used to implement the IATE model into the two-fluid model is presented. A three-field two-fluid model is proposed with modifications made to the governing equations of mass, momentum, and energy. Particularly, the interfacial forces including the drag, lift, wall lubrication, and turbulent dispersion forces are discussed in detail.

The turbulence model is described in Chapter 4. Two types of the turbulence model, i.e., the standard and RNG models, are discussed.

Chapter 5 primarily shows the studies on the model validation when the one-group IATE model is implemented. Different flow conditions, including the air-water bubbly flows in a circular pipe and a confined channel, as well as liquid-liquid two-component flows in a circular pipe, are used for the purpose of validation. A set of model coefficients in the one-group IATE model is suggested for three-dimensional simulations.

In Chapter 6, a mathematical property is discussed, namely the well-posedness of the proposed numerical model. The characteristics of the one-dimensional model are
studied employing the momentum flux parameters, which help achieve the hyperbolicity of the model.

In Chapter 7, the two-fluid model equipped with two-group IATE model is validated by modeling cap-bubbly and churn-turbulent flows in a confined flow channel. Also, the effects of the interfacial forces on the lateral phase distributions in two-phase flows are investigated.

Chapter 8 presents the conclusions based on the previous chapters and provides recommendations for future work.
Chapter 2. Interfacial Area Transport Equations

This chapter provides an introduction to the interfacial area transport equation, the development of two types of IATE model, namely, the one-group IATE model and two-group IATE model, as well as a discussion on the important bubble interaction mechanisms in two-phase flows.

2.1. Background

Historically, an empirical approach based on two-phase flow regimes (shown in Figure 2.1) and regime transition criteria (Mishima and Ishii, 1984), was applied to calculate the interfacial area concentration. In this approach, flow regime transition criteria are based on bubble Reynolds number ($Re_b$) and viscous number ($N_\mu$), defined as

$$Re_b = \frac{\rho_f v_r D_d}{\mu_f} \quad (2.1)$$

and

$$N_\mu = \frac{\mu_f}{\left(\rho_f \sigma \sqrt{\frac{\sigma}{g \Delta \rho}}\right)^{1/2}} \quad (2.2)$$

Here, $\rho_f$, $v_r$, $D_d$, $\mu_f$, $\sigma$, $g$, and $\Delta \rho$ are respectively the density of the liquid (continuous) phase, magnitude of the relative velocity between the two phases, fluid particle (bubble or droplet) diameter, dynamic viscosity of the liquid (continuous) phase,
surface tension between the two phases, gravitational acceleration, and density difference between the two phases. Hibiki and Ishii (2000a) pointed out that this modeling approach, developed based on limited flow conditions, was applicable only when the flow was in steady state and fully developed. This approach also intrinsically introduces artificial discontinuities at flow regime transition, possibly with numerical instability.

![Flow regime map proposed by Mishima and Ishii (1984)](image)

Figure 2.1. Flow regime map proposed by Mishima and Ishii (1984)

In view of the shortcomings of the empirical approach, dynamic approaches, analogous to the Boltzmann transport equation, have been recently developed. One method is called the population balance equation, which is a transport equation for the number density function of the bubbles (Millies and Mewes, 1999). Both break-up and coalescence kernel functions have been proposed. Lehr and Mewes (2001) evaluated the
population balance equation using the concept of self-similarity to reduce the numerical effort and showed acceptable agreement. Another method is called the interfacial area transport equation, which was proposed to predict the evolution of the interfacial area concentration as a function of space and time (Ishii, 1975; Kocamustafaogullari and Ishii, 1995) and is used in the present work. In the formulation of the IATE, no assumption was made on the interface configuration, which helped to minimize the need for predetermining the flow regime transition in many phenomenological models and remedy numerical oscillatory behavior. As addressed by Hibiki and Ishii (2000a), the IATE, in theory, was capable of solving the interfacial area concentration in any flow regime dynamically and accurately if the mechanisms of bubble (or droplet) interactions, which served as the source/sink terms in the IATE, could be correctly furnished.

Simultaneously, to understand the dynamics of bubble interactions thoroughly, a considerable number of experiments of two-phase flows have been conducted in various flow passage configurations with different channel sizes, including circular pipes, annulus, and rectangular ducts, as well as with different flow orientations, such as upward and downward (Kocamustafaogullari and Wang, 1991; Ohnuki and Akimoto, 1996; Hassan et al., 1998; Suzanne et al., 1998; Barrau et al., 1999; Kashinsky and Randin, 1999; Kim, 1999; Wu and Ishii, 1999; Kim et al., 2000; Fu, 2001; Hibiki et al., 2001; Sun, 2001; Garnier et al., 2002; Hibiki et al., 2003). It was generally observed that depending on the flow conditions, the shapes of bubbles can be very different. In order to classify the bubble shapes in a two-phase flow system, four length scales are first defined as follows:
Sauter mean diameter:

\[ D_{sm} = \frac{6B_d}{A_i}, \]  
(2.3)

Drag diameter:

\[ D_d = \frac{6B_d}{4A_d}, \]  
(2.4)

Equivalent diameter:

\[ D_e \equiv \left( \frac{6}{\pi} \right)^{1/3} \]  
(2.5)

Surface diameter:

\[ D_s \equiv \left( \frac{A_i}{\pi} \right)^{1/2}, \]  
(2.6)

where \( B_d, A_i, \) and \( A_d \) are the volume, surface area, and projected area of a typical fluid particle (bubble or droplet).

As the number density of the gas (dispersed) phase and the interfacial area concentration are respectively given by \( N_d = \alpha_d / B_d \) and \( a_i = N_d A_i \), the interfacial area concentration can be expressed in different forms such as

\[ a_s = \frac{6\alpha_d}{D_{sm}} = \frac{6\alpha_d}{D_d} \left( \frac{D_d}{D_{sm}} \right). \]  
(2.7)

In gas-liquid two-phase flows, bubbles are separated into five different categories, namely, spherical, distorted, cap, Taylor (slug), and churn-turbulent. Bubbles with different shapes and sizes are expected to have different characteristics in the drag,
motion, and interaction mechanisms. The size distribution of bubbles may be modeled using the bubble distribution function, which is yet limited in practical applications. In that respect, a multi-group approach, analogous to the multi-group concept in the neutron transport theory, is a necessary and reasonable approximation. The bubble size is basically bounded by two limits, i.e., the lower limit determined by the bubble generation mechanism and fluid properties, and the upper limit mainly governed by the bubble surface instability. Three length scales, i.e., the spherical bubble limit \( D_{d, s} \), maximum distorted bubble limit \( D_{d, \text{max}} \), and maximum cap bubble limit \( D_{c, \text{max}} \) are proposed in order to determine the upper or lower limit of bubbles. They are defined as (Ishii and Zuber, 1979)

\[
D_{d, s} = 4\sqrt{\frac{2\sigma}{g\Delta \rho}} \left( \frac{\mu_f^2}{\sqrt{\rho_f^2 \sigma^3/(g\Delta \rho)}} \right)^{1/6},
\]

(2.8)

\[
D_{d, \text{max}} = 4\sqrt{\frac{\sigma}{g\Delta \rho}},
\]

(2.9)

and

\[
D_{c, \text{max}} = 40\sqrt{\frac{\sigma}{g\Delta \rho}}.
\]

(2.10)

Here, the maximum cap bubble limit is based on the Kelvin-Helmholtz and Rayleigh-Taylor instabilities.

As a result, a two-group approach has been proposed in the literature (Hibiki and Ishii, 2000b; Ishii and Kim, 2004). In the two-group approach, \( D_{d, \text{max}} \) is considered as the
transition length scale between Group-1 and Group-2 bubbles. Small spherical and
distorted bubbles with a diameter less than $D_{d,\text{max}}$ fall into Group-1; whereas larger cap,
Taylor, and churn-turbulent bubbles are categorized as Group-2 bubbles. When larger
bubbles grow to such an extent that the bubble size exceeds $D_{c,\text{max}}$, the bubbles become
unstable due to the interfacial instability along the leading nose of the bubble analogous
to Kelvin-Helmholtz instability. Thus, bubbles having a size greater than $D_{c,\text{max}}$ cannot
be sustained and will disintegrate into typically two cap or churn-turbulent bubbles very
quickly. As emphasized by Sun (2001), the two-group approach would inevitably
introduce some errors into the modeling; however, these errors can be corrected provided
that the major mechanisms of the bubble interactions were captured.

2.2. Interfacial area transport equation

The theoretical interfacial area transport equation was derived from the fluid
particle number density transport equation and established by Kocamustafaogullari and
Ishii (1995) as

$$\frac{\partial a_i}{\partial t} + \nabla \cdot (a_i \vec{v}_i) - \frac{\vec{V}}{V} \int_{V_{\text{min}}}^{V_{\text{max}}} f(V, x, t) V dA_i = \sum_j \phi_j + \phi_{\text{ph}}, \quad (2.11)$$

Here, the interfacial velocity, $\vec{v}_i$, which represents the interfacial area-weighted velocity
of the fluid particles, is defined as

$$\vec{v}_i(x, t) = \frac{\int_{V_{\text{min}}}^{V_{\text{max}}} f(V, x, t) A_i(V) \vec{v}(V, x, t) dV}{\int_{V_{\text{min}}}^{V_{\text{max}}} f(V, x, t) A_i(V) dV}, \quad (2.12)$$
where \( f(V, x, t) \) is the bubble density distribution function about a position \( x \) at a given time \( t \). The terms on the right hand side of Eq. (2.11) account for the contributions to the interfacial area concentration due to fluid particle (bubble or droplet) interaction mechanisms (\( \phi_j \)), and due to the phase changes caused by nucleation, evaporation, or condensation (\( \phi_{ph} \)). If isothermal adiabatic two-phase flow is considered, the second term (\( \phi_{ph} \)) is neglected.

As discussed in Section 1.1, the mean motion of two-phase flow strongly depends on the small-scale motion, requiring an understanding of the interactions of each bubble (or droplet) with the surrounding fluid as well as with each other. The mechanisms of bubble (or droplet) interactions in two-phase flow have been investigated since the late 19\(^{th}\) century. It was shown that the interactions usually depended on the flow conditions, fluid properties, and geometry of the flow channel. Furthermore, it was shown that all the mechanisms could be approximately categorized into the following eight classifications (Kim, 1999; Hibiki and Ishii, 2000b; Fu, 2001; Hibiki et al., 2001; Sun, 2001; Ishii and Kim, 2004): (1) coalescence between the fluid particles (bubbles or droplets) due to random collisions driven by turbulent eddies, (2) coalescence between the fluid particles due to wake entrainment, (3) disintegration of the fluid particles caused by turbulent eddy impact, (4) shearing-off of small fluid particles at the rim of large cap, slug or churn-turbulent fluid particles, (5) breakup of large cap and churn-turbulent fluid particles induced by flow instabilities, (6) collision due to velocity gradient near the wall region,
collision due to different rise velocity of fluid particles in different sizes, and breakup caused by laminar viscous force.

Typically, the possibility of collision among multiple (more than two) fluid particles is low compared to that of the binary collision. Thus, a binary collision is reasonably assumed. Categories (7) and (8) are neglected for an air-water system while category (6) is exclusively important in the region extremely close to the wall. Consequently, one-group and two-group IATEs were developed for air-water two-phase flows. The one-group IATE model includes interactions (1)-(3) that dominate in bubbly flows, and is therefore applicable in bubbly flows (Wu et al., 1998b; Kim, 1999); whereas, the two-group IATE model includes interactions (1)-(5), which collectively play an important role in flow regimes beyond bubbly flows (Smith, 2002; Fu and Ishii, 2003a; Sun et al., 2004a). In what follows, the fluid particle interaction mechanisms are investigated according to different flow regimes in order to complete the formulation of the one-group IATE model discussed in Section 2.3 and the two-group IATE model discussed in Section 2.4.

2.3. One-group IATE

The one-group IATE model is established by Wu et al. (1998b) and Kim (1999) as

\[
\frac{\partial a_i}{\partial t} + \nabla \cdot \left( a_i \vec{v}_i \right) = \frac{2}{3} \left( \frac{a_i}{\alpha} \right) \left( \frac{\partial \alpha}{\partial t} + \nabla \cdot \left( \alpha \vec{v}_g \right) - \eta_{ph} \right) + \frac{1}{3\psi} \left( \frac{\alpha}{a_i} \right)^2 \sum_j R_j + \phi_{ph}. \tag{2.13}
\]

Here, \( \vec{v}_g, \eta_{ph}, R_j, \) and \( \psi \) are, respectively, the bubble (or droplet) velocity, gas phase volume change rate due to phase change, bubble (or droplet) number density change rate...
due to the $j^{th}$ bubble (or droplet) interaction, and bubble (or droplet) shape factor. The first term on the right hand side in Eq. (2.13) accounts for the effects of pressure on the expansion or contraction of the gas phase. $\psi$ is defined as $\psi = \frac{1}{36\pi} \left( \frac{D_{sm}}{D_e} \right)^3$. The value of $D_{sm}$ is equal to that of $D_e$ for a spherical shape of fluid particle. If a gas-liquid bubbly flow system is considered, the fluid particle is a bubble.

To start with the discussions on the bubble interaction mechanisms, a parameter called the Weber number ($We$) is first defined as the ratio of the particle turbulent inertial energy to the surface energy as: $We = \rho_f |\bar{v}_t|^2 D_{avg}/\sigma$, where $\bar{v}_t$ and $D_{avg}$ are the turbulent velocity of the liquid phase and average bubble diameter, respectively. The critical value, $We_{cr}$, is used to describe a condition where the cohesive and disruptive forces balance. If the turbulent eddies are strong enough to overcome the surface tension force of the bubbles, i.e., $We$ is larger than $We_{cr}$, the disintegration of the bubbles caused by the impact of turbulence eddies will occur, contributing to the generation of the interfacial area concentration as (Wu et al., 1998b; Kim, 1999)

$$R_{II} = \frac{C_{II} \psi \left( a_i^4 |\bar{v}_l|^6 \right)}{6 \left( \frac{\alpha^3}{a_i^3} \right)} \sqrt{1 - \frac{We_{cr}}{We} \exp(-\frac{We_{cr}}{We})}, \text{ if } We > We_{cr}. \quad (2.14)$$

Collision of the bubbles should happen before the coalescence takes place, resulting in the occurrence of coalescence determined by both the bubble collision events and the probability of collisions resulting in coalescence. In history, the coalescence was treated as a two-stage process (Coulaloglou and Tavlarides, 1977): first, a small amount
of liquid between the bubbles at the collision was trapped; next, the liquid film between contacting surfaces was drained, followed by the rupture of the film. In bubbly flows, the dominant mechanisms of the bubble coalescence are either caused by the turbulence-driven random collision or due to the wake entrainment.

One mechanism of the bubble coalescences in bubbly flows is caused by turbulence-driven random collisions. The bubble collision is assumed to take place in an isotropic turbulence system. This phenomenon is therefore similar to the intermolecular collisions in an ideal gas, and the collision frequency is calculated using the kinetic theory of gas molecules. The two colliding bubbles are assumed to have the same size. The constitutive relation of $R_{WE}$ is given as (Wu et al., 1998b; Kim, 1999)

$$R_{RC} = -36\psi^2 C_{RC} \times \alpha^4 \left| \frac{\partial}{\partial t} \right| \left[ 1 - \exp \left( -\frac{C\alpha^{1/3} \alpha^{1/3} \alpha^{1/3}}{\left( \alpha^{1/3} - \alpha^{1/3} \right)} \right) \right].$$

In the above closure model, $\alpha_{max}$ is the void fraction at the bubble maximum packing. The adjustable coefficient $C_{RC}$ is used to account for the coalescence efficiency instead of the complicated model applying film drainage theory.

The other mechanism of the bubble coalescences in bubbly flows is due to the entrainment of the following bubbles in the wake region of a preceding bubble, resulting in the loss of the interfacial area concentration. A critical distance has been discovered between the following and leading bubbles, within which the following bubbles will make collision with the leading bubble without exception, if time is allowed. The critical distance ($L_c$) is generally proposed as
\[ L_c \sim 5D_d^3, \]  

(2.16)

where \( D_d \) is the diameter of the leading bubble. The mechanism, \( R_{WE} \), is proportional to the relative velocity between the liquid (continuous) and gas (dispersed) phases, \( \vec{v}_r \), and can be modelled as (Wu et al., 1998b; Kim, 1999)

\[ R_{WE} = -36\psi^2C_{WE}C_D^{1/3} \frac{a_4^4|\vec{v}_r|}{\alpha^2}, \]  

(2.17)

where \( C_D \) is the drag coefficient.

In Eqs. (2.14), (2.15), and (2.17), \( C_{TI}, C_{WE}, C_{RC} \) and \( C \) are model coefficients determined experimentally by comparing the values of the interfacial area concentration obtained from numerical calculations to those from the experimental data.

2.4. \textit{Two-group IATE}

In the flow regimes beyond bubbly flows, the substantial differences in sizes and shapes of bubbles complicate the bubble interactions, requiring that the one-group IATE be extended to the two-group IATE model, which is formulated as (Hibiki and Ishii, 2000b; Fu, 2001; Sun, 2001; Fu and Ishii, 2003a; Ishii and Kim, 2004; Sun et al., 2004a)

\[
\begin{align*}
\frac{\partial a_{i,1}}{\partial t} + \nabla \cdot (a_{i,1} \vec{v}_{i,1}) &= \left[ \frac{2}{3} - \chi \left( \frac{D_{c1}}{D_{sm,1}} \right)^2 \right] \left[ \frac{a_{i,1}}{\alpha_1} \right] \frac{\partial \alpha_1}{\partial t} + \nabla \cdot \left[ \alpha_1 (\vec{v}_{g,1}) - \eta_{ph,1} \right] \\
&+ \Phi_{ph,1} + \sum_j \Phi_{j,1},
\end{align*}
\]  

(2.18)

and
\[
\frac{\partial \alpha_{i,2}}{\partial t} + \nabla \cdot \left( \alpha_{i,2} \vec{v}_{i,2} \right) = \frac{2}{3} \left( \frac{a_{i,2}}{\alpha_{2}} \right) \left( \frac{\partial \alpha_{2}}{\partial t} + \nabla \cdot \left( \alpha_{2} \vec{v}_{g,2} \right) \right) - \eta_{ph,2} + \nabla \cdot \left( \alpha_{2} \vec{v}_{g,2} \right) - \eta_{ph,2} + \chi \left( \frac{D_{cl}}{D_{sm,1}} \right)^2 \left( \frac{a_{i,1}}{\alpha_{1}} \right) \left( \frac{\partial \alpha_{1}}{\partial t} + \nabla \cdot \left( \alpha_{1} \vec{v}_{g,1} \right) \right) - \eta_{ph,1} + \Phi_{ph,2} + \sum_{j} \Phi_{j,2},
\]

where \( D_{cl} \) is the volume-equivalent diameter of a bubble having the critical volume.

\( D_{sm,n} \) is the Sauter mean diameter defined as

\[
D_{sm,n} = 6 \frac{\alpha_{n}}{a_{i,n}},
\]

(2.20)

where the subscript \( n \ (n = 1 \text{ or } 2) \) refers to Group-\( n \) bubble. \( \eta_{ph,n} \), \( \Phi_{ph,n} \), and \( \Phi_{j,n} \) denote, respectively, the void fraction source/sink due to phase change, interfacial area concentration source/sink due to phase change, and interfacial area concentration source/sink due to bubble interactions for Group-\( n \) bubbles. The inter-group transfer coefficient \( (\chi) \), which is usually between 0 and 2 depending on the bubble distributions, takes into account the inter-group void transport at the group boundary due to expansion and compression of bubbles. \( \chi \) is calculated based on the Group-1 bubble size probability distribution \( (f) \) as

\[
\chi = \frac{fV_{c}}{\int_{V_{min}}^{V_{c}} f dV} = \frac{fV_{c}}{n_{1}},
\]

(2.21)

Here, \( n_{1} \) is the bubble number density for Group-1 bubbles. \( f_{c} \) and \( V_{c} \) are the bubble number density distribution and bubble volume at the group boundary between the two
groups, respectively. However, it is usually very complicated to get the bubble number density distribution with respect to the bubble volume, as discussed by Sun (2001).

In addition, the following relations exist (Sun et al., 2003):

\[ \alpha = \alpha_1 + \alpha_2, \quad (2.22) \]
\[ a_i = a_{i1} + a_{i2}, \quad (2.23) \]
\[ \bar{v}_g = \frac{\alpha_1 \bar{v}_g}{\alpha_1 + \alpha_2} + \frac{\alpha_2 \bar{v}_g^2}{\alpha_1 + \alpha_2}, \quad (2.24) \]

Similar to the discussions on the one-group IATE model, appropriate closure laws of \( \Phi_{j,n} \) should be carefully established through theoretical modeling of the bubble interaction mechanisms as to close the two-group IATE model. As the size of the bubble increases, the transport mechanisms are further complicated due to additional phenomena such as shearing-off and surface instability.

First of all, the bubble coalescence due to turbulent-driven collision is considered. There are four kinds of bubble collisions driven by turbulent eddies: coalescence of two Group-1 bubbles to generate a Group-1 bubble, coalescence of two Group-1 bubbles to generate a Group-2 bubble, coalescence between a Group-1 bubble and a Group-2 bubble to create a Group-2 bubble, and coalescence of two Group-2 bubbles to generate a Group-2 bubble.

Similarly, there are four types of bubble coalescence due to wake entrainment: coalescence of two Group-1 bubbles to produce a Group-1 bubble, coalescence of two Group-1 bubbles to provide a Group-2 bubble, coalescence of a Group-1 bubble and a

It is noted that there are other mechanisms resulting in bubble coalescence, such as buoyancy and laminar shear. These mechanisms are not very important in the gas-liquid two-phase flows in nuclear power plant applications, and therefore they are not considered in this dissertation.

For the mechanism of bubble breakup due to turbulent impact, binary breakup is assumed. During this process, appropriate eddy size is required, since very small eddies do not provide sufficient energy to make significant effects on the bubble motion while much larger eddies simply transport bubbles without leading to significant relative motion. Eddies responsible for bubble breakup are usually assumed to be bounded by 20% and 100% of the bubble size.

The phenomenon of bubble breakup due to surface instability is important in the flow regimes ranging from the Taylor (slug) flow regime to the churn-turbulent regime (Mishima and Ishii, 1984). This mechanism is mainly caused by the interfacial wave instability developed at the gas-liquid interface (Kocamustafogullari et al., 1984; Miller et al., 1993). The initial growth of interfacial wave instability is due to the Kelvin-Helmholtz instability and later driven by Rayleigh-Taylor instability. As Group-2 bubbles exceed the maximum stable bubble limit, the bubble breakup takes place.

The phenomenon of shearing-off of small bubbles at the rim of large bubbles occurs when the disruptive force (interfacial shear force) pulling at the rim of the cap exceeds the cohesive surface tension force of the large bubbles. The sizes of shear-off
bubbles can be analyzed based on the captured images. It has been determined that the
distribution information is too complicated to be utilized in the model, and a mean
diameter related to the bubble velocity is usually used.

Sun (2001) undertook a detailed investigation on the inter-group (between the
two-groups) and intra-group (within the same group) bubble interaction mechanisms, of
which the contributions to the generation and loss of the interfacial area concentration for
Group-1 and Group-2 bubbles are summarized in Table 2.1.
<table>
<thead>
<tr>
<th>Mechanisms</th>
<th>Group interactions</th>
<th>Contributions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbulent disintegration</td>
<td>(1)-&gt;(1)+(1)</td>
<td>Source in Group-1, $\Phi_{T1.1}^{(1)}$</td>
</tr>
<tr>
<td>Turbulent disintegration</td>
<td>(2)-&gt;(1)+(1)</td>
<td>Source in Group-1, $\Phi_{T1.1}^{(2,11)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Sink in Group-2, $\Phi_{T2.2}^{(2,11)}$</td>
</tr>
<tr>
<td>Turbulent disintegration</td>
<td>(2)-&gt;(1)+(2)</td>
<td>Source in Group-1, $\Phi_{T1.1}^{(2,12)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Sink in Group-2, $\Phi_{T2.2}^{(2,12)}$</td>
</tr>
<tr>
<td>Turbulent disintegration</td>
<td>(2)-&gt;(2)+(2)</td>
<td>Source in Group-2, $\Phi_{T2.2}^{(2)}$</td>
</tr>
<tr>
<td>Random Collision</td>
<td>(1)+(1)-&gt;(1)</td>
<td>Sink in Group-1, $\Phi_{RC,1}^{(1)}$</td>
</tr>
<tr>
<td>Random Collision</td>
<td>(1)+(1)-&gt;(2)</td>
<td>Sink in Group-1, $\Phi_{RC,1}^{(11,2)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Source in Group-2, $\Phi_{RC,2}^{(11,2)}$</td>
</tr>
<tr>
<td>Random Collision</td>
<td>(1)+(2)-&gt;(2)</td>
<td>Sink in Group-1, $\Phi_{RC,1}^{(12,2)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Source in Group-2, $\Phi_{RC,2}^{(12,2)}$</td>
</tr>
<tr>
<td>Random Collision</td>
<td>(2)+(2)-&gt;(2)</td>
<td>Sink in Group-2, $\Phi_{RC,2}^{(2)}$</td>
</tr>
<tr>
<td>Wake entrainment</td>
<td>(1)+(1)-&gt;(1)</td>
<td>Sink in Group-1, $\Phi_{WE,1}^{(1)}$</td>
</tr>
<tr>
<td>Wake entrainment</td>
<td>(1)+(1)-&gt;(2)</td>
<td>Sink in Group-1, $\Phi_{WE,1}^{(11,2)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Source in Group-2, $\Phi_{WE,2}^{(11,2)}$</td>
</tr>
<tr>
<td>Wake entrainment</td>
<td>(1)+(2)-&gt;(2)</td>
<td>Sink in Group-1, $\Phi_{WE,1}^{(12,2)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Source in Group-2, $\Phi_{WE,2}^{(12,2)}$</td>
</tr>
<tr>
<td>Wake entrainment</td>
<td>(2)+(2)-&gt;(2)</td>
<td>Sink in Group-2, $\Phi_{WE,2}^{(2)}$</td>
</tr>
<tr>
<td>Shearing-off</td>
<td>(2)-&gt;(1)+(2)</td>
<td>Source in Group-1, $\Phi_{SO,1}^{(2,12)}$</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Sink in Group-2, $\Phi_{SO,2}^{(2,12)}$</td>
</tr>
<tr>
<td>Surface instability</td>
<td>(2)-&gt;(2)+(2)</td>
<td>Source in Group-2, $\Phi_{SI,2}^{(2)}$</td>
</tr>
</tbody>
</table>

Table 2.1 Summary of source and sink of the interfacial area concentration in the two-group IATE (Sun, 2001)

The expressions of these models are summarized as follows (Sun, 2001):

For turbulent impact:
\[ \Phi_{TI}^{(1)} = 0.12C_{TI}^{(1)} \varepsilon^{1/3} (1 - \alpha) a_{n1}^{5/3} \exp \left( - \frac{W_{e,TT1}}{W_{e1}} \right) \sqrt{1 - \frac{W_{e,TT1}}{W_{e1}}}; \]

\[ \Phi_{TI,1}^{(2,1)} = \Phi_{TI,1}^{(2,11)} + \Phi_{TI,1}^{(2,12)} \]

\[ = 2.71C_{TI}^{(2)} \varepsilon^{1/3} G^{1/2} \alpha_2^2 (1 - \alpha) \frac{R_c^{3/3}}{R_m^{7/3}} \exp \left( - \frac{W_{e,TT2}}{W_{e2}} \right) \sqrt{1 - \frac{W_{e,TT2}}{W_{e2}}}; \]

\[ \Phi_{TI,2}^{(2,11)} = \Phi_{TI,2}^{(2,11)} + \Phi_{TI,2}^{(2,12)} + \Phi_{TI,2}^{(2)} \]

\[ = 1.4C_{TI}^{(2)} \varepsilon^{1/3} G \frac{R_{m8}^{2/3}}{R_{m2}^{1/3}} (1 - \alpha) \left( 1 - 2 R_c' \right) \exp \left( - \frac{W_{e,TT2}}{W_{e2}} \right) \sqrt{1 - \frac{W_{e,TT2}}{W_{e2}}}. \]

For random collision:

\[ \Phi_{RC,1}^{(1)} = \Phi_{RC,1}^{(1)} + \Phi_{RC,1}^{(11)} \]

\[ = -0.17C_{RC}^{(1)} \varepsilon^{1/3} \alpha_{\max}^{1/3} a_{n1}^{5/3} \left( 1 - \frac{\alpha_{\max}^{1/3} a_{n1}^{5/3}}{\alpha_{\max}^{1/3} - \alpha_1^{1/3}} \right) \left( 1 - \exp \left( -C_{RC1} \frac{\alpha_{\max}^{1/3} a_{n1}^{5/3}}{\alpha_{\max}^{1/3} - \alpha_1^{1/3}} \right) \right); \]

if \( D_{c1} < 1.5, \)

\[ \Phi_{RC,2}^{(11,2)} = 0.68C_{RC}^{(1)} \varepsilon^{1/3} \alpha_{\max}^{1/3} \alpha_{n1}^{5/3} \left( 1 - \frac{\alpha_{\max}^{1/3} a_{n1}^{5/3}}{\alpha_{\max}^{1/3} - \alpha_1^{1/3}} \right) \]

\[ \times \left[ 1 + 0.7G^{7/6} \frac{a_{ii}}{\alpha_1} \left( \frac{\sigma}{g \Delta \rho} \right)^{-1/3} \left( 1 - \frac{2}{3} D_{c1} \right) \right]; \]

\[ \Phi_{RC,1}^{(11,2)} = -4.85C_{RC}^{(11,2)} \varepsilon^{1/3} \alpha_{\max}^{1/3} \alpha_{n1}^{5/3} \frac{R_{m2}^{2/3}}{R_m^{7/3}} \left( 1 - \frac{\alpha_{\max}^{1/3} a_{n1}^{5/3}}{\alpha_{\max}^{1/3} - \alpha_1^{1/3}} \right) \]

\[ \times \left[ 1 + 0.7G^{7/6} \frac{a_{ii}}{\alpha_1} \left( \frac{\sigma}{g \Delta \rho} \right)^{-1/3} \left( 1 - \frac{2}{3} D_{c1} \right) \right]; \]
\[ \Phi_{RC,2}^{(12,2)} = 13.6 C_{RC}^{(12,2)} \frac{e^{1/3} \alpha_{1}^{5/3} \alpha_{2}^{2}}{R_{m_{2}}^{2/3} G} \left( 1 + \frac{10.3 G}{R_{m_{2}}} \right) \left[ 1 - \exp \left( -C_{RC1} \frac{\alpha_{1}^{1/3} \alpha_{1}^{1/3}}{\left( \alpha_{1,max}^{1/3} - \alpha_{1}^{1/3} \right)} \right) \right] ; \]

\[ \Phi_{RC}^{(2)} = -13.6 C_{RC}^{(2)} \frac{\alpha_{2}^{2/3} e^{1/3}}{W_{2}^{2/3}} \frac{R_{m_{2}}^{4/3}}{1 - 2.0 R_{c}^{*} + \frac{9.0 G}{R_{m_{2}}}} \left[ 1 - \exp \left( -C_{RC2} \alpha_{2}^{1/2} \right) \right] . \]

For wake entrainment:

\[ \Phi_{WE,1}^{(1*)} = \Phi_{WE,1}^{(1)} + \Phi_{WE,1}^{(11,2)} \]

\[ = -0.27 C_{WE}^{(1)} u_{r_{1}} C_{D1}^{1/3} a_{2}^{2} ; \]

for \( D_{c1}^{*} < 1.5, \)

\[ \Phi_{WE,2}^{(11,2)} = 1.08 C_{WE}^{(11,2)} u_{r_{1}} C_{D1}^{1/3} \frac{\alpha_{1} a_{1}}{G} \left( 1 - \frac{2}{3} D_{c1}^{*} \right) \left[ 1 + 0.7 G^{2/3} \left( \frac{a_{r_{1}}}{\alpha_{1}} \right)^{2} \left( \frac{\sigma}{g \Delta \rho} \right)^{-1/3} \right] ; \]

\[ \Phi_{WE,1}^{(12,2)} = -4.35 C_{WE}^{(12,2)} \sqrt{g C_{D2} G} \frac{a_{r_{1}} \alpha_{2}}{R_{m_{2}}} ; \]

\[ \Phi_{WE,2}^{(12,2)} = 26.1 C_{WE}^{(12,2)} \alpha_{1} \alpha_{2} \sqrt{g C_{D2} G} \frac{1}{R_{m_{2}}} \left( 1 + 4.31 \frac{G}{R_{m_{2}}} \right) ; \]

\[ \Phi_{WE,2}^{(2)} = -15.9 C_{WE}^{(2)} \frac{\alpha_{2}^{2}}{R_{m_{2}}^{2}} \sqrt{g C_{D2} G} \left( 1 + 0.51 R_{c}^{*} \right) . \]

For shearing-off:

\[ \Phi_{SO,1}^{(2,12)} = 64.51 C_{SO} C_{d}^{2} \frac{\alpha_{2} \nu_{r_{1}}}{G R_{m_{2}}} \left[ 1 - \left( \frac{We_{c,SO}}{We_{m_{2}}} \right)^{3} \right] ; \]
\[ \Phi_{SO,2}^{(2,12)} = -21.50C_{SO}C_d^3 \left( \frac{\sigma}{\rho_f} \right)^{3/5} \frac{\alpha_2}{\eta^{1/5}} \left( \frac{G^{8/5}}{R_{m,2}} \right)^{1/3} \left[ 1 - \left( \frac{W_{e,SO}}{W_{e,m,2}} \right)^3 \right] + 3.24G \left( \frac{W_{e,SO}}{W_{e,m,2}} \right)^2 \].

For surface instability:

\[ \Phi_{SI,2}^{(2)} = 1.25\alpha_2^2 \left( \frac{\sigma}{g \Delta \rho} \right)^{-1} \times \left[ C_{RC}^{(2)} \left( \frac{\sigma}{W^2} \right) \right]^{7/6} \left[ 1 - \exp \left( -C_{RC2} \alpha_2^{1/2} \right) \right] \left[ \left( \frac{\sigma}{g \Delta \rho} \right) \right]^{7/6} + 2.3 \times 10^{-4} C_{WE}^{(2)} \sqrt{C_D g G} \].

In the above models, there are adjustable coefficients, \( C_d, C_{RC1}, C_{RC2}, W_{e,TI1}, \)

\( W_{e,TI2}, W_{e,SO}, C_{RC}^{(1)}, C_{RC}^{(12,2)}, C_{RC}^{(2)}, C_{WE}^{(1)}, C_{WE}^{(12,2)}, C_{WE}^{(2)}, C_{SO}, C_{TI}^{(1)}, \) and \( C_{TI}^{(2)} \), which should be determined based on experiments using a systematic approach.

Therefore, \( \Phi_{i,1} \) and \( \Phi_{i,2} \) are proposed as: (Sun, 2001)

\[ \Phi_{i,1} = \Phi_{TI,1}^{(1)} + \Phi_{TI,1}^{(2,11)} + \Phi_{TI,1}^{(2,12)} + \Phi_{RC,1}^{(1)} + \Phi_{RC,1}^{(12,2)} + \Phi_{WE,1}^{(1)} + \Phi_{WE,1}^{(12,2)} + \Phi_{WE,1}^{(2)} + \Phi_{SO,1}^{(2,12)} \]

and

\[ \Phi_{i,1} = \Phi_{TI,2}^{(2,11)} + \Phi_{TI,2}^{(2,12)} + \Phi_{RC,2}^{(2)} + \Phi_{RC,2}^{(11,2)} + \Phi_{RC,2}^{(12,2)} + \Phi_{WE,2}^{(2)} + \Phi_{WE,2}^{(11,2)} + \Phi_{WE,2}^{(12,2)} + \Phi_{SO,2}^{(2,12)} \]

+ \( \Phi_{SI,2}^{(2)} \).
Chapter 3. Technical Approach

3.1. Implementation of IATE into Fluent

An investigation of the Fluent 6.3.33 code indicates that the bubble size must be specified by users as a constant or a function. In addition, the Fluent 6.3.33 code does not take into account the interactions among fluid particles and between fluid particles and turbulent eddies, which affect the interfacial structure of the two-phase flow. To model the evolution of the interfacial structure dynamically, the interfacial area concentration parameter is introduced into the Fluent code as a user-defined scalar (UDS), which is solved with its default transport equation in order to facilitate the flexibility and expand the capabilities of the Fluent code. When multiphase flow is simulated, two kinds of UDS, i.e. UDS per phase and UDS of mixture, can be specified associated with different levels of computational cells.

If the UDS \( \Phi \) is defined in the gas phase domain in the Fluent code, the transport equation for \( \Phi \) is given as (Fluent 6.3 User’s Guide, 2006):

\[
\frac{\partial (\alpha \rho_g \Phi)}{\partial t} + \nabla \cdot \left( \alpha \rho_g \vec{v}_g \Phi - \alpha \Gamma_g \nabla \Phi \right) = S_g, \tag{3.1}
\]

where \( \Gamma_g \) and \( S_g \) are the diffusion coefficient and source terms for \( \Phi \), respectively. The first term on the left hand side of Eq. (3.1) indicates the temporal evolution of \( \Phi \); the second term on the left hand side is the convection and diffusion of \( \Phi \). Given appropriate initial and boundary conditions, the value of \( \Gamma_g \), and the closure laws for \( S_g \), the Fluent
The code solves the transport equation of UDS in the same way that the Fluent code does for default scalars defined in the code.

The methodology to incorporate the two-group IATE model into the two-fluid model in the Fluent code is based on Eq. (3.1). The interfacial area concentration of Group-\(n\), \(a_{i,n}\), is defined as the UDS in the gas phase domain in the Fluent code and then substituted into Eq. (3.1). Equation (3.1) is then rewritten as

\[
\frac{\partial \left( \alpha_n \rho g a_{i,n} \right)}{\partial t} + \nabla \cdot \left( \alpha_n \rho g a_{i,n} \Gamma_{g,n} \nabla a_{i,n} \right) = S_{g,n}. \tag{3.2}
\]

On the other hand, if it is assumed that \(a_{i,n} (x,t) \approx \tilde{a}_{i,n} (x,t)\), the two-group IATE model given in Section 2.4 can be reformulated as:

for Group-1

\[
\frac{\partial a_{i,1}}{\partial t} + \nabla \cdot \left( a_{i,1} \tilde{v}_{g,1} \right) = \left[ \frac{2}{3} - \chi \left( D_{c1} \right)^2 \left( \frac{a_{i,1}}{\alpha_1} \right) \right] \frac{\partial \alpha_1}{\partial t} + \nabla \cdot \left( \alpha_1 \tilde{v}_{g,1} \right) - \eta_{ph,1} + \Phi_{ph,1} + \sum_j \Phi_{j,1}, \tag{3.3}
\]

and for Group-2

\[
\frac{\partial a_{i,2}}{\partial t} + \nabla \cdot \left( a_{i,2} \tilde{v}_{g,2} \right) = \frac{2}{3} \left( \frac{a_{i,2}}{\alpha_2} \right) \frac{\partial \alpha_2}{\partial t} + \nabla \cdot \left( \alpha_2 \tilde{v}_{g,2} \right) - \eta_{ph,2} + \Phi_{ph,2} + \sum_j \Phi_{j,2}. \tag{3.4}
\]
If one compares Eqs. (3.3) and (3.4) to Eq. (3.2), the diffusion coefficient \( \Gamma_{g,n} \) must be set equal to zero, for which the physical interpretation is that there is no diffusion of the interfacial area concentration in the flow field. By multiplying the two-group IATE model with \( \alpha_i \rho_g \) on both sides, the source term shown on the right hand side of Eq. (3.2) is determined as:

for Group-1

\[
S_{g,1} = a_{i,1} \left[ \frac{\partial (\alpha_i \rho_g)}{\partial t} + \vec{v}_{g,1} \nabla \cdot (\alpha_i \rho_g) \right] + a_{i,1} \rho_g \left[ \frac{2}{3} - \chi \left( \frac{D_{c1}}{D_{sm,1}} \right)^2 \frac{\partial \alpha_1}{\partial t} + \nabla \cdot (\alpha_1 \vec{v}_{g,1}) - \eta_{ph,1} \right] + \rho_1 \left( \Phi_{ph,1} + \sum_j \Phi_{j,1} \right),
\]

and for Group-2

\[
S_{g,2} = a_{i,2} \left[ \frac{\partial (\alpha_i \rho_g)}{\partial t} + \vec{v}_{g,2} \nabla \cdot (\alpha_i \rho_g) \right] + a_{i,1} \rho_g \left[ \frac{2}{3} \frac{\partial \alpha_2}{\partial t} + \nabla \cdot (\alpha_2 \vec{v}_{g,2}) - \eta_{ph,2} \right] + a_{i,1} \rho_g \left\{ \chi \left( \frac{D_{c1}}{D_{sm,1}} \right)^2 \frac{\partial \alpha_1}{\partial t} + \nabla \cdot (\alpha_1 \vec{v}_{g,1}) - \eta_{ph,1} \right\} + \rho_2 \left( \Phi_{ph,2} + \sum_j \Phi_{j,2} \right).
\]

If it is adiabatic flow without phase change effect, the two-group IATE model can be further simplified as:

for Group-1
\[
\frac{\partial a_{i,1}}{\partial t} + \nabla \cdot \left( a_{i,1} \vec{v}_{g,1} \right) = \left( \frac{2}{3} - \chi \left( \frac{D_{cl}}{D_{sm,1}} \right)^2 \right) \left( \frac{a_{i,1}}{\alpha_1} \right) \left( \frac{\partial \alpha_1}{\partial t} + \nabla \cdot \left( \alpha_1 \vec{v}_{g,1} \right) \right) + \sum_j \Phi_{j,1}, \quad (3.7)
\]

and for Group-2
\[
\frac{\partial a_{i,2}}{\partial t} + \nabla \cdot \left( a_{i,2} \vec{v}_{g,2} \right) = \left( \frac{2}{3} \right) \left( \frac{a_{i,2}}{\alpha_2} \right) \left( \frac{\partial \alpha_2}{\partial t} + \nabla \cdot \left( \alpha_2 \vec{v}_{g,2} \right) \right) + \chi \left( \frac{D_{cl}}{D_{sm,1}} \right)^2 \frac{a_{i,1}}{\alpha_1} \left( \frac{\partial \alpha_1}{\partial t} + \nabla \cdot \left( \alpha_1 \vec{v}_{g,1} \right) \right) + \sum_j \Phi_{j,2}. \quad (3.8)
\]

Then the source term shown on the right hand side of Eq. (3.2) is determined as:

for Group-1
\[
S_{g,1} = -\left( \alpha_1 a_{i,1} \rho_g \right) \nabla \cdot \vec{v}_{g,1} + a_{i,1} \rho_g \left( \frac{2}{3} - \chi \left( \frac{D_{cl}}{D_{sm,1}} \right)^2 \right) \left( \nabla \cdot \left( \alpha_1 \vec{v}_{g,1} \right) \right) + \alpha_1 \rho_g \sum_j \Phi_{j,1}, \quad (3.9)
\]

and for Group-2
\[
S_{g,2} = -\left( \alpha_2 a_{i,2} \rho_g \right) \nabla \cdot \vec{v}_{g,2} + \frac{2}{3} a_{i,2} \rho_g \left( \nabla \cdot \left( \alpha_2 \vec{v}_{g,2} \right) \right) + \frac{a_{i,1} \alpha_2 \rho_g \chi}{\alpha_1} \left( \frac{D_{cl}}{D_{sm,1}} \right)^2 \left( \nabla \cdot \left( \alpha_1 \vec{v}_{g,1} \right) \right) + \alpha_2 \rho_g \sum_j \Phi_{j,2}. \quad (3.10)
\]

To implement the two-group IATE model into the two-fluid model, the first step is to code Eqs. (3.5) and (3.6) (or Eqs. (3.9) and (3.10) for adiabatic flow) in a program written by C and then compile the IATE model in the Fluent code. Three fields, namely, Group-1 bubbles as field-1, Group-2 bubbles as field-2, and the liquid (continuous) phase as field-3, are assumed in the numerical model. The two-group IATE model is solved for \( a_{i,n} \), coupled with the mass, momentum, and energy conservation equations in the three-
dimensional, three-field, two-fluid model. The effects of $a_{i,n}$ are further propagated into
the calculations of the interfacial momentum transfer and turbulence model, which will
be discussed later. This process is carried out in an iterative manner till the solutions of
interest in the flow field have converged. At this point, the groundwork for implementing
the two-group IATE model into the Fluent code has been built.

3.2. Continuity equations of three-field two-fluid model

In the three-field two-fluid model, mass transfer occurs not only between the gas
and liquid phases when there is phase change, but also between Group-1 and Group-2
bubbles due to intra- and inter-group bubble interactions. The continuity equation for the
gas phase is therefore separated into two equations that govern the mass conservation of
Group-1 and Group-2 bubbles, respectively, as

$$\frac{\partial (\alpha_g \rho_g)}{\partial t} + \nabla \cdot \left( \alpha_g \rho_g \bar{v}_{g,n} \right) = \Gamma_{g,n}. \quad (3.11)$$

It can be expanded as

for Group-1

$$\frac{\partial (\alpha_{g1} \rho_g)}{\partial t} + \nabla \cdot \left( \alpha_{g1} \rho_g \bar{v}_{g,1} \right) = \Gamma_{g,1} - \Delta \dot{m}_{12}, \quad (3.12)$$

and for Group-2

$$\frac{\partial (\alpha_{g2} \rho_g)}{\partial t} + \nabla \cdot \left( \alpha_{g2} \rho_g \bar{v}_{g,2} \right) = \Gamma_{g,2} + \Delta \dot{m}_{12}. \quad (3.13)$$

Here, $\Delta \dot{m}_{12}$ is the net inter-group mass transfer rate from Group-1 to Group-2 bubbles
and is modeled as (Sun, 2001)
\[
\Delta \dot{m}_{12} = \rho_g \left\{ \sum_j \eta_{j,2} + \chi \left( \frac{D_{c1}}{D_{sm,1}} \right)^2 \nabla \cdot \left( \alpha_1 \vec{v}_{s,1} \right) \right\}.
\]

(3.14)

In the above equation, \( \eta_{j,2} \) is the net volume transfer from Group-1 bubbles to Group-2 bubbles originating from the mechanisms of bubble coalescence and disintegration, which have been discussed in Section 2.4. It is the summation of the following models given as (Sun, 2001)

\[
\eta_{RC,2}^{(12)} = 3.4C_{RC}^{(1)} \frac{\varepsilon^{1/3} \alpha_1^{2/3} \alpha_{i,1}^{1/3}}{\alpha_{i,\max}^{1/3}} \left[ 1 - \frac{2}{3} D_{c1}^* \right] 1 - \exp \left( -C_{RC1} \frac{\alpha_{i,\max}^{1/3}}{\alpha_{i,\max}^{1/3} - \alpha_1^{1/3}} \right), \quad \text{for } D_{c1}^* < 1.5
\]

\[
\eta_{RC,2}^{(122)} = 4.85C_{RC}^{(122)} \frac{\varepsilon^{1/3} \alpha_1^{5/3} \alpha_{2}^{2/3}}{R_{m2}^{2/3}} \left[ 1 - \exp \left( -C_{RC1} \frac{\alpha_{i,\max}^{1/3}}{\alpha_{i,\max}^{1/3} - \alpha_1^{1/3}} \right) \right],
\]

\[
\eta_{WE,2}^{(112)} = 5.40C_{WE}^{(112)} C_{D1}^{1/3} u_c \alpha_1 \alpha_{i,1} \left[ 1 - \frac{2}{3} D_{c1}^* \right], \quad \text{for } D_{c1}^* < 1.5
\]

\[
\eta_{WE,2}^{(122)} = 4.35C_{WE}^{(122)} \sqrt{gC_{D2} G} \frac{\alpha_1 \alpha_2}{R_{m2}}.
\]

\[
\eta_{SO,2}^{(2,12)} = -10.75C_{SO}^{(2)} C_d^{3/5} \left( \frac{\sigma}{\rho_f G} \right)^{3/5} \frac{\alpha_2}{v_{rb}^{1/5} R_{m2}} \left[ 1 - \left( \frac{We_{c,SO}}{We_{m2}} \right)^3 \right],
\]

\[
\eta_{TT,2}^{(2,1)} = -0.34C_{TT}^{(2)} \varepsilon^{1/3} G \alpha_2 \left( 1 - \alpha \right) \frac{R_{c}^{4/3}}{R_{m2}^{5/3}} \left( 1 - R_c^{6/3} \right) \exp \left( -\frac{We_{c,TT2}}{We_c} \right) \sqrt{1 - \frac{We_{c,TT2}}{We_c}}.
\]

For the liquid phase, the mass conservation equation is given as
where $\Gamma_f$ satisfies

$$\Gamma_f = -\left(\Gamma_{g,1} + \Gamma_{g,2}\right).$$

(3.16)

In adiabatic flow, there is no phase change (mass transfer) between the gas and liquid phases, resulting in the following relation:

$$\Gamma_{g,1} = \Gamma_{g,2} = \Gamma_f = 0.$$  

(3.17)

3.3. Momentum equations of three-field two-fluid model

3.3.1. Governing equations

The interfacial area concentration, $a_{k,n}$, is linked with the three-field two-fluid model in the Fluent code through the interfacial momentum transfer terms in the ensemble-averaged momentum equation for phase-$k$, which is written as follows: (Ishii and Hibiki, 2006)

$$\frac{\partial \left( \alpha_k \rho_k \bar{v}_k \right)}{\partial t} + \nabla \cdot \left( \alpha_k \rho_k \bar{v}_k \bar{v}_k \right) = -\nabla \left( \alpha_k p_k \right) + \nabla \cdot \left[ \alpha_k \left( \bar{\mathbf{F}}_k^p + \bar{\mathbf{F}}_k^T \right) \right] + \alpha_k \rho_k \bar{g}
+ \Gamma_k \bar{v}_{i,k} + p_{t,k} \nabla \alpha_k - \nabla \alpha_k \cdot \bar{\mathbf{r}}_{i,k} + \bar{\mathbf{F}}_{i,k},$$

(3.18)

where $\bar{\mathbf{F}}_{i,k}$ is the generalized interfacial force. Eq. (3.18) can be expanded as:

for Group-1
\[ \frac{\partial}{\partial t} \left( \alpha_i \rho_i \vec{v}_{g,i} \right) + \nabla \cdot \left( \alpha_i \rho_i \vec{v}_{g,i} \vec{v}_{g,i} \right) = -\nabla \left( \alpha_i p_{g,i} \right) + \nabla \left[ \alpha_i \left( \vec{F}_m + \vec{F}_T \right) \right] + \alpha_i \rho_i \vec{g} \\
+ \left( \Gamma_{g,i} - \Delta \dot{m}_{12} \right) \vec{v}_{l,g_i} + p_{l,g_i} \nabla \alpha_i \quad (3.19) \]

for Group-2

\[ \frac{\partial}{\partial t} \left( \alpha_2 \rho_2 \vec{v}_{g,2} \right) + \nabla \cdot \left( \alpha_2 \rho_2 \vec{v}_{g,2} \vec{v}_{g,2} \right) = -\nabla \left( \alpha_2 p_{g,2} \right) + \nabla \left[ \alpha_2 \left( \vec{F}_m + \vec{F}_T \right) \right] + \alpha_2 \rho_2 \vec{g} \\
+ \left( \Gamma_{g,2} + \Delta \dot{m}_{12} \right) \vec{v}_{l,g2} + p_{l,g2} \nabla \alpha_2 \quad (3.20) \]

and for the liquid phase

\[ \frac{\partial}{\partial t} \left( \alpha_j \rho_j \vec{v}_f \right) + \nabla \cdot \left( \alpha_j \rho_j \vec{v}_f \vec{v}_f \right) = -\alpha_j \nabla \vec{p}_f + \nabla \cdot \left( \alpha_j \vec{F}_m + \alpha_j \rho_j \vec{g} \right) \\
- \nabla \alpha_j \cdot \vec{F}_{i,f} \quad (3.21) \]

Here, the conservation of the mixture momentum provides the momentum-jump condition as:

\[ \vec{F}_{i,f} = -\left( \vec{F}_{i,g1} + \vec{F}_{i,g2} \right) \quad (3.22) \]

Ishii and Hibiki (2006) suggested the generalized interfacial be formulated as a linear combination of various known interfacial forces. For Group-\( n \) bubbles, it is written as:

\[ \vec{F}_{i,gn} = \vec{F}_{d,gn} + \vec{F}_{l,gn} + \vec{F}_{em,gn} + \vec{F}_{B,gn} + \vec{F}_{W,gn} + \vec{F}_{TD,gn} \quad (3.23) \]
where $\vec{F}_{d,g,n}$, $\vec{F}_{l,g,n}$, $\vec{F}_{em,g,n}$, $\vec{F}_{B,g,n}$, $\vec{F}_{W,g,n}$, and $\vec{F}_{TD,g,n}$ are the standard drag, lift, virtual mass, Basset (or history), wall lubrication (or wall lift), and turbulent dispersion forces on Group-$n$ bubbles.

The phase change at the bubble surface contributes to the interfacial momentum transfer in two different ways. First of all, there is a direct effect of momentum carried by the mass undergoing the phase change process. Secondly, there is an indirect effect on the drag coefficient due to the change of size or shape of the bubble and modification of the boundary layer around the fluid particles.

In adiabatic flows, where there is no mass exchange between the gas and liquid phases, the momentum equation for Group-$n$ bubbles is simplified as:

$$
\frac{\partial (\alpha_n \rho_g \vec{v}_{g,n})}{\partial t} + \nabla \cdot \left( \alpha_n \rho_g \vec{v}_{g,n} \vec{v}_{g,n} \right) = -\alpha_n \nabla p_{g,n} + \nabla \cdot \left( \alpha_n \vec{\tau}_{g,n} \right) + \alpha_n \rho_g \vec{g} + \left( -1 \right)^n \Delta \dot{m}_{12} \vec{v}_{i,gn} - \nabla \alpha_n \vec{\tau}_{i,gn} + \vec{F}_{i,gn} \quad (3.24)
$$

3.3.2. Discussion on drag force

The correlations of the drag force coefficient for single-particle and multi-particle systems are usually formulated for steady-state and adiabatic conditions. It is postulated that the transient effect on the momentum exchange term can be taken into account by the transient forces using an essential linear constitutive relation. As shown in Eq. (3.23), the additional interfacial forces due to the inertia effect and the development of a boundary layer in a transient flow are considered separately. Therefore, it is indirectly assumed that the standard drag force coefficient discussed in the following analysis could also be used for transient conditions.
In a single-particle system, the drag force coefficient depends not only on the flow regimes but also on the nature of the particles, including solid particle, droplet or bubble. The similarity hypothesis is made for a multi-particle system. The standard drag force acting on a Group-\(n\) bubble, \(\vec{F}_{d,gn}\), is similar to the skin and form drag force. It is a function of the drag force coefficient \((C_{D,n})\), relative velocity of the bubble with respect to the surrounding liquid (continuous) phase \((\vec{v}_{r,n})\), and bubble drag diameter \((D_{d,n})\). Making use of the definition of the bubble Sauter mean diameter \((D_{sm,n})\), \(\vec{F}_{d,gn}\) is written as:

\[
\vec{F}_{d,gn} = -\frac{\alpha_{a,n} A_d}{2B_d} C_{D,n} \rho_f \vec{v}_{r,n} \mid \vec{v}_{r,n} \mid = -\frac{\alpha_{a,n}}{8} C_{D,n} \rho_f \vec{v}_{r,n} \mid \vec{v}_{r,n} \mid \left(\frac{D_{sm}}{D_d}\right)_n,
\]

which is used in the simulations instead of the default model provided by the Fluent code, in which a constant bubble diameter is generally assumed.

In gas-liquid two-phase flow systems, the drag coefficient is modeled differently in various flow regimes, including viscous, distorted-particle, slug, and churn-turbulent flow regimes. As proposed by Ishii and Mishima (1984), the drag force coefficient in the viscous regime is given as:

\[
C_D = \frac{24}{\text{Re}_b} \left(1 + 0.1 \text{Re}_b^{0.75}\right).
\]

In the distorted-particle regime, the drag force coefficient is provided as:

\[
C_D = \frac{2}{3} f(\alpha) D_d \sqrt{\frac{g \Delta \rho}{\sigma}}.
\]
where $f(\alpha)$ is a function and determined based on the dynamic viscosity of fluid particles. $f(\alpha)$ can be given as:

for $\mu_f \gg \mu_g$, $f(\alpha) = (1 - \alpha)^{-0.5}$;

for $\mu_f \sim \mu_g$, $f(\alpha) = (1 - \alpha)^{-1.0}$;

for $\mu_f \ll \mu_g$, $f(\alpha) = (1 - \alpha)^{-1.5}$.

Furthermore, the drag force coefficient in slug flow is given as:

$$C_D = 9.8 (1 - \alpha)^3.$$  \hfill (3.28)

Finally, in churn-turbulent flow regime, the drag force coefficient is provided as:

$$C_D = \frac{8}{3} (1 - \alpha)^2.$$  \hfill (3.29)

The drag force coefficient model suggested by Tomiyama (1998) for slightly-contaminated air-water two-phase flow is given based on two dimensionless numbers, namely, the Eotvos number ($Eo_n$) and bubble Reynolds number ($Re_{b,n}$), which are defined, respectively, as

$$Eo_n = \frac{g \Delta \rho D_{d,n}^2}{\sigma}$$  \hfill (3.30)

and

$$Re_{b,n} = \frac{\rho_f \left| \ddot{\rho}_{c,n} \right| D_{d,n} \mu_f}{\mu_f}$$  \hfill (3.31)

for Group-$n$ bubbles. Therefore, the drag force coefficient is provided as
This drag force coefficient model is used in bubbly flow or for Group-1 bubbles in flow regimes beyond bubbly flow.

3.3.3. Discussion on lift force

Analogous to the rotation of spherical particles in a viscous shear flow, the velocity gradient leads to the lift force on bubbles, $\vec{F}_{l,n}$, which is normal to the bubble relative velocity direction. Studies (Zun, 1980; Drew and Lahey, 1987) have shown that the major contributions to the lift force include the relative velocity between a particle and an ambient fluid, shear rate of an ambient fluid, particle rotational speed, and the surface boundary condition (non-slip or slip at the particle surface). In view of this, the shear-lift force model (Mei and Klausner, 1994) and lift force caused by slanted wake (Tomiyama et al., 2002) were proposed.

The expression for the lift force is usually given by (Auton, 1987)

$$\vec{F}_{l,gm} = -C_{l,n} \alpha_n \rho_f \vec{v}_{r,n} \times \left( \nabla \times \vec{v}_f \right),$$

(3.33)

where $C_{l,n}$ is the lift force coefficient. It usually falls in the range between 0.01 and 0.5 in bubbly flows (Wang et al., 1987).

More comprehensive research related to $C_{l,n}$ has been recently performed. Hibiki and Ishii (2007) found out that the deformation of a particle caused the lift force modifications through the associated wake modification and modified interactions with the surrounding flow structures. Thus, the lift force coefficient was given as:
\[ C_{i,n} = \xi_\infty \sqrt[2]{\left(C_{i,\infty}^{\text{low} \text{Re}_\infty \left(\text{Re}_\infty, G_{\infty}\right)} \right)^2 + \left(C_{i,\infty}^{\text{high} \text{Re}_\infty \left(\text{Re}_\infty\right)} \right)^2}, \quad (3.34) \]

where \( \xi_\infty \) is a modification factor based on existing experimental data. The bubble drag diameter, \( D_d \), is a key parameter to correlate the modification factor. The ratio of the bubble drag diameter to the bubble diameter at the distorted bubble limit, \( \bar{D}_{d,\infty}^* \), is defined as

\[ \bar{D}_{d,\infty}^* = \frac{D_d}{D_{dc}} = \frac{Eo^{1/2}}{4}. \quad (3.35) \]

Physically, the decreased bubble diameter reduces the bubble distortion, thus, the asymptotic value of \( \xi_\infty \) might be assumed to be unity at \( \bar{D}_{d,\infty}^* \rightarrow 0 \). It is seen that for \( \bar{D}_{d,\infty}^* \leq 1 \), it falls into the spherical or distorted bubble regime; while, for \( \bar{D}_{d,\infty}^* \geq 1 \), cap or slug bubbles are formed.

Another model of the lift force coefficient was proposed by Tomiyama (1998). It is given as

\[ C_{i,n} = \begin{cases} \min \left[0.288 \tanh \left(0.121 \text{Re}_b \right), f\left(Eo_{b,n}\right)\right], & \text{if } Eo_{b,n} < 4 \\ f\left(Eo_{b,n}\right), & \text{if } 4 \leq Eo_{b,n} \leq 10 \\ -0.29, & \text{if } Eo_{b,n} > 10 \end{cases} \quad (3.36) \]

where

\[ f\left(Eo_{b,n}\right) = 0.00105Eo_{b,n}^3 - 0.0159Eo_{b,n}^2 - 0.0204Eo_{b,n} + 0.474. \quad (3.37) \]
If we define the maximum horizontal dimension of a bubble, $D_{H,n}$, which is calculated as

$$D_{H,n} = D_{d,n} \left(1 + 0.163 E_{b,n}^{0.0757}\right)^{1/3},$$

the modified Eotvos number, $E_{b,n}$, is defined as

$$E_{b,n} = \frac{g(\rho_f - \rho_s)D_{H,n}^2}{\sigma}. \quad (3.38)$$

Since both $E_{b,n}$ and $Re_{b,n}$ are functions of the bubble size, the lift force becomes a function of the bubble size as well.

3.3.4. Discussion on wall lubrication (wall lift) force

The transverse migration of bubbles influenced by walls in vertical flow was studied. Zun (1980) discussed that there might be several mechanisms, which had been previously proposed by others, to explain the phenomena near the wall, such as the Zhukovski forces acting on the bubbles as spinning rigid spheres, influence of the liquid velocity gradient, static pressure change over the cross section of the channel due to liquid turbulence, and the Magnus force due to the circulation of liquid around the bubble together with the Bernoulli force resulting from the stronger back flow on the wall side of the bubble. In addition, Rouhani (1976) proposed the hypothesis of rolling vortices generation near walls as a theoretical explanation for a wall void peaking if there was one.

In the study of Antal et al. (1991), the wall lubrication force was due to the velocity distribution change around the fluid particles near a wall. When a rising bubble comes close to a wall, the normally uniform drainage of the fluid around the bubble changes dramatically. In the region close to the wall, the non-slip condition slows the
drainage rate between the bubble and the wall; whereas the drainage rate will increase on the opposite side. This phenomenon of the asymmetric drainage of the liquid around the bubble in the vicinity of the wall brings a hydrodynamic force, which floats a journal in its bearing housing. It is therefore called wall lubrication or wall lift force, which tends to move the bubble away from the wall. However, no analytical three-dimensional solution of the flow between a bubble and a wall is available to describe this phenomenon, based on author’s knowledge.

Antal et al. (1991) deduced an approximate two-dimensional solution of the wall lubrication force on a sphere based on the complex potential function of flows between a cylinder and a wall. They discussed that the theoretical wall lubrication force was a polynomial function with different coefficients. With the help of the PHOENICS computer code, the wall lubrication force was simplified as a function of the first two terms to satisfactorily fit the numerical results as

\[
\bar{F}_{W,\gamma n} = \frac{2\alpha_n \rho_f}{D_{d,n}} \left| \nu_{\nu|n} \right|^2 C_{w1,n} + C_{w2,n} \left( \frac{D_{d,n}}{2d_{bw}} \right) \bar{n}\nu, 
\]

where \(d_{bw}\) and \(\bar{n}\nu\) are the distance between the bubble and the wall and the unit outward normal vector of the wall surface, respectively. \(\bar{\nu}_{\nu|n}\) is the relative velocity parallel to the wall for Group-\(n\) bubbles and is defined as

\[
\bar{\nu}_{\nu|n} = \left( \bar{\nu}_{g,n} - \bar{\nu}_f \right) - \left[ \bar{n}\nu \cdot \left( \bar{\nu}_{g,n} - \bar{\nu}_f \right) \right] \bar{n}\nu. 
\]

The coefficients are given as
The main effect of the wall lubrication force is to ensure the zero void condition found experimentally near vertical walls, while there is no significant effect on the phase distribution far away from the wall.

3.3.5. Discussion on turbulent dispersion force

The turbulent dispersion force is due to the bubble motion produced by the turbulent energy of the liquid phase (Lahey et al., 1993; Ishii and Hibiki, 2006). This force is driven by the void fraction gradient and tends to flatten the void fraction distribution. Analogous to the molecular dispersion force, the turbulent dispersion force is modeled by Lahey et al. (1993) as

$$\vec{F}_{TD,gn} = -C_{T,n} \rho_j k_f \nabla \alpha_n,$$  

(3.43)

where $k_f$ is the total turbulent kinetic energy of the liquid phase, and $C_{T,n}$ is an adjustable coefficient given as

$$C_{T,n} = 0.1.$$  

(3.44)

Lopez de Bertodano et al. (2006) established the model of bubble-induced turbulent diffusion force, which could be generalized as

$$\vec{F}_{TD,gn}^{BI} = \frac{1}{\tau_{d,n}} \left( \rho_g + C_{em,gn} \rho_j \right) \bar{u}_{g,n} \nabla \alpha_n,$$  

(3.45)
where $\tau_{d,n}$ is the time constant of Group-$n$ bubbles. Eq. (3.45) can be further formulated as

$$\vec{F}_{TD,gn}^{\text{t}} = -\frac{3}{4} C_{DB,n} \rho_f C_{T,n}^* \alpha_{u} \frac{\vec{v}}{r,n} \left| \frac{\vec{v}}{r,n} \right| \nabla \alpha_{u}.$$  

Here, $C_{DB,n}$ is a constant determined experimentally, and $C_{T,n}^*$ is related to the drag force coefficient and bubble diameter. Lopez de Bertodano et al. (2006) emphasized that the bubble-induced turbulent diffusion force was important when there were large bubbles in two-phase flow.

3.3.6. Discussion on transient forces

Two-phase flow also physically experiences other forms of forces, such as Basset (history) force ($\vec{F}_{B,gn}^h$) and virtual mass force ($\vec{F}_{vm,gn}^v$). The Basset force was first emphasized by Boussinesq (1885) under the creeping flow condition. Later, Basset (1888a and 1888b) performed independent work on deriving this history integral force, and obtained an expression of the force identical to that provided by Boussinesq (1885). However, people usually called this history force “Basset force” given the chronological precedence of Boussinesq’s work. The virtual mass force becomes important when a particle accelerates relative to the liquid (continuous) phase such that the inertia of the liquid (continuous) phase mass encountered by the accelerating particles exerts a virtual mass force on the particle. As the “added mass” of the liquid is accelerated, a resistance to the particle acceleration is induced, and the virtual mass force is generated. The pioneering work was done by Poisson (1832), followed by Green (1836) and Clebsch
(1856). The transient forces are important not only to provide accurate estimation of flow distributions, but also to stabilize the numerical solutions in general (Michaelides, 1997). In the current study, since the flow is at quasi-steady state, the transient forces are not included.

3.4. **Enthalpy equations of three-field two-fluid model**

In the three-field two-fluid model, the enthalpy equation for phase-\(k\) is given as (Ishii and Hibiki, 2006):

\[
\frac{\partial \left( \alpha_k \rho_k H_k \right)}{\partial t} + \nabla \cdot \left( \alpha_k \rho_k \vec{v}_k H_k \right) = -\nabla \cdot \left[ \alpha_k \left( \bar{q}_k + \bar{q}_k^f \right) \right] + \frac{D_k \left( \alpha_k p_k \right)}{Dt} + \Gamma_k H_{i,k} \nonumber \\
+ a_i q''_{i,k} - p_{i,k} \frac{D_k \alpha_k}{Dt} + \phi_k. \tag{3.47}
\]

It can be further written as:

for Group-1

\[
\frac{\partial \left( \alpha_1 \rho_{1,g} H_{g,1} \right)}{\partial t} + \nabla \cdot \left( \alpha_1 \rho_{1,g} \vec{v}_{1,g} H_{g,1} \right) = -\nabla \cdot \left[ \alpha_1 \left( \bar{q}_{1,g,1} + \bar{q}_{1,g,1}^f \right) \right] + \frac{D_{g_1} \left( \alpha_1 p_{g,1} \right)}{Dt} \\
+ \left( \Gamma_{g,1} + \Delta \hat{m}_{12} \right) H_{i,g,1} \\
+ a_{i,1} q''_{i,1,g} - p_{i,g,1} \frac{D_{g_1} \alpha_{g,1}}{Dt} + \phi_{g,1}. \tag{3.48}
\]

for Group-2

\[
\frac{\partial \left( \alpha_2 \rho_{g,2} H_{g,2} \right)}{\partial t} + \nabla \cdot \left( \alpha_2 \rho_{g,2} \vec{v}_{g,2} H_{g,2} \right) = -\nabla \cdot \left[ \alpha_2 \left( \bar{q}_{g,2} + \bar{q}_{g,2}^f \right) \right] + \frac{D_{g_2} \left( \alpha_2 p_{g,2} \right)}{Dt} \\
+ \left( \Gamma_{g,2} + \Delta \hat{m}_{12} \right) H_{i,g,2} \\
+ a_{i,2} q''_{i,2,g} - p_{i,g,2} \frac{D_{g_2} \alpha_{g,2}}{Dt} + \phi_{g,2}. \tag{3.49}
\]
and for the liquid phase

\[ \frac{\partial (\alpha_f \rho_f \bar{H}_f)}{\partial t} + \nabla \cdot (\alpha_f \rho_f \bar{v}_f \bar{H}_f) = -\nabla \cdot \left[ \alpha_f (\bar{q}_f + \bar{q}_f^T) \right] + \frac{D_g (\alpha_f \rho_f)}{Dt} + \Gamma_f H_{i,f} + a_{i,f} q'''_{i,f} - p_{i,f} \frac{D_g \alpha_f}{Dt} + \phi_{i,f}. \]  

(3.50)

Here, it satisfies

\[ a_{i,f} q'''_{i,f} + \Gamma_f H_{i,f} = -(a_{i,1} q'''_{i,g1} + \Gamma_{g,1} H_{i,g1} + a_{i,2} q'''_{i,g2} + \Gamma_{g,2} H_{i,g2}). \]  

(3.51)

The energy equations are omitted if the flow is under isothermal condition.

3.5. Discussion on bubble velocity

In two-phase flow, the void fraction weighted average of the quantity \( F \) for phase-\( k \) is introduced as

\[ \left\langle\left\langle F \right\rangle\right\rangle = \frac{\left\langle \alpha_k F \right\rangle}{\left\langle \alpha_k \right\rangle}, \]  

(3.52)

which is not a function across the cross section of the flow channel. Here, \( \left\langle \right\rangle \) is introduced as the average over the cross sectional area of the flow channel (\( A \)) of \( F \) and defined as

\[ \left\langle F \right\rangle = \frac{1}{A} \int_A F dA. \]  

(3.53)

Additional variables due to the velocity difference between the two phases, which usually depend on bubble size, are defined. One variable is the relative velocity (\( \bar{v}_r \)) between the gas phase velocity (\( \bar{v}_g \)) and liquid phase velocity (\( \bar{v}_f \)) and is given as
\[ \vec{v}_r = \vec{v}_g - \vec{v}_f. \]  

Using a force balance between the buoyancy force and the drag force, Ishii and Zuber (1979) provided the relation of the relative velocity in bubbly flows as

\[ |\vec{v}_r| = \sqrt{\frac{4 D_a \Delta \rho g (1 - \alpha)}{3 C_D \rho_f}}, \]  

where \( C_D \) is the drag coefficient, discussed previously.

Figure 3.1. A cap bubble rising in an infinite liquid

Some studies were also performed on the velocity of a large bubble rising in an infinite liquid, as illustrated in Figure 3.1. The shape of a fluid particle is assumed to be a spherical cap, of which the upper surface is virtually indistinguishable from a sphere and the lower surface is unsteady and fluctuating about a horizontal plane. It is found that the relative velocity of spherical-cap bubbles is related to their apparent radius of curvature. Using the Bernoulli’s equation, it is given as

\[ |\vec{v}_r| = \eta \sqrt{gr}, \]  

54
where \( r \) is the apparent radius of curvature of the upper part of the bubble and \( \eta \) is a constant. Different researchers have given different values of \( \eta \). For instance, Rosenberg (1950) suggested an experimental value of 0.645. While, Davies and Taylor (1950) presented a theoretical evaluation and suggested a value of 2/3. A second approximation of the velocity of a large bubble rising in an infinite liquid was performed by Collins (1966). He derived it from a linear perturbation of the first approximation and showed a good agreement with the experimental results when \( \eta \) was equal to 0.636.

Another variable is the drift velocity with respect the superficial velocity of the mixture \((j)\), \(\vec{V}_{kj}\), which is defined as

\[
\vec{V}_{kj} = \vec{v}_k - j.
\]  

(3.57)

Thus, void fraction weighted velocity of the gas phase can be expressed as

\[
\left\langle \left\langle \vec{v}_{g} \right\rangle \right\rangle = \frac{\left\langle \vec{v}_g \alpha_g \right\rangle}{\left\langle \alpha_g \right\rangle} = \frac{\left\langle j_g \right\rangle}{\left\langle \alpha_g \right\rangle} = \frac{\left\langle \alpha_g j_g \right\rangle}{\left\langle \alpha_g \right\rangle} + \frac{\left\langle \alpha_g \vec{V}_{gj} \right\rangle}{\left\langle \alpha_g \right\rangle} = C_0 \left\langle j \right\rangle + \frac{\left\langle \alpha_g \vec{V}_{gj} \right\rangle}{\left\langle \alpha_g \right\rangle} = C_0 \left\langle j \right\rangle + \left\langle \left\langle \vec{V}_{gj} \right\rangle \right\rangle.
\]  

(3.58)

Here, \( C_0 \) is called the distribution parameter, defined as

\[
C_0 = \frac{\left\langle \alpha_g j_g \right\rangle}{\left\langle \alpha_g \right\rangle \left\langle j \right\rangle}.
\]  

(3.59)
In round pipes, $C_o$ is usually chosen in the range between 1.0 and 1.5 for fully established bubbly flows. In the slug and churn-turbulent flows, $C_o$ is usually chosen as 1.18. In rectangular ducts, $C_o$ is proposed by Ishii (1977) as

$$C_o = 1.35 - 0.35 \sqrt{\frac{\rho_g}{\rho_f}}. \quad (3.60)$$

The correlations of the void fraction weighted drift velocity also depend on the flow channel configurations and flow regimes. For example, for the slug flow in a pipe, $\langle \langle \hat{V}_{s1} \rangle \rangle$ is given as (Ishii, 1977)

$$\langle \langle \hat{V}_{s1} \rangle \rangle = 0.35 \left[ \frac{g \Delta \rho D}{\rho_f} \right]^{1/2}, \quad (3.61)$$

while in the churn-turbulent flow, it is given as (Ishii, 1977)

$$\langle \langle \hat{V}_{s1} \rangle \rangle = 1.53 \left[ \frac{\sigma g \Delta \rho}{\rho_f^2} \right]^{1/4}. \quad (3.62)$$

Here, $D$ is the inner diameter of the circular pipe. For flows in a rectangular duct, Griffith (1964) pointed out that the drift velocity of a cap or slug bubble in stagnant flow was determined based on the dimension of the flow channels, and proposed the void fraction weighted drift velocity as

$$\langle \langle \hat{V}_{s1} \rangle \rangle = \left[ 0.23 + 0.13 \frac{G}{W} \right] \sqrt{\frac{\Delta \rho g W}{\rho_f}}, \quad (3.63)$$
where $G$ and $W$ are the gap and width of the flow channel, respectively, with $W$ being larger than $G$. 
Chapter 4. \( k - \varepsilon \) Turbulence Model

It is essential to choose appropriate turbulence models in the two-phase flow simulations since mechanistic models of the bubble interactions rely strongly on the turbulent parameters, such as the turbulent kinetic energy dissipation rate. There are ongoing efforts to develop appropriate turbulence models for two-phase flows; nevertheless, no widely accepted model currently exists. Despite the anisotropic features of some two-phase flows such as cap-bubbly flows, \( k - \varepsilon \) turbulence model is deliberately proven to provide a decent approximation of Large-Eddy Simulation (LES) and Reynolds stress model (Laborde-Boutet et al., 2009). In this chapter, different types of \( k - \varepsilon \) turbulence models are investigated.

4.1. Governing equations of \( k - \varepsilon \) turbulence model

The magnitude of the turbulent velocity, \( v_t \), is evaluated based on the Kolmogorov’s universal equilibrium theory in the inertial sub-range of isotropic homogeneous turbulence as (Batchelor, 1951; Rotta, 1972; Hinze, 1975):

\[
v_t = 1.4 \varepsilon_f^{1/3} D_d^{1/3},
\]

which is a function of the turbulence kinetic energy dissipation rate of the liquid phase, i.e. \( \varepsilon_f \).
The general governing equations in the $k - \varepsilon$ turbulence to model the turbulence kinetic energy ($k$) and its dissipation rate ($\varepsilon$) for phase-$p$ are given as (Batchelor, 1951; Launder and Spalding, 1972; Fluent 6.3 User’s Guide, 2006):

$$\frac{\partial}{\partial t}\left(\alpha_p \rho_p k_{p,p}\right) + \nabla \cdot \left(\alpha_p \rho_p k_{p,p} \mathbf{v}_{p,p}\right) = \nabla \cdot \left[ \alpha_p \left( \frac{\theta_{k,p} \mu_p + \mu_{\text{eff},p}}{\sigma_{k,p}} \right) \nabla k_p \right]$$

$$+ \alpha_p G_{k,p} + \alpha_p G_{b,p} - \alpha_p \rho_p \varepsilon_p - \alpha_p Y_{M,p} + \Phi_{k,p}, \tag{4.2}$$

and

$$\frac{\partial}{\partial t}\left(\alpha_p \rho_p \varepsilon_{p,p}\right) + \nabla \cdot \left(\alpha_p \rho_p \varepsilon_{p,p} \mathbf{v}_{p,p}\right) = \nabla \cdot \left[ \alpha_p \left( \frac{\theta_{\varepsilon,p} \mu_p + \mu_{\text{eff},p}}{\sigma_{\varepsilon,p}} \right) \nabla \varepsilon_p \right]$$

$$+ \rho_p \varepsilon_p \left( C_1 S - C_2 \frac{\varepsilon_p}{k_p + \sqrt{\mu_p \varepsilon_p / \rho_p}} \right)$$

$$+ \alpha_p \frac{\varepsilon_p}{k_p} \left( C_{1,\varepsilon} \theta_{2,\varepsilon,p} G_{k,p} - C_{2,\varepsilon} \theta_{3,\varepsilon,p} \rho_p \varepsilon_p \right)$$

$$+ \alpha_p \frac{\varepsilon_p}{k_p} \left( C_{1,\varepsilon} C_{4,\varepsilon} G_{b,p} - \alpha_p R_{\varepsilon,p} + C_{3,\varepsilon} \Phi_{\varepsilon,p} \right). \tag{4.3}$$

Here, $G_{k,p}$, $G_{b,p}$, and $Y_{M,p}$, on the right hand side of Eq. (4.2), are the production of turbulence kinetic energy due to the mean velocity gradients, generation of turbulence kinetic energy due to buoyancy, and contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate for phase-$p$, respectively.

$G_{k,p}$ is modeled as:

$$G_{k,p} = -\rho_p v_{i,p} v_{j,p} \frac{\partial v_{j,p}}{\partial x_i}. \tag{4.4}$$
It can also be evaluated in a manner consistent with the Boussinesq hypothesis as:

\[ G_{k,p} = \mu_{i,p} S^2, \]  

(4.5)

where \( \mu_{i,p} \) is the eddy viscosity. \( S \) is the modulus of the mean rate-of-strain tensor and is defined as

\[ S = \sqrt{\frac{2S_{ij}S_{ij}}{}} \]  

(4.6)

with \( S_{ij} = \frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) \).

The effect of the buoyancy on turbulence kinetic energy dissipation rate is determined by \( C_{4,\epsilon} \), which is calculated as

\[ C_{4,\epsilon} = \tanh \left| \frac{v_\parallel}{v_\perp} \right|, \]  

(4.7)

where \( v_\parallel \) and \( v_\perp \) are the components of the flow velocity parallel and perpendicular to the gravitational vector, respectively.

In addition, the quantities \( \sigma_{k,p} \) and \( \sigma_{\epsilon,p} \) are the effective Prandtl numbers for \( k \) and \( \epsilon \), respectively. Other parameters will be discussed later when each turbulence model is investigated.

The \( k - \epsilon \) turbulence model provides the Reynolds stress tensor, which can be provided as (Batchelor, 1951)

\[ \rho_p v'_p \otimes v'_p = -\frac{2}{3} \left( \rho_p k_p + \rho_p \mu_{i,p} \nabla \times \vec{v}_p \right) I + \rho_p \mu_{i,p} \left( \nabla \vec{v}_p + \left( \nabla \vec{v}_p \right)^T \right) \]  

(4.8)
or
\[ \rho_p \frac{\overline{v_i^t v_j^t}}{} = -2 \left( \rho_p \frac{\partial v_{i,p}}{\partial x_i} + \rho_p \frac{\partial v_{i,j,p}}{\partial x_j} \right) \delta_{ij} + \rho_p \mu_{i,j,p} \left( \frac{\partial v_{i,j,p}}{\partial x_i} - \frac{\partial v_{i,j,p}}{\partial x_j} \right). \] (4.9)

4.2. Standard \( k-\varepsilon \) turbulence model

The standard \( k-\varepsilon \) turbulence model is a semi-empirical model for fully turbulence flows. The transport equation for \( k \) is derived from the exact equation, while the transport equation for \( \varepsilon \) is obtained by comparing it to its mathematical counterpart using physical reasoning. The turbulence source terms in Eqs. (4.2) and (4.3) are related according to

\[ \Phi_{\varepsilon,p} = \frac{\varepsilon_p}{k_p} \Phi_{k,p}. \] (4.10)

In general, if the standard \( k-\varepsilon \) turbulence model is applied, the terms in Eqs. (4.2) and (4.3) are given as (Fluent 6.3 User’s Guide, 2006)

\[ G_{b,p} = 0, \quad Y_{M,p} = 0, \quad \mu_{eff,p} = \mu_{t,p}, \quad C_1 = C_2 = 0. \] (4.11)

4.2.1. Dispersed model

In the dispersed model, the transport equations of turbulent kinetic energy and its dissipation rate for the liquid (continuous) phase are solved, i.e., \( p = f \). Let subscript \( d \) refers to the gas (dispersed) phase. The source term is then given as

\[ \Phi_{k,p} = K_{dp} \left( \overline{v_p^t v_d^t} + \overline{v_r^t v_d^t} \right), \] (4.12)

or
\[ \Phi_{k,p} = K_{dp} \left( k_{dp} - 2k_p + \bar{v}_r \cdot \bar{v}_{dr} \right). \]  

(4.13)

Here, \( \bar{v}_r \) and \( \bar{v}_{dr} \) are the relative velocity and drift velocity, respectively. The drift velocity is evaluated in the Fluent code according to

\[ \bar{v}_{dr} = - \left( \frac{D_d^{dp}}{\sigma_{dp} \alpha_d} \nabla \alpha_d - \frac{D_p}{\sigma_{dp} \alpha_p} \nabla \alpha_p \right), \]  

(4.14)

where \( \sigma_{dp} \) is defined as the dispersion Prandtl number, of which the default value is 0.75. \( D_d \) and \( D_p \) are the diffusivities with respect to the gas and liquid phases. It is usually assumed that

\[ D_d = D_p = D_{t,dp} = \frac{1}{3} k_{dp} \tau_{t,dp}, \]  

(4.15)

In Eqs. (4.13) and (4.15), \( k_{dp} \) is the covariance of the velocities of the liquid and gas phases, which is given as:

\[ k_{dp} = 2k_p \left( \frac{b + \eta_{dp}}{1 + \eta_{dp}} \right). \]  

(4.16)

Here, \( \eta_{dp} \) is the ratio between two characteristic times and formulated as

\[ \eta_{dp} = \frac{\tau_{t,dp}}{\tau_{F,dp}}. \]  

(4.17)

\( \tau_{F,dp} \) is the characteristic particle relaxation time connected with inertial effects acting on the liquid phase and is defined as
\[ \tau_{F,dp} = \alpha_d \rho_p K_{dp}^{-1} \left( \frac{\rho_d}{\rho_p} + C_V \right), \]  

(4.18)

\( \tau_{t,dp} \) is the Lagrangian integral time scale calculated along particle trajectories and is defined as

\[ \tau_{t,dp} = \frac{\tau_{t,p}}{\sqrt{1 + C_\beta \xi^2}}, \]  

(4.19)

Here, \( \tau_{t,p} \) is the characteristic time of the energetic turbulent eddies. The following relations are applied to calculate the parameters in Eq. (4.19) as:

\[ \tau_{t,p} = \frac{3}{2} C_{\mu,p} \frac{k_p}{\varepsilon_p}, \]  

(4.20)

\[ \xi = \frac{\bar{v}_r}{L_{t,p}}, \]  

(4.21)

\[ L_{t,p} = \sqrt{\frac{3}{2} C_{\mu,p} \frac{k_p^{3/2}}{\varepsilon_p}}, \]  

(4.22)

\[ C_\beta = 1.8 - 1.35 \cos^2 \theta. \]  

(4.23)

The term \( L_{t,p} \) in Eqs. (4.21) and (4.22) is the length scale of the turbulent eddies. The term \( \theta \) in Eq. (4.23) is the angle between the mean particle velocity and the mean relative velocity. Finally, \( b \) is given as

\[ b = \left( 1 + C_V \right) \left( \frac{\rho_d}{\rho_p} + C_V \right)^{-1}, \]  

(4.24)
where $C_v$ is the added-mass coefficient.

In Eqs. (4.12) and (4.18), $K_{dp}$ is the exchange coefficient for fluid-fluid flows, including gas-liquid and liquid-liquid mixtures. In the Fluent code, it is written as:

$$K_{dp} = \frac{\alpha_d \alpha_p \rho_p \rho_f f}{\tau_p}, \quad \text{(4.25)}$$

where $f$ and $\tau_p$ are the drag function and particulate relaxation time, respectively. They are defined as

$$f = \frac{C_D \text{Re}}{24}, \quad \text{(4.26)}$$

and

$$\tau_p = \frac{\rho_p D_d^2}{18 \mu_p}, \quad \text{(4.27)}$$

where $\text{Re}$ is the Reynolds number. Thus, $K_{dp}$ is rewritten as

$$K_{dp} = \frac{3 \alpha_d \alpha_p \rho_p C_D}{4 D_d} \left| \vec{v}_d \right|. \quad \text{(4.28)}$$

It is noted that Eq. (4.28) is also used in the model of drag force in the Fluent code. However, an additional term, $\alpha_p$, appears compared to the model of drag force proposed by other studies. In view of this, we construct the model of the exchange coefficient as

$$K_{dp} = \frac{3 \alpha_d \rho_p C_D}{4 D_d} \left| \vec{v}_r \right|, \quad \text{(4.29)}$$

which is consistent with most studies.
The corresponding turbulent parameters for the gas phase are provided using Tchen-theory correlations based on the values of the liquid phase as

\[
k_d = k_p \left( \frac{b^2 + \eta_{dp}}{1 + \eta_{dp}} \right). \tag{4.30}
\]

Finally, the following values are used for some parameters in Eqs. (4.2) and (4.3) if the dispersed model is used:

\[
\theta_{1,e,p} = 0, \quad \theta_{2,e,p} = 1, \quad \theta_{3,e,p} = 1, \quad \theta_{k,p} = 0, \quad R_{e,p} = 0. \tag{4.31}
\]

4.2.2. Per-phase model

The per-phase model takes into account the coupling terms in intrinsic turbulence and pseudo-turbulence in two ways, which means turbulence could be induced by gas phase into liquid phase and vice versa. The transport equations (Eqs. (4.2) and (4.3)) are solved for both gas and liquid phases. The source terms in Eqs. (4.2) and (4.3) are therefore given as

\[
\Phi_{k,p} = K_{dp} \left( C_{dp} k_d - C_{pd} k_p \right) - K_{dp} \frac{\mu_{d,p}}{\alpha_{d} \sigma_{d}} \nabla \alpha_d + K_{dp} \frac{\mu_{t,p}}{\alpha_{p} \sigma_{p}} \nabla \alpha_p, \tag{4.32}
\]

where \( \sigma_k \) is the turbulent Prandtl number for phase-\( k \) and is defined as

\[
\sigma_k = \frac{\varepsilon_M}{\varepsilon_H}. \tag{4.33}
\]

Here, \( \varepsilon_M \) and \( \varepsilon_H \) are the eddy diffusivities for momentum transfer and heat transfer. The turbulent Prandtl number depends on the Prandtl number of the fluid based on experimental data. Here, using the Reynolds analogy, we apply
\[ \sigma_p = \sigma_d = 1. \] (4.34)

The parameters in Eq. (4.32) are given as

\[ C_{dp} = 2, \quad C_{pd} = 2 \frac{\eta_{dp}}{1 + \eta_{dp}}. \] (4.35)

The viscosity without the bubble induced turbulence is given as

\[ \mu_{\tau,p} = \rho_p C_{\mu,p} \frac{k^2}{\varepsilon_p}, \] (4.36)

where \( C_{\mu,p} = 0.09 \). If the bubble-induced turbulence is considered, the two-phase turbulent viscosity, \( \mu_{\tau,p} \), is customized based on Lahey’s model (2005) as:

\[ \mu_{\tau,p} = C_{\mu} \frac{k^2}{\varepsilon_p} + 0.6 D_d \alpha_d |\vec{v}_r|, \] (4.37)

The constitutive relation of \( \Phi_k \) is furnished by

\[ \Phi_{k,p} = \frac{3}{4D_d} \alpha_d \rho_p C_{\nu_p} \left[ \frac{2k_p (b - 1)}{1 + \eta_{dp}} + \vec{v}_r \cdot \vec{v}_d \right]. \] (4.38)

Finally, the following values are used in Eqs. (4.2) and (4.3):

\[ \theta_{k,p} = 0, \quad \theta_{1,c,p} = 0, \quad \theta_{2,c,p} = 1, \quad \theta_{3,c,p} = 1, \quad R_{c,p} = 0; \]
\[ C_{1,c} = 1.44, \quad C_{2,c} = 1.92, \quad C_{3,c} = 1.2, \quad \sigma_{k,p} = 1.0, \quad \sigma_{c,p} = 1.3. \] (4.39)

4.3. \textit{RNG k – \varepsilon} turbulence model

The RNG \( k – \varepsilon \) turbulence model is also derived from the instantaneous Navier-Stokes equations. In contrast to the standard \( k – \varepsilon \) model, the “renormalization group” (RNG) method is used, providing the additional term in Eq. (4.3) as
\[
R_{\varepsilon,p} = \frac{C_{\mu,p} \rho_p \eta_p^3 \left(1 - \frac{\eta_p}{\eta_0}\right) \varepsilon_p^2}{1 + \beta \eta_p^3}.
\] (4.40)

In Eq. (4.40), the following relations are given as:

\[
\eta_p = \frac{S k_p}{\varepsilon_p}, \quad \eta_0 = 4.38, \quad \beta = 0.012.
\] (4.41)

Generally, the following values are used in Eqs. (4.2) and (4.3) for RNG model:

\[
\begin{align*}
\Phi_{k,p} &= \Phi_{\varepsilon,p} = 0; \\
C_1 &= C_2 = 0; \\
\theta_{k,p} &= 0, \quad \theta_{1,\varepsilon,p} = 0, \quad \theta_{2,\varepsilon,p} = 1, \quad \theta_{3,\varepsilon,p} = 1; \\
\mu_{\text{eff},p} &= \mu_{t,p}, \quad \sigma_{k,p} = 1.393, \quad \sigma_{\varepsilon,p} = 1.393; \\
G_{k,p} &= 0, \quad Y_{m,p} = 0; \\
C_{\mu,p} &= 0.0845, \quad C_{1,\varepsilon} = 1.42, \quad C_{2,\varepsilon} = 1.68.
\end{align*}
\] (4.42)

In this study, different turbulence models will be applied according to the flow conditions.
Chapter 5. Model Validation of One-group IATE

5.1. PC-SIMPLE algorithm

In CFD codes, there are two basic types of meshes, namely, structured mesh and unstructured mesh. Data in structured mesh is arranged in adjacent cells while data in unstructured mesh is scattered throughout the whole domain with additional connectivity relationships. In view of this, unstructured mesh provides more geometric flexibility and freedom in terms of the storage and access of the data and is usually employed in the Fluent code.

A variable in unstructured mesh is mapped to a storage maker that specifies its memory location. It was discussed by Vasquez and Ivanov (2000) that one could not solve multiphase flow problems by simply increasing the number of variables and equations since they were all coupled. Therefore, Vasquez and Ivanov (2000) developed an algorithm for solving general multiphase flow problems in multidimensional unstructured meshes, which was called Phase Coupled Semi-Implicit Method for Pressure-Linked Equation, or PC-SIMPLE, for short.

The PC-SIMPLE algorithm is an extension of the SIMPLE algorithm such that a brief introduction to the SIMPLE algorithm is provided here first. The SIMPLE algorithm was originally developed by Patankar and Spalding (1972) as a guess-and-correct procedure. With an initial guess of the flow field, the velocities are first computed from momentum equations and then used in the pressure correction equation to obtain the
pressure. Based on the discrepancy between the guessed field and the computed field, the variables are then updated with appropriate under-relaxation parameters. It is always an iterative procedure.

Similar to the SIMPLE algorithm, ensemble averaged equations for mass, momentum, energy, and/or turbulence with closure relations for each phase are also solved in the PC-SIMPLE algorithm (Vasquez and Ivanov, 2000). One difference of the PC-SIMPLE algorithm from the SIMPLE algorithm lies in the existence of interfacial coupling terms in the conservation equations, which can be treated explicitly, semi-implicitly, such as the Partial Elimination Algorithm (Spalding, 1980), or implicitly. Attention is also paid to the application of the total volume continuity in the pressure-velocity coupling in the PC-SIMPLE algorithm, which helps avoid bias towards a heavy phase.

5.2. **Mesh generation**

All the meshes of the present numerical models are generated using the integrated solid modeling and meshing commercial program GAMBIT. The mesh refinement is performed by successively adjusting the number of cells to increase the mesh density. The numerical model with a finer mesh resolves more physical features in an appropriate fashion, but requires more iterations for convergence. The criterion of the grid independence is based on a small relative error of important hydrodynamic parameters. An optimization between an accurate solution with adequate details and an acceptable computational efficiency should be achieved.
5.3. **Boundary conditions and convergence criteria**

Fluent code utilizes a segregated solver to evaluate the linearized system of the equations in the two-fluid model using the Gauss–Seidel method. The variables for each phase in the momentum equations are decoupled from those for all other phases using the full elimination algorithm. It has been observed, experimentally, that the inlet turbulence can sometimes significantly influence the downstream flow. The initial estimation of turbulent kinetic energy and dissipation rate are supplied based on empirical correlations in the Fluent code, which are related to the turbulence intensity as

\[ I = 0.16 \text{Re}^{-1/8} \],

where \( \text{Re} \) is the Reynolds number for the liquid phase based on the hydraulic diameter. The static gauge pressure at the outlet boundary was specified based on the experimental data. The boundary conditions at the walls are internally computed by the Fluent code, which obviates the need for boundary condition inputs.

All simulations are conducted in double precision to obtain high accuracy. The iteration procedure continues until the scaled residuals of all variables are sufficiently small (usually less than \( 10^{-4} \)). The global imbalance of mass for each phase is also monitored, which should be reduced from its original value by several (usually larger than four) orders of magnitude.

5.4. **Model validation: air-water bubbly flows in a circular pipe**

5.4.1. **Flow conditions**

Three-dimensional simulations were performed for co-current upward air-water bubbly flows in a vertical pipe with an inner diameter of 48.3 mm. The relevant
experiments were conducted by Fu (2001). In the experiment, the local flow data were acquired at three axial locations, i.e., \( z / D = 5, 30 \), and 55, using multi-sensor conductivity probes, which have a measurement uncertainty less than \( \pm 10\% \) for the void fraction and interfacial area concentration (Kim, 1999). Here, \( D \) is the inner diameter of the pipe and \( z \) is the vertical distance measured from the inlet (i.e., the exit of bubble injector).

Table 5.1 summarizes the experimental conditions, including the superficial velocities of the gas and liquid phases, void fraction, interfacial area concentration, and bubble Sauter mean diameter at the location of 5 pipe diameters away from the inlet, i.e., \( z / D = 5 \). The averaged superficial velocities of the gas (air) and liquid (water) phases, i.e., \( \langle j_g \rangle \) and \( \langle j_l \rangle \), range from 0.039 to 1.275 m/s, and 0.064 to 5.1 m/s, respectively. All of these flows fall in the bubbly flow regime on a flow regime map (Mishima and Ishii, 1984), as shown in Figure 5.1.

Also, the bubbly flow condition can be examined by considering two geometrical bubble scales that bound the limits of the diameter for small bubbles, i.e., the maximum spherical bubble limit \( (D_{ds}) \) and maximum distorted bubble limit \( (D_{d,\text{max}}) \), as introduced in Section 2.1. Bubbles, when they are small, are in perfect spherical shape without wobbling motion until their diameters exceed \( D_{ds} \). Beyond this size, bubbles start to become distorted. Furthermore, bubbles will transition to cap, slug or churn-turbulent bubbles when the bubble diameter is larger than \( D_{d,\text{max}} \). Under the current air-water flow condition, \( D_{ds} \) and \( D_{d,\text{max}} \) are calculated approximately as 2 and 10.7 mm, respectively. It
is evident from Table 5.1 that the initial bubble Sauter mean diameter is below $D_{d,max}$. In addition, the bubble Sauter mean diameters for all the flow conditions, except for Runs 5 and 10, are approximately 2 to 3 mm.

<table>
<thead>
<tr>
<th>Run #</th>
<th>$\langle j_g \rangle$ (m/s)</th>
<th>$\langle j_l \rangle$ (m/s)</th>
<th>$\langle \alpha \rangle$ (%)</th>
<th>$\langle a_i \rangle$ (m$^{-1}$)</th>
<th>$\langle D_{sm} \rangle$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Run-2</td>
<td>0.039</td>
<td>0.682</td>
<td>2.21</td>
<td>58.0</td>
<td>2.3</td>
</tr>
<tr>
<td>Run-3</td>
<td>0.136</td>
<td>0.682</td>
<td>9.37</td>
<td>180</td>
<td>3.1</td>
</tr>
<tr>
<td>Run-4</td>
<td>0.138</td>
<td>2.336</td>
<td>3.74</td>
<td>94.8</td>
<td>2.4</td>
</tr>
<tr>
<td>Run-5</td>
<td>0.506</td>
<td>2.336</td>
<td>12.8</td>
<td>171</td>
<td>4.5</td>
</tr>
<tr>
<td>Run-6</td>
<td>0.538</td>
<td>5.10</td>
<td>5.75</td>
<td>193</td>
<td>1.8</td>
</tr>
<tr>
<td>Run-7</td>
<td>1.234</td>
<td>5.10</td>
<td>11.7</td>
<td>260</td>
<td>2.7</td>
</tr>
<tr>
<td>Run-10</td>
<td>1.275</td>
<td>2.607</td>
<td>25.7</td>
<td>166</td>
<td>9.3</td>
</tr>
<tr>
<td>Run-14</td>
<td>0.039</td>
<td>0.064</td>
<td>11.8</td>
<td>295</td>
<td>2.4</td>
</tr>
<tr>
<td>Run-16</td>
<td>0.039</td>
<td>0.20</td>
<td>7.03</td>
<td>188</td>
<td>2.2</td>
</tr>
<tr>
<td>Run-17</td>
<td>0.133</td>
<td>0.20</td>
<td>25.0</td>
<td>559</td>
<td>2.7</td>
</tr>
</tbody>
</table>

Table 5.1 Flow conditions at $z / D = 5$

Figure 5.1. Flow conditions in the flow regime map (Mishima and Ishii, 1984)
5.4.2. *Simulations with model coefficients from Ishii et al. (2002)*

As pointed out earlier, efforts have been made to determine the IATE model coefficients by comparing numerical results to experimental measurements. One of these efforts was made by Ishii et al. (2002), who used the one-dimensional two-fluid model and a one-dimensional one-group IATE model (based on the three-dimensional IATE models discussed in Eqs. (2.13)-(2.15) and (2.17)) to calculate the phase distributions for bubbly flows in medium-sized circular pipes, and suggested values for the coefficients of the one-dimensional one-group IATE model. Their study showed acceptable predictions of flow parameters along the flow direction. The IATE model coefficients suggested by Ishii et al. (2002) are shown as follows:

Turbulent impact: \( C_{Tt} = 0.0085; \ W_{efr} = 6.0; \)

Wake entrainment: \( C_{WE} = 0.002; \)

Random collision: \( C_{RC} = 0.004; \ C = 3.0; \ \alpha_{\text{max}} = 0.75. \)

Its consistency and universal applicability have been validated by several studies, including the one by Fu and Ishii (2003b).

In the current study, three-dimensional numerical calculations were first performed assuming that the coefficients from the one-dimensional model benchmark are applicable to the three-dimensional simulations. After a careful mesh sensitivity study, it was found that for the pipe test section, 380,160 cells with 900 nodes along the pipe axial direction (over a height of 3 m) were sufficient. A similar mesh sensitivity study can be found in the study carried out by Wang and Sun (2009). Because of bubbly flows, the dispersed model of the standard \( k - \varepsilon \) turbulence model was applied. Lateral profiles of
the void fraction, interfacial area concentration, and bubble velocity at $z / D = 5$
obtained by Fu (2001) were applied as the inlet boundary conditions. These profiles were
not uniform in the radial direction.

Differences between the code predictions ($\langle a_{i}^{\text{num}} \rangle$) and the measurements ($\langle a_{i}^{\text{exp}} \rangle$) of the area-averaged interfacial area concentration are quantified using the
relative error, which is defined as:

$$\text{Error} = \frac{\langle a_{i}^{\text{num}} \rangle - \langle a_{i}^{\text{exp}} \rangle}{\langle a_{i}^{\text{exp}} \rangle} \times 100 \text{ [%].} \tag{5.2}$$

As shown in Figure 5.2, the relative errors at the locations of $z / D = 30$ and 55 are over
50% for the four experimental runs shown. The interfacial area concentration is always
overestimated in the simulation for these flow conditions, which implies that the source
term in the one-group IATE is over-predicted.

![Figure 5.2. Relative error of the interfacial area concentration using model coefficients from Ishii et al. (2002)](image)
5.4.3. Discussion on the three-dimensional model

There are two possible issues when the calibrated one-dimensional IATE model is used for three-dimensional analysis. The first issue is attributed to the averaging process used to obtain the one-dimensional IATE model from the three-dimensional IATE model. In the averaging process, the covariance term representing the difference between the average of the product of two variables and the product of two averaged variables was neglected, i.e., \( \text{COV} \langle AB \rangle = \langle AB \rangle - \langle A \rangle \langle B \rangle = 0 \) (Kim, 1999). The other issue is related to the source term of the one-group IATE in Eq. (2.13) or similarly in Eq. (3.9), which includes the velocity gradient in the form of \(-a_i \alpha \rho_g \nabla \cdot \vec{v}_g\). This term is treated as \(-a_i \alpha \rho_g \frac{\partial v_{gz}}{\partial z}\) in the one-dimensional form. However, it should be \(-a_i \alpha \rho_g \left( \frac{\partial v_{gz}}{\partial x} + \frac{\partial v_{gy}}{\partial y} + \frac{\partial v_{gz}}{\partial z} \right)\) in a three-dimensional model. It is clearly seen that the additional contribution, i.e., from the term \( \frac{\partial v_{gz}}{\partial x} + \frac{\partial v_{gy}}{\partial y} \), is omitted in the one-dimensional model. These two issues would not exist if the lateral flow distributions were uniform, which, however, is not true for the current flow conditions.

Figure 5.3 shows the velocity profile across the cross section of the test section in Runs 5, 6, 10, and 16. It is noted that for all the plots here, locations \( r / R = 0 \) and 1 represent respectively the centerline and wall of the pipe, where \( r \) and \( R \) are the radial position and pipe radius. The predicted profiles by Fluent code are in fairly satisfactory
agreement with the measurements and are apparently not uniform. The velocity gradient effect is especially important for the flow very near the wall.

In addition, during the calibration process of the coefficients for the one-dimensional IATE model, the bubble velocities were obtained by interpolation using either a linear or a second-order polynomial fit based on the measured bubble velocities

Figure 5.3. Bubble velocity profiles from experiments and simulations: (a) Run 5, (b) Run 6, (c) Run 10, and (d) Run 16
(Ishii et al., 2002). The errors from the estimations of gas velocity might propagate through the IATE model, resulting in model coefficients with errors.

Therefore, the model coefficients calibrated by Ishii et al. (2002) are inappropriate for three-dimensional simulations. A new set of the IATE model coefficients needs to be developed for three-dimensional simulations.

5.4.4. Testing on model coefficients with one-dimensional simulation

A study was carried out to examine the model coefficients that were obtained by Ishii et al. (2002) through a quasi-one-dimensional simulation. In this study, a three-dimensional simulation of Run 10 was performed, but only the velocity gradient in the $z$-direction (axial direction) was included in the term of $- \left( a_i \alpha \rho_g \right) \nabla \cdot \vec{v}^g$, i.e., $- \left( a_i \alpha \rho_g \right) \frac{\partial v^g}{\partial z}$ was used to calculate the term.

Figure 5.4(a) clearly shows that the predicted interfacial area concentration in the radial direction at the elevation of $z / D = 55$ is in good agreement with the experimental data. The predicted void fractions at $z / D = 55$ from the Fluent code with and without the IATE model are plotted along with the experimental data in Figure 5.4(b) for comparison. The core void peak observed in the experiment is captured when the one-group IATE model was incorporated, which is illustrated more clearly in Figure 5.4(c) by the contour plot of the void fraction from the Fluent with the one-group IATE model. This exercise basically demonstrated that the IATE model coefficients from Ishii et al.
(2002) work reasonably well in this simulation, where the radial bubble velocity profile is considered uniform, i.e., the flow can be considered quasi one-dimensional.

Figure 5.4. Lateral distributions in Run 10 from simulations and experiments at the location \( z / D = 55 \): (a) the interfacial area concentration, (b) the void fraction, and (c) counter of the void fraction from Fluent code with one-group IATE model

5.4.5. Suggestions on model coefficients for three-dimensional IATE model

The exercise in Section 5.4.4 indicates that it is indispensable to determine appropriate values for the model coefficients in Eqs. (2.14), (2.15), and (2.17) for a three-
dimensional IATE model. The methodology of determining these coefficients is based on the experimental observations that the different bubble interaction mechanisms are predominant in different flow conditions. The coefficient for one specific bubble interaction term is possible to be estimated quasi-independently, if for certain flow conditions, this term is significant and other bubble interactions are either known or negligible. For instance, for flows having a low flow rate, the dominant bubble interaction phenomenon is typically the wake entrainment coalescence, in which following bubbles inside the wake region of a preceding bubble catch up and coalesce with the preceding bubble. When the superficial liquid velocity becomes larger, an additional mechanism that would appear first is the random collision coalescence due to the higher liquid turbulent intensity. When the superficial liquid velocity continues to increase such that the inertia of a turbulent eddy overcomes the surface tension energy at a bubble interface, the bubble breakup phenomenon due to the turbulent impact starts to take place.

The coefficients of $W_{e_{cr}}$, $C_r$, and $\alpha_{\text{max}}$ in Eqs. (2.13)-(2.15) and (2.17) are assumed the same as the values suggested by Ishii et al. (2002). The process of identifying the other model coefficients is illustrated as follows:

1. Estimate $C_{WE}$ when $j_g$ and $j_f$ are low;

2. Estimate $C_{RC}$ when $j_g$ is high and $j_f$ is still low. Here, $C_{WE}$ is pre-determined in step 1;
3. Estimate $C_{TI}$ when $\dot{J}_g$ and $\dot{J}_f$ are high. Here, $C_{WE}$ and $C_{AE}$ are determined in the previous two steps;

4. Check these adjustment coefficients for all flow conditions;

5. Adjust the coefficients iteratively until the relative errors between predictions and experimental data approach their minimum.

As a result, the following model coefficients yield the best fit to the experimental data in our three-dimensional simulations. The relative errors between the numerical and experimental results of the area-averaged interfacial area concentration are within 15%, as shown in Figure 5.5.

Turbulent impact: $C_{TI} = 0.005$, $We_{cr} = 6.0$;

Wake entrainment: $C_{WE} = 0.006$;

Random collision: $C_{RC} = 0.013$, $C = 3.0$, $\alpha_{max} = 0.75$.

Figure 5.5. Relative errors of interfacial area concentration using the suggested model coefficients
In addition, the predicted interfacial area concentration values using different coefficients at the location $z / D = 55$ are compared to the experimental data in Figure 5.6(a) for Run 5 and in Figure 5.6(b) for Run 6. It is clearly seen that in both runs, the interfacial area concentration values using the coefficients suggested by Ishii et al. (2002) are overestimated, especially near the wall region. A distinct wall peak of interfacial area concentration arises due to the contributions of the sharp velocity decrease close to the wall.

5.4.6. Study on the lift force

The shear-induced lift force, proportional to the vorticity of the liquid phase, is important for phase distributions in two-phase flows. The study on the lift force was performed using three different available models: (1) Model 1: simulation without the IATE model and without lift force ($C_l = 0$); (2) Model 2: simulation without the IATE model and with a constant lift force coefficient; and (3) Model 3: simulation with the
IATE model and with the lift force coefficient given by Eq. (3.36), which was proposed by Tomiyama (1998). The coefficients in the IATE model suggested in Section 5.4.5 were used here.

Figure 5.7 shows the void fractions calculated by the three aforementioned models and a comparison with the experimental data acquired by Fu (2001) at $z / D = 55$ for Runs 2 and 5. In Models 1 and 2, the bubble size is considered to be constant, which is initially defined at the inlet. The lift force coefficient can therefore be determined based on the initial bubble size using Tomiyama’s model given by Eq. (3.36), and it results in a value of about 0.25 for Model 2 in Runs 2 and 5. As we compare the predictions between Models 1 and 2 (the lift force coefficient was changed from 0 to 0.25), Model 2 provides a slightly higher void fraction in the wall region (local wall peak), which indicates that the lift force pushes small bubbles towards to the wall in the
current upward flows. In the Fluent simulation with the IATE model implemented (Model 3), the lift force coefficient is a function of bubble size and therefore changes as the flow develops. It can be clearly seen that the results of Model 3 are generally in better agreement with experimental data for both flow conditions.

5.4.7. Comparisons of results

Three-dimensional simulations were performed for all the flow conditions with the coefficients suggested in Section 5.4.5, and the simulation results are reported in Figures 5.8-5.10.

As shown in Figure 5.8, the implementation of the one-group IATE model considerably improves Fluent’s predictive capability in the lateral phase distributions, except for Runs 16 and 17. Run 16 has low superficial velocities and low void fraction. It was observed that in this run the axial pressure drop, which leads to bubble expansion, was a major contributor to the change of the void fraction along the flow direction. The bubble size in Run 16 was very close to \( D_{ds} \) and therefore the bubbles were fairly stable and did not actively interact with others in the neighborhood, i.e., bubble interactions became negligible. The distributions of the void fraction along the radial direction were almost flat except near the wall region, where a small peak appeared, as shown in Figure 5.8(e). This phenomenon could be captured by the Fluent code, regardless of whether or not the one-group IATE model was applied. In Run 17, turbulent eddy impact was not strong enough to break up bubbles due to the relatively low superficial velocity of the liquid phase. In contrast, bubble coalescence took place, induced by both the random collision and wake entrainment, producing relatively larger bubbles, such as cap and slug
bubbles. Consequently, Run 17 is close to the flow regime transition region, where the bubble transport mechanisms are more complicated (Sun et al., 2004a). Therefore, the one-group IATE model is not capable of describing these additional bubble interactions due to the existence of large bubbles, requiring the application of the two-group IATE model for Run 17.

As the interfacial area concentration was introduced in the Fluent code, the predictions of interfacial area concentration were plotted in Figure 5.9 to help understand bubble interaction mechanisms and validate the models. Predictions of the interfacial area concentration from the Fluent code with the IATE model match the experimental results qualitatively and quantitatively. For instance, it can be seen that the peak of the interfacial area concentration in the wall region in Run 3 is captured by the simulation. A weak core peak of the interfacial area concentration is observed in Runs 5 and 6; while a relatively flat profile is shown in the other runs. A sharp decrease close to the wall occurs in all runs, since the interfacial area concentration on the wall is forced to zero.
Figure 5.8. Predictions of void fraction with comparison to experimental data at $z / D = 55$: (a) Run 3, (b) Run 5, (c) Run 6, (d) Run 10, (e) Run 16, and (f) Run 17.
Figure 5.9. Predictions of interfacial area concentration with comparison to experimental data at \( z / D = 55 \): (a) Run 3, (b) Run 5, (c) Run 6, (d) Run 10, (e) Run 16, and (f) Run 17
Figure 5.10. Predictions of gas velocity with comparison to experimental data at $z / D = 55$: (a) Run 3, (b) Run 5, (c) Run 6, (d) Run 10, (e) Run 16, and (f) Run 17
Finally, comparisons of the bubble velocity for each run are provided in Figure 5.10. Generally speaking, simulations from the Fluent code with the IATE model are in better agreement with the experimental data, except for Run 6.

5.5. Model validation: air-water bubbly flows in a duct

5.5.1. Description of experiments

Another study was performed to test the capability of the Fluent code with the one-group IATE model for air-water bubbly flows in a confined channel. Based on a literature survey, it was decided to use the experimental data acquired by Kim (1999) for comparison with the code calculations. A short description of the experiments is herein provided for the benefit of better explaining the numerical model.

The experiments focused on performing the measurements of local parameters, such as the bubble velocity, void fraction, interfacial area concentration, and bubble number frequency for upward air-water vertical two-phase flows in a rectangular flow channel (Kim, 1999). De-mineralized water and air, denoted as the liquid and gas phases, respectively, with varied superficial liquid (water) velocities, \( j_l \), and superficial gas (air) velocities, \( j_g \), were introduced from the bottom into a confined rectangular duct with a cross section of 200 mm (width) × 10 mm (gap). The experiments were performed at a constant temperature of 20 °C and under the atmospheric pressure. Through six two-phase mixture injection sites, which were arranged by offsetting them with each other by an equal distance below the test section inlet, a uniform injection condition was approximately achieved. The local measurements were taken using miniature double-sensor conductivity probes having a measurement uncertainty less than 10%.
5.5.2. **Numerical model and flow conditions**

In the simulations, air was modeled as an ideal gas, of which the density was related to the pressure to account for the pressure drop along the flow duct. The rectangular duct was represented by a three-dimensional model, which has the dimensions of 200 mm ($x$) $\times$ 10 mm ($y$) $\times$ 2700 mm ($z$) with 2700 mm being the duct height. After the evaluation of different mesh sizes for the current two-phase flow conditions, a hexahedral mesh containing $100 \times 10 \times 1000$ cells for the above computational domain was chosen.

Due to considerable difficulties in obtaining reliable experimental data in flow conditions with either very low or very high void fractions using local measurement instruments, experimental data with void fractions in an intermediate range, e.g., between about 4% and 25%, were selected for the current validation study. Two flow conditions were consequently chosen to be simulated. Table 5.2 shows these two conditions at the location of $z / D_h = 34.8$, where $D_h$ is the hydraulic diameter of the duct. Uniform inlet boundary conditions were applied using the averaged values obtained from the measurements at $z / D_h = 34.8$.

<table>
<thead>
<tr>
<th>Run #</th>
<th>$\langle j_x \rangle$ (m/s)</th>
<th>$\langle j_y \rangle$ (m/s)</th>
<th>$\langle \alpha \rangle$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>R-1</td>
<td>0.95</td>
<td>0.14</td>
<td>11.0</td>
</tr>
<tr>
<td>R-2</td>
<td>4.42</td>
<td>0.62</td>
<td>7.8</td>
</tr>
</tbody>
</table>

Table 5.2 Measurements at location $z/D_h = 34.8$ in a rectangular duct
The following model coefficients determined for the rectangular test section by Kim (1999) were adopted in this study:

Turbulent impact: $C_{TI} = 0.026; We_{cr} = 8.0$;

Wake entrainment: $C_{WE} = 0.042$;

Random collision: $C_{RC} = 0.003; C = 3.0; \alpha_{max} = 0.75$.

It should be noted that these coefficients were suggested from a one-dimensional calibration by Kim (1999).

5.5.3. **Comparison of results**

The flow behaviors at the location $z/D_H = 88.2$ in Run R-1 and $z/D_H = 141.7$ in Run R-2 are compared with the experimental data, as shown in Figures 5.11 and 5.12. In the figures presented in this section, locations $x/W = 0$ and 1 represent the wall and the centerline of the duct in the width direction ($x$-direction), respectively (i.e., $W = 100$ mm). It was observed in the experiments that the phase distribution in the gap direction ($y$-direction) was fairly uniform, except at the regions adjacent to the wall. Therefore, to make the comparison clearer, the line-averaged results (in the $y$-direction) are reported here.
Figure 5.11. Comparisons of numerical results with the experimental data (Kim, 1999) at $z/D_{H} = 88.2$ for Run R-1: (a) void fraction, (b) interfacial area concentration, and (c) bubble Sauter mean diameter.
The wall peak of the void fraction observed in the experiment of Run R-1 is qualitatively captured in the calculations with the IATE model, but with a notable difference between the predictions, both with and without the lift force, and the experimental data, as shown in Figure 5.11(a). Again, the lift force tends to push small bubbles to the wall region, resulting in a relatively lower void fraction in the center region compared to the results without the lift force. Meanwhile, the probability of bubble coalescence is enhanced near the wall region in the calculation with the lift force due to a relatively larger bubble number concentration, which leads to an increase in the average bubble size and therefore a reduction in the wall peak of the interfacial area concentration, as shown in Figure 5.11(b). Also note that some fluctuations along the $x$-direction exist in the void fraction calculations when both the IATE and lift force are considered.

In Run R-2, a significant difference existed between the liquid and gas velocities. The superficial liquid velocity was 4.42 m/s and the flow condition was close to the bubbly flow to finely-dispersed bubbly flow transition. The lift force is included in all the simulations shown in Figure 5.12 for Run R-2. The time marching method was applied, which will be discussed in Chapter 7 in detail. Several time marching steps were used and a time step of 0.0005 second was adopted.
Figure 5.12. Comparisons of numerical results with the experimental data (Kim, 1999) at $z/D_H = 141.7$ for Run R-2: (a) void fraction, (b) interfacial area concentration, and (c) bubble Sauter mean diameter
As indicated in Figure 5.12(a), a flat profile is obtained for the void fraction in the simulation without the IATE model, whereas the introduction of the IATE model helps capture the wall peak reasonably well. According to the experimental observation (Kim, 1999), a significant bubble relative motion generated additional turbulent fluctuations, which caused the flow to be slightly oscillatory. However, the present simulation with the IATE model is not able to reproduce the oscillatory phenomenon. In addition, an extremely strong shear stress in the vicinity of the wall was observed experimentally (Kim, 1999), which contributed to the bubble disintegration into smaller ones, as implied in Figure 5.12(c). The interfacial area concentration close to the wall was not well-predicted by the Fluent code, which leads to an opposite trend for the bubble Sauter mean diameter, as shown in Figure 5.12(c). Therefore, a further study on the wall boundary condition is necessitated to improve the predictions.

Furthermore, to analyze the effects of individual contributions from the bubble interaction mechanisms on the change of the interfacial area concentration for Run R-2, three additional simulations have been carried out to include just one individual source/sink term in the one-group IATE model in each simulation, as shown in Figure 5.13. A time step of 0.0005 second was adopted in these simulations. It is clear that the bubble breakup due to the impact of turbulent eddies influences the results most significantly among the three bubble interactions. Furthermore, the bubble breakup mechanism due to the impact of turbulent eddies acts as the source term in the IATE model whereas the two bubble coalescence mechanisms behave as sink terms.
Figure 5.13. Evaluation of the individual bubble interaction contributions at \( z/D_h = 141.7 \) for Run R-2.

5.6. Model validation: liquid-liquid two-component flows in a pipe

5.6.1. Background

Recent advancements in space explorations have brought more focus on the potential applications of two-phase flows in a reduced-gravity/microgravity environment (Fowle, 1981; Rankin and Marshall, 1983; Keshock, 1987; Colin et al., 1991; Chahed et al., 2002; Takamasa et al., 2004). For example, the latent heat due to the phase change in two-phase flow can be utilized in a heat removal system to improve its capacity and efficiency, which is important to an advanced spacecraft design. In the past, to investigate the characteristics of gas-liquid two-phase flows under reduced-gravity conditions, most of the experiments were performed either in a drop tower, a parabolic flight or a sounding-rocket, all of which were of high cost. In view of this, a more practical and economic experimental approach was developed using a ground-based facility, in which
two immiscible fluids of very similar density were used to simulate the reduced buoyancy force resulting from the suppressed gravitational field (Nigmatulin et al., 2000; Vasavada et al., 2007). One such experimental study was conducted by Vasavada et al. (2007, 2009), who used two immiscible liquids, namely, water as the continuous phase and Therminol 59® as the dispersed phase. It was pointed out by the authors that the acquired experimental data agreed with the published data obtained from air-water systems in parabolic flights and therefore were helpful in understanding both gas-liquid two-phase flow under reduced-gravity conditions and liquid-liquid two-component flow.

5.6.2. Description of experiments

The goal of this study is to examine the predictive capability of the Fluent code with the one-group IATE model for liquid-liquid two-component flows by comparing the simulation results to the data obtained from the experiments performed by Vasavada et al. (2007). The experiments were carried out to measure local flow parameters of co-current liquid-liquid two-component flows in a vertical circular pipe having an inner diameter of 25.4 mm and a height of 2.8 m. Water and Therminol 59®, were introduced from a mixing chamber below the test section and flowed upward adiabatically at 20°C and the atmospheric pressure. Water was the continuous phase with a density of 998 kg/m³. The flow rates of water were measured by a magnetic flowmeter within an uncertainty of ±1.0% and a rotameter within an uncertainty of ±3.0%. Therminol 59®, an organic engineering fluid, was the dispersed phase with a density of 972 kg/m³ at the experimental condition. The flow rates of Therminol 59® were measured using a rotameter with an inaccuracy of ±3.0% if the flow rate was low, and an inline paddle
wheel flowmeter with an inaccuracy of ±2.0% if the flow rate was high. Four-sensor conductivity probes were employed to measure local two-phase flow variables at two axial locations of $z / D = 30$ and 58, respectively. At each axial location, ten measurements were taken along the radial direction. The benchmark studies showed that the four-sensor conductivity probes measured the drop velocity, drop volumetric fraction (void fraction), and interfacial area concentration with an uncertainty of ±5.0%, ±7.0%, and ± 8.0 ~ 12.0%, respectively.

As aforementioned, the shape of the bubbles/drops may be determined using three length scales, namely, the maximum spherical bubble limit ($D_{d}$), maximum distorted bubble limit ($D_{d,\text{max}}$), and maximum cap bubble limit ($D_{c,\text{max}}$), which are are 8.9, 50.5, and 505.0 mm, respectively, for the current flow conditions. It is noted that the pipe inner diameter 25.4 mm is much smaller than the maximum distorted bubble limit. Therefore, the large-size cap-shape drops will elongate in the axial direction as they grow and reach a shape similar to the slug bubbles as the void fraction increases to a certain value, which depends on the flow conditions and fluid properties.

5.6.3. Numerical model and flow conditions

Numerical simulations were performed to simulate the above liquid-liquid flow experiments. Water and Therminol 59® were considered incompressible and immiscible with a density difference of 2.7% at the room temperature. The dynamic viscosities of water and Therminol 59® were 0.001 and 0.00686 kg/m-s, respectively (Vasavada et al., 2007). The area-averaged experimental data acquired at the location $z / D = 30$ was
applied as the uniform inlet boundary condition, and the atmospheric pressure was used as the outlet boundary condition. A circular pipe 2.1-m high was modeled since the inlet of the test section in the numerical model was located at $z / D = 30$ in the physical model. Simulations including 9 flow conditions covered dispersed drop flow and drop-to-slug flow transition regimes, with the area-averaged void (drop) fractions ranging from 3 to 30%. Table 5.3 lists the cross-sectional area-averaged data for each flow condition at $z / D = 30$ acquired by Vasavada et al. (2007).

For the model coefficients of the one-group IATE model, the following values suggested by Vasavada et al. (2009) were adopted in the simulations:

- Turbulent impact: $C_{TI} = 0.034; W_{cr} = 6.0$;
- Wake entrainment: $C_{WE} = 0.002$;
- Random collision: $C_{RC} = 0.0021; C = 3.0; \alpha_{\text{max}} = 0.52$.

<table>
<thead>
<tr>
<th>Run #</th>
<th>$\langle j_x \rangle$ (m/s)</th>
<th>$\langle j_d \rangle$ (m/s)</th>
<th>$\langle \alpha \rangle$ (%)</th>
<th>$\langle a_i \rangle$ (m$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L-1</td>
<td>0.215</td>
<td>0.012</td>
<td>0.048</td>
<td>73</td>
</tr>
<tr>
<td>L-2</td>
<td>0.209</td>
<td>0.050</td>
<td>0.159</td>
<td>238</td>
</tr>
<tr>
<td>L-3</td>
<td>0.343</td>
<td>0.050</td>
<td>0.125</td>
<td>235</td>
</tr>
<tr>
<td>L-4</td>
<td>0.305</td>
<td>0.112</td>
<td>0.278</td>
<td>264</td>
</tr>
<tr>
<td>L-5</td>
<td>0.496</td>
<td>0.056</td>
<td>0.102</td>
<td>101</td>
</tr>
<tr>
<td>L-6</td>
<td>0.496</td>
<td>0.112</td>
<td>0.220</td>
<td>180</td>
</tr>
<tr>
<td>L-7</td>
<td>0.745</td>
<td>0.056</td>
<td>0.084</td>
<td>86</td>
</tr>
<tr>
<td>L-8</td>
<td>0.742</td>
<td>0.112</td>
<td>0.167</td>
<td>137</td>
</tr>
</tbody>
</table>

Table 5.3 Measurements at the location of $z / D = 30$ for liquid-liquid flows (Vasavada et al., 2007)
5.6.4. Comparison of results

Table 5.4 shows that the mass imbalance for the eight simulations reaches at least $10^{-4}$ in magnitude compared to the mass flow rate at the inlet. For all the plots in this section, locations $r/R = 0$ and 1 represent the centerline and wall of the pipe, where $r$ and $R$ are the radial position and pipe radius, respectively.

<table>
<thead>
<tr>
<th>Run #</th>
<th>Mass in (kg/s)</th>
<th>Mass out (kg/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>L-1</td>
<td>0.11465</td>
<td>0.11465</td>
</tr>
<tr>
<td>L-2</td>
<td>0.13031</td>
<td>0.13031</td>
</tr>
<tr>
<td>L-3</td>
<td>0.19809</td>
<td>0.19809</td>
</tr>
<tr>
<td>L-4</td>
<td>0.20937</td>
<td>0.20937</td>
</tr>
<tr>
<td>L-5</td>
<td>0.27843</td>
<td>0.27842</td>
</tr>
<tr>
<td>L-6</td>
<td>0.30598</td>
<td>0.30598</td>
</tr>
<tr>
<td>L-7</td>
<td>0.40437</td>
<td>0.40437</td>
</tr>
<tr>
<td>L-8</td>
<td>0.43041</td>
<td>0.43041</td>
</tr>
</tbody>
</table>

Table 5.4 Comparisons of computed mass outflow rates to the inflow rates

As discussed in Section 3.3.3, the velocity gradient in the continuous phase and the relative velocity between different phases in two-phase flows give rise to the shear-induced lift force, which usually contributes to the radial phase distributions (Auton, 1987). As shown in the previous sections, the lift force tends to push small bubbles to the wall region in upward gas-liquid two-phase bubbly flows. For liquid-liquid two-component flows, the effect of the lift force on the phase distribution was investigated by using the conventional Fluent code without the one-group IATE model.

As shown in Figure 5.14, numerical predictions for Run L-3 using different lift force coefficient values, i.e., $C_l = 0$ and 0.5, did not result in an appreciable difference at
the location of $z/D = 58$. This was because the difference of the axial velocity between water and Therminol 59® along the radial direction was not significant, as shown in Figure 5.15, resulting in a low relative velocity. Additional studies performed for other runs yielded the same conclusion, which agreed with Chahed et al. (2002) under the microgravity condition. Thus, it might be reasonable to set the lift force to zero in the momentum equations for the remaining simulations.

Figure 5.14. Comparisons of the radial void fraction distributions using different lift force coefficients for Run L-3 at $z/D = 58$
Figure 5.15. Numerical predictions of radial profiles of the axial velocities of water and Therminol 59® for Run L-3 at $z / D = 58$: (a) $C_t = 0$ and (b) $C_t = 0.5$

As discussed earlier, the lateral void fraction profile may be classified as: core peaking, intermediate peaking, wall peaking, and a flat distribution. Figure 5.16 illustrates the code calculations of the void fraction and interfacial area concentration along with the corresponding experimental data (Vasavada et al., 2007) for Runs L-1 and L-2 at $z / D = 58$, for which the superficial velocity of the continuous phase was similarly low (~ 0.2 m/s); while the superficial velocity of the dispersed phase in Run L-2 was approximately four times that in Run L-1. Two simulation models are shown in the plots, namely, Fluent without IATE and Fluent with IATE, which, respectively, stand for the conventional Fluent code without the IATE model and the Fluent code with the one-group IATE model.
Figure 5.16. Radial profiles of local flow parameters at $z / D = 58$: (a) void fraction for Run L-1, (b) interfacial area concentration for Run L-1, (c) void fraction for Run L-2, and (d) interfacial area concentration for Run L-2

As illustrated in Figure 5.16(a) and Figure 5.16(c), a distinctive wall peak of the void fraction and a relatively flat distribution away from the wall as observed in the experiments, were qualitatively captured in the simulations, regardless of whether or not the IATE model was applied. However, it was apparent that the simulations with the Fluent code incorporated with the one-group IATE model predicted the lateral phase
distribution slightly better than the Fluent code without the IATE model. The small improvement made by the implementation of the IATE model could be explained based on the observations of the drop behavior from the experiment (Vasavada et al., 2007). In these flow conditions, small drops did not significantly interact with others with a similar size. In other words, neither the coalescence nor breakup of the dispersed phase was very active and made considerable contributions to the change of the interfacial structure.

In addition, the predicted radial distributions of the interfacial area concentration were in reasonable agreement with the experimental data, as shown in Figure 5.16(b) and Figure 5.16(d). The value of interfacial area concentration was not defined explicitly in the conventional Fluent code and therefore was not provided here. Compared to the area-averaged interfacial area concentration given at $z / D = 30$, i.e., 73 and 238 m$^{-1}$ for Runs L-1 and L-2, respectively, as shown in Table 5.3, the computed values of the area-averaged interfacial area concentration at $z / D_h = 58$ decreased to 70 and 180 m$^{-1}$, respectively. The loss of the interfacial area concentration was attributed to the coalescence of the drops, which was mainly due to the wake entrainment (Vasavada et al., 2009). As the superficial velocity of the dispersed phase increased, the local Weber number increased, promoting drop coalescence due to the wake entrainment.
Figure 5.17. Radial profiles of local flow parameters at $z / D = 58$: (a) void fraction for Run L-3, (b) void fraction for Run L-5, (c) void fraction for Run L-7, and (d) velocity of Therminol 59® for Run L-7.

If we keep the superficial velocity of the dispersed phase in Run L-2 constant but increase the superficial velocity of the continuous phase, the lateral void fraction profile would exhibit different characteristics. As shown in Figure 5.17, the predictions by the Fluent code with the one-group IATE model reproduced the experimental data generally better than the conventional Fluent approach. The void fraction profiles were identified as
the intermediate peaking, flat distribution, and core peaking for Runs L-3, L-5, and L-7, respectively. The difference in void peak locations was attributed mainly by the transversal pressure induced by the gradient of the turbulence in the radial direction. In addition, Figure 5.17(d) provided the drop velocity radial profile for Run L-7 at $z/D = 58$. Since the density of Therminol 59® was considered to be constant, the mass flow rate of Therminol 59® was analyzed by integrating the product of the drop velocity and void (drop volumetric) fraction over the entire pipe cross-sectional area.

When the superficial velocity of the dispersed phase reached a relatively high value as in the case of Run L-6 ($\langle j_d \rangle = 0.112$ m/s), or when the superficial velocity of the continuous phase became large as in the case of Run L-8 ($\langle j_c \rangle = 0.742$ m/s), a significant core (center) peak for the void fraction was captured by the Fluent code with the one-group IATE model. In contrast, it was unlikely for Fluent without the IATE model to predict the lateral void fraction distribution, as shown in Figure 5.18.
Figure 5.18. Radial profiles of local flow parameters at $z/D = 58$: (a) void fraction for Run L-6, (b) interfacial area concentration for Run L-6, (c) void fraction for Run L-8, and (d) interfacial area concentration for Run L-8.

In both runs, the velocity might be sufficiently high to promote the bubble coalescence induced by the wake entrainment, which was considered as the predominantly interaction mechanisms. In other words, the wake entrainment mechanism for drop coalescence could be enhanced by increasing either the continuous or dispersed phase velocity, which increased the Weber number. However, Figure 5.18 also

106
demonstrated that the void core peaking was under-predicted by Fluent even with the one-group IATE model compared to the experimental data.

It was observed experimentally that in reduced-gravity two-phase flows, there were three main flow regimes, namely, bubbly (dispersed drop in the current experiment), slug and annular flows, for which different criteria had been applied to characterize the flow regime transitions (Vasavada et al., 2007). One widely used criterion was based on the critical void fraction, which was highly dependent on the pipe size. It was observed by Vasavada et al. (2007) that in their experiments the critical void fraction at the flow regime transition boundary between bubbly and slug flows was approximately 45% for pipes with inner diameters below 25.4 mm and about 25% for pipe sizes above 25.4 mm. The next study was therefore performed to investigate the lateral phase distribution for the conditions where the area-averaged void fraction was larger than 25%. As shown in Figure 5.19, the core peaking of the void fraction observed in the experiment for Run L-4 is fairly well captured by the Fluent with the IATE model.

![Figure 5.19. Radial profiles of the void fraction at $z/D = 58$ for Run L-4](image)

Figure 5.19. Radial profiles of the void fraction at $z/D = 58$ for Run L-4
5.7. Conclusions

In this chapter, the one-group IATE model is successfully implemented into Fluent, with the expectation of improving the predictions of phase distributions in different two-phase flow conditions. Three sets of experimental data were used to validate the Fluent with IATE model.

The first study focuses on the re-calibration of the three-dimensional IATE model in air-water bubbly flow. New IATE model coefficients are suggested, with which numerical results obtained in the three-dimensional simulations show good agreement with the experimental data.

The following studies indicate that the coefficients in the one-group IATE model from a one-dimensional model calibration work reasonably well in the three-dimensional simulations of air-water bubbly flows in a confined flow channel and liquid-liquid two-component flows in a circular pipe. This is mainly because of the relatively uniform velocity distributions across the cross section of the flow channels.

In addition, effects of the lift force on the lateral phase distributions are discussed. The lift force is important in air-water bubbly flows; whereas it becomes negligible in the liquid-liquid two-component flow discussed due to the insignificant relative velocity between water and Therminol 59®.

In summary, it was demonstrated that the simulations with the Fluent code together with the one-group IATE model predict the phase distributions more accurately than the conventional Fluent code without the IATE model in a dispersed two-phase flow.
system. However, it was also shown that the application of the one-group IATE model is limited to bubbly and dispersed drop flows. Larger bubbles/drops encountered in flow regime transition region and flow regimes beyond bubbly flows have substantial differences in their transport mechanisms from small bubbles and drops. It indispensably requires the application of the two-group IATE model for simulations of general two-phase flows.
Chapter 6. Well-posedness Study of Three-field Two-fluid Model

6.1. Background

A successful model proposed for solving physical problems must first satisfy four principles, i.e., equipresence, well-posedness, frame invariance, and fulfillment of the second law of thermodynamics. Mathematically, a well-posed problem means that its solution should exist, be unique, and depend continuously on variables. Insights into the field of the well-posedness of the proposed numerical model are therefore of great significance.

As discussed earlier, some CFD codes, such as CFX and Fluent, and some reactor system safety analysis codes, such as RELAP5, TRACE, and CATHARE, employ the two-fluid model for two-phase flow simulations. In contrast to the single-phase Eulerian model, which has real characteristic roots inherently guaranteed by the second law of thermodynamics, the standard form of the partial differential equations in the two-fluid model may not be strictly hyperbolic as an initial value problem (Gidaspow, 1974; Jones and Prosperetti, 1985). Moreover, the infinite instability growth rate may exist when two-phase flows are modeled with the two-fluid model, which violates the observation that the energy originating from perturbation continuously decays due to the local fluctuations (energy cascade and dissipation), resulting in the naturally steady equilibrium of the flow in different flow regimes. These lead to the possibility of the partial differential equations of the two-fluid model being ill-posed.
In the literature, two fundamental technical approaches were utilized to remedy the ill-posedness of the two-fluid model (Pokharna et al., 1997; Dinh et al., 2003). The first approach is more realistic, in which additional terms representing physical mechanisms, such as the pressure difference between the phases (Hancox et al., 1980), virtual mass force, surface tension force (Brauner and Maron, 1992; Chung, 2007), and Reynolds stress (Harlow and Besnard, 1985), are incorporated into the conservation equations. However, difficulties were encountered in both constructing reliable constitutive relations for these terms and resolving the short wavelengths at which these physical mechanisms become dominant. The other approach is to regularize the model mathematically or numerically. For example, the ill-posedness of the two-fluid model can be remedied by either applying a preconditioning mass matrix (Zanotti et al., 2007) or adding an artificial numerical damping (Pokharna et al., 1997). The disadvantage of the second approach lies in the possibility of introducing non-physical dynamic behaviors.

It is realized that many nuclear reactor safety system analysis codes, such as RELAP5 (Ransom et al., 1995) and TRAC (TRAC-PF1/MOD1 user manual, 1986), use a one-dimensional two-fluid model for modeling two-phase flows. Song and Ishii (2000) reported that the stable region of a well-posed one-dimensional two-fluid model could be evaluated by introducing so-called momentum flux parameters, which helped preserve the information of the local flow structures, in which the void fraction profile is coupled with the velocity profile over the cross section of a flow channel. In addition, the IATE model discussed in Chapter 2 can potentially replace the flow regime-based correlations/models for the interfacial area concentration and further dynamically model
the flow regime transitions. The three-field two-fluid model with the implementation of
the IATE model is called “two-fluid-IATE model” hereafter.

6.2. Governing equations

The current work focuses on discussing the well-posedness of the standard one-
dimensional two-fluid-IATE model, which can be obtained directly by area-averaging the
three-dimensional two-fluid-IATE model. To quantify the coupling effect of the local
void fraction and velocity distributions, the momentum flux parameter $C_{v,k}$ is defined for
Field-$k$ (Song and Ishii, 2000):

$$C_{v,k} = \frac{\langle \alpha_k v_k^2 \rangle}{\langle \alpha_k \langle v_k \rangle \rangle^2} = \frac{\left( \int_A \alpha_k v_k^2 dA \right) \left( \int_A \alpha_k dA \right)}{\left( \int_A \alpha_k v_k dA \right)^2},$$

where $v_k$ is the one-dimensional velocity of Field-$k$. Here, the signs $\langle \rangle$ and $\langle \langle \rangle \rangle$ are
introduced to represent the area averaging and phase fraction weighted area averaging,
respectively. In the conventional one-dimensional two-fluid model, $C_{v,k}$ is assumed to be
unity, potentially resulting in an ill-posed one-dimensional two-fluid model.

To highlight the role that the momentum flux parameters play in the process of
regularization, we assume that the density of each phase does not change appreciably,
both spatially and temporally. Dropping the signs $\langle \rangle$ and $\langle \langle \rangle \rangle$ for simplicity, the area-
averaged continuity and momentum equations of the three-field two-fluid model and two-
group IATEs for an adiabatic incompressible two-phase flow can be written as:
\[
\frac{\partial \alpha_1}{\partial t} + v_1 \frac{\partial \alpha_1}{\partial z} + \alpha_1 \frac{\partial v_1}{\partial z} = - \frac{\Delta \dot{m}_{12}}{\rho_1}, \tag{6.2}
\]

\[
\frac{\partial \alpha_2}{\partial t} + v_2 \frac{\partial \alpha_2}{\partial z} + \alpha_2 \frac{\partial v_2}{\partial z} = \frac{\Delta \dot{m}_{12}}{\rho_2}, \tag{6.3}
\]

\[- \frac{\partial \alpha_1}{\partial t} - v_3 \frac{\partial \alpha_1}{\partial z} - \frac{\partial \alpha_2}{\partial t} - v_3 \frac{\partial \alpha_2}{\partial z} + \left(1 - \alpha_1 - \alpha_2\right) \frac{\partial v_3}{\partial z} = 0, \tag{6.4}\]

\[
\rho_1 v_1 \frac{\partial \alpha_1}{\partial t} + \rho_1 C_{r,1} v_1^2 \frac{\partial \alpha_1}{\partial z} + \alpha_1 \rho_1 \frac{\partial v_1}{\partial t} + 2 \alpha_1 \rho_1 C_{r,1} v_1 \frac{\partial v_1}{\partial z} + \alpha_1 \frac{\partial p}{\partial z} = M_{i,1}^*, \tag{6.5}
\]

\[
\rho_2 v_2 \frac{\partial \alpha_2}{\partial t} + \rho_2 C_{r,2} v_2^2 \frac{\partial \alpha_2}{\partial z} + \alpha_2 \rho_2 \frac{\partial v_2}{\partial t} + 2 \alpha_2 \rho_2 C_{r,2} v_2 \frac{\partial v_2}{\partial z} + \alpha_2 \frac{\partial p}{\partial z} = M_{i,2}^*, \tag{6.6}
\]

\[- \rho_3 v_3 \frac{\partial \alpha_1}{\partial t} - \rho_3 C_{r,3} v_3^2 \frac{\partial \alpha_1}{\partial z} - \rho_3 v_3 \frac{\partial \alpha_2}{\partial t} - \rho_3 C_{r,3} v_3^2 \frac{\partial \alpha_2}{\partial z} + \left(1 - \alpha_1 - \alpha_2\right) \frac{\partial v_3}{\partial z} + 2 \left(1 - \alpha_1 - \alpha_2\right) \rho_3 \frac{\partial p}{\partial z} = M_{i,3}^*, \tag{6.7}\]

\[
- \frac{2}{3} - \chi \left(\frac{D_e}{D_{sm,1}}\right)^2 \left(\frac{a_{i,1}}{\alpha_1}\right) \frac{\partial \alpha_1}{\partial t} - \frac{2}{3} - \chi \left(\frac{D_e}{D_{sm,1}}\right)^2 \left(\frac{a_{i,1}}{\alpha_1}\right) v_1 \frac{\partial \alpha_1}{\partial z}
\]

\[
+ \frac{1}{3} + \chi \left(\frac{D_e}{D_{sm,1}}\right)^2 a_{i,1} \frac{\partial v_1}{\partial t} + \frac{\partial a_{i,1}}{\partial t} + v_1 \frac{\partial a_{i,1}}{\partial z} = \Phi_1, \tag{6.8}
\]

\[
- \chi \left(\frac{D_e}{D_{sm,1}}\right)^2 \left(\frac{a_{i,1}}{\alpha_1}\right) \frac{\partial \alpha_1}{\partial t} - \chi \left(\frac{D_e}{D_{sm,1}}\right)^2 \left(\frac{a_{i,1}}{\alpha_1}\right) v_1 \frac{\partial \alpha_1}{\partial z}
\]

\[
- \left(\frac{2a_{i,2}}{3\alpha_2}\right) \frac{\partial \alpha_2}{\partial t} - \left(\frac{2a_{i,2}}{3\alpha_2}\right) v_2 \frac{\partial \alpha_2}{\partial z} + \frac{1}{3} a_{i,2} \frac{\partial v_2}{\partial t} + \frac{\partial a_{i,2}}{\partial t} + v_2 \frac{\partial a_{i,2}}{\partial z} = \Phi_2. \tag{6.9}
\]

Here, the subscripts 1, 2, and 3 denote Field-1 (Group-1 dispersed fluid particles: drops or bubbles), Field-2 (Group-2 dispersed fluid particles), and Field-3 (continuous phase),
respectively. Here, $p$, $\rho_k$, $\Delta m_{12}$, $M^r_{i,k}$, $\chi$, $D_c$, $D_{sm}$ and $\Phi_k$ are the pressure, density of Field-$k$, net inter-group mass transfer rate from Group-1 to Group-2 fluid particles, generalized interfacial force of Field-$k$, coefficient accounting for the inter-group void transport at the group boundary, critical fluid particle diameter at the group boundary, fluid particle Sauter mean diameter, and interfacial area concentration source/sink rate for Field-$k$, respectively.

In this model, $\rho_1$ may be assumed identical to $\rho_2$ since Field-1 and Field-2 fluid particles are the same fluid at almost identical temperature and pressure, but with different particle sizes. In a gas-liquid two-phase flow, Group-1 and Group-2 fluid particles are small (spherical and distorted bubbles) and large (cap, slug and churn-turbulent) bubbles, respectively (Ishii and Kim, 2004; Sun et al., 2004a). In addition, there is no mass transfer considered between two different kinds of fluids due to the adiabatic assumption. In other words, no mass transfer takes place either between Field-1 and Field-3 or between Field-2 and Field-3. It is also noted that the phase-to-interface pressure difference is neglected, which means a single pressure is shared by all the phases.

In the literature, the contributions of $M^r_{i,k}$ to the regularization of the two-fluid model have attracted the attention of many researchers (Harlow and Besnard, 1985; Brauner and Maron, 1992). It was suggested that the inclusion of $M^r_{i,k}$ including the
virtual mass force and drag force could help render the model into a hyperbolic form. However, as emphasized by Song and Ishii (2000), to construct an appropriate correlation of $M'_{i,k}$ that could be applicable in any circumstances remained a challenge. Noting the argument that $M'_{i,k}$ usually tends to stabilize the two-fluid model, the analysis of the model hyperbolicity would be conservative if one adopts an algebraic form for $M'_{i,k}$ since the contribution of $M'_{i,k}$ to stabilizing the model will then not be credited in the characteristic analysis.

6.3. Characteristic analysis

A characteristic analysis for the modified one-dimensional two-fluid-IATE model was performed in order to study its hyperbolicity. The analysis provides information on the limiting short wavelength behavior. If a vector $\mathbf{x} = \left(\alpha_1, \alpha_2, v_1, v_2, v_3, p, a_{i,1}, a_{i,2}\right)^T$ is defined, the governing equations of the system can be rewritten in the form of matrix as

$$
\left[ A \right] \frac{\partial \mathbf{x}}{\partial t} + \left[ B \right] \frac{\partial \mathbf{x}}{\partial z} = \left[ C \right],
$$

(6.10)

where $[A]$ and $[B]$ are the coefficient matrices. The necessary condition for the model to be a well-posed initial value problem is that the set of partial differential equations is hyperbolic, i.e., the characteristic equation $\left\| [A] \lambda - [B] \right\| = F(\lambda) = 0$ has real roots for $\lambda$. The complex conjugate values for the eigenvalue $\lambda$ lead to the elliptic equations, which are mathematically ill-posed. $F(\lambda)$ is rearranged and simplified to

$$
g(\lambda) = g_1(\lambda) - g_2(\lambda),
$$

(6.11)
where the corresponding polynomials are given as below:

\[ g_{i1}(\lambda) = \rho_1 g_{11}(\lambda) g_{12}(\lambda), \]

\[ g_{11}(\lambda) = \lambda^2 - 2C_{v,3} v_3 \lambda + C_{v,3}^2, \]

\[ g_{12}(\lambda) = (\alpha_1 + \alpha_2) \lambda^2 - 2\left(\alpha_1 C_{v,2} v_2 + \alpha_2 C_{v,3} v_1\right) \lambda + \left(\alpha_1 C_{v,2}^2 + \alpha_2 C_{v,3} v_1^2\right), \]  

\[ g_2(\lambda) = -(1 - \alpha_1 - \alpha_2) \rho_1 g_{21}(\lambda) g_{22}(\lambda), \]

\[ g_{21}(\lambda) = \lambda^2 - 2C_{v,1} v_1 \lambda + C_{v,1}^2, \]

\[ g_{22}(\lambda) = \lambda^2 - 2C_{v,2} v_2 \lambda + C_{v,2}^2. \]

Note that \( F(\lambda) \) is replaced by \( g(\lambda) \) since four out of the eight roots for \( F(\lambda) = 0 \) are guaranteed to be real roots.

Considering the fact that \( \rho_1 \) and \( \rho_2 \) are positive and \( (1 - \alpha_1 - \alpha_2) \) is constrained to being between zero and unity to maintain its physical meaning, we recognize that the coefficient of the highest order of \( g(\lambda) \), i.e., the 4th order, should always be positive. All roots of \( g(\lambda) \) are real if the following two requirements are satisfied:

1. \( g'(\lambda) = 0 \) has three real roots \( \lambda_1, \lambda_2, \) and \( \lambda_3 \) (let \( \lambda_1 > \lambda_2 > \lambda_3 \)) ;

2. \( g(\lambda_2) > 0, g(\lambda_1) < 0, g(\lambda_3) < 0. \)

It is realized that to solve the eigenvalues, a 3rd-order polynomial equation must be solved, from which the expression of its roots are usually very complicated and lengthy.
This analytical approach is not practical due to the complication of solving a 3rd-order polynomial equation.

Alternatively, based on available experimental data of a certain two-phase flow configuration, the momentum flux parameters could be constructed as a function of the void fraction (and perhaps other flow variables), reducing the numbers of undetermined variables in \( g(\lambda) \). The plots of \( g(\lambda) \) therefore could be given, from which the hyperbolic property of \( g(\lambda) \) can be studied graphically. If there are four intersections between \( g(\lambda) \) and the real axis, then equation \( g(\lambda) = 0 \) will have four real roots for \( \lambda \). More details are given in the next section.

6.4. Results and discussions: a case study

To demonstrate the feasibility of the approach discussed earlier, \( g(\lambda) \) is analyzed for a specific two-phase flow as a case study. Since the compressibility of fluids is not considered here for simplicity, it is appropriate to take a liquid-liquid slug flow as an example. One relevant experiment in the literature was performed by Vasavada (2008). In this experiment, two immiscible fluids, namely, water and Therminol 59®, flowed upward adiabatically in a vertical pipe with an inner diameter of 25.4 mm at the room temperature. Therminol 59®, an organic engineering fluid, was the dispersed phase having a density of 972 kg/m³ at 20°C. Based on the sizes of droplets, the organic droplets were classified into Field-1 and Field-2, with small droplets being Field-1. Water was the continuous phase as Field-3 with a density of 998 kg/m³ at 20°C. Local flow variables in 17 different flow conditions were measured at three measurement elevations.
along the flow direction with $z/D = 13, 67, \text{ and } 121$, respectively (Vasavada, 2008). Table 6.1 lists the cross-sectional area-averaged data for each flow condition at $z/D = 13$.

<table>
<thead>
<tr>
<th>Run #</th>
<th>$\langle \alpha_1 \rangle$ (%)</th>
<th>$\langle \alpha_2 \rangle$ (%)</th>
<th>$\langle v_1 \rangle$ (m/s)</th>
<th>$\langle v_2 \rangle$ (m/s)</th>
<th>$\langle \nu_{g,avg} \rangle$ ** (m/s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>24.96</td>
<td>5.98</td>
<td>0.36</td>
<td>0.37</td>
<td>0.37</td>
</tr>
<tr>
<td>14</td>
<td>38.93</td>
<td>8.16</td>
<td>0.38</td>
<td>0.33</td>
<td>0.37</td>
</tr>
<tr>
<td>15</td>
<td>32.69</td>
<td>14.78</td>
<td>0.49</td>
<td>0.46</td>
<td>0.49</td>
</tr>
<tr>
<td>16</td>
<td>20.41</td>
<td>0.11</td>
<td>0.45</td>
<td>0.16***</td>
<td>0.45</td>
</tr>
<tr>
<td>17</td>
<td>24.15</td>
<td>6.87</td>
<td>0.52</td>
<td>0.50</td>
<td>0.52</td>
</tr>
<tr>
<td>18</td>
<td>26.14</td>
<td>10.95</td>
<td>0.55</td>
<td>0.57</td>
<td>0.55</td>
</tr>
<tr>
<td>19</td>
<td>19.90</td>
<td>20.12</td>
<td>0.64</td>
<td>0.64</td>
<td>0.64</td>
</tr>
<tr>
<td>20</td>
<td>15.84</td>
<td>0.14</td>
<td>0.62</td>
<td>0.07***</td>
<td>0.61</td>
</tr>
<tr>
<td>21</td>
<td>22.30</td>
<td>1.90</td>
<td>0.57</td>
<td>0.51</td>
<td>0.55</td>
</tr>
<tr>
<td>22</td>
<td>20.17</td>
<td>3.39</td>
<td>0.75</td>
<td>0.77</td>
<td>0.76</td>
</tr>
<tr>
<td>23</td>
<td>16.99</td>
<td>17.39</td>
<td>0.85</td>
<td>0.82</td>
<td>0.84</td>
</tr>
<tr>
<td>24</td>
<td>17.64</td>
<td>1.05</td>
<td>0.71</td>
<td>0.55</td>
<td>0.71</td>
</tr>
<tr>
<td>25</td>
<td>14.37</td>
<td>1.78</td>
<td>0.84</td>
<td>0.90</td>
<td>0.85</td>
</tr>
<tr>
<td>26</td>
<td>22.23</td>
<td>0.32</td>
<td>0.79</td>
<td>0.81</td>
<td>0.79</td>
</tr>
<tr>
<td>27</td>
<td>13.13</td>
<td>0.14</td>
<td>1.58</td>
<td>0.41***</td>
<td>1.58</td>
</tr>
<tr>
<td>28</td>
<td>11.87</td>
<td>0.91</td>
<td>1.56</td>
<td>1.59</td>
<td>1.56</td>
</tr>
<tr>
<td>29</td>
<td>19.27</td>
<td>2.29</td>
<td>1.69</td>
<td>1.84</td>
<td>1.70</td>
</tr>
</tbody>
</table>

*: The Run #’s are consistent with Vasavada (2008);
**: The averaged velocity was void fraction weighted velocity of Therminol 59® provided by Vasavada (2008);
***: Due to the small sampling numbers of group-2 droplets, these velocity data are considered not statistically sound.

Table 6.1 Area-averaged data for Runs 13-29 at $z/D = 13$ (Vasavada, 2008)
Figure 6.1. $C_{v,k}$ vs. the total void (drop) fraction $\alpha$: (a) $C_{v,1}$, (b) $C_{v,2}$, and (c) $C_{v,3}$
The momentum flux parameter $C_{r,k}$ ($k = 1, 2, \text{ and } 3$) are calculated according to the experimental data (Vasavada, 2008) when the total void fraction of the organic drops, $\alpha$ ($\alpha = \alpha_1 + \alpha_2$), is in the range between 0.1 and 0.6.

The results are given in Figure 6.1, where $C_{r,k}$ is plotted versus $\alpha$. From the plots, the relationship between $C_{r,k}$ and $\alpha$ could be determined. Figure 6.1(a) illustrates that $C_{r,1}$ is a relatively weak function of $\alpha$. Most of $C_{r,1}$ data points fall into a narrow band around 1.5 except two points having a magnitude between 2 and 2.5. After a further investigation of the measured data, it is found out that the experimental data from the measurements in the flow conditions associated with these two data points had zero values for the Group-2 void fraction at several radial locations. This indicates that the flow might be in the bubbly-to-slug transition region instead of slug flows. Considering the difficulties in obtaining accurate measurements in flow transition regions, it might be reasonable to discard those two points and assume $C_{r,1} \simeq 1.5$. In Figure 6.1(b), although it shows a scattered distribution when $\alpha$ is small, $C_{r,2}$ follows the power law profile of $\alpha$ to a good approximation as $\alpha$ becomes larger, which corresponds to the slug flow conditions of interest. Other data fitting methods of constructing the correlation of $C_{r,2}$, such as a linear function or higher order polynomials are also investigated, which generally provide a smaller value of $R^2$. The $R^2$ value is a measure of how good the curve fit is to the data and is bounded between zero and unity. A higher value of $R^2$
always provides a better fit of the regression to the data set. Finally, as shown in Figure 6.1(e), $C_{v,3}$ fits a 2nd-order polynomial of $\alpha$ well.

In addition, it is reasonable to assume that the velocities of the different phases are the same, i.e., $v_1 = v_2 = v_3 = v$, because of the similar densities between water and Therminol 59® (The density difference between the two fluids is about 2.7% at 20°C). Since the velocity for each phase follows similar turbulent velocity profile along the radial direction of the pipe, this assumption could also be partially verified from comparisons of the area-averaged velocities between Group-1 and Group-2 drops, as shown in Table 6.1. In most runs, $v_1$ is approximately equal to $v_2$, except for three runs, i.e., Runs 16, 20, and 27. In these three runs, it is shown that the void fraction of Group-2 droplets is significantly smaller than that of Group-1 droplets. Also, the average velocity of the dispersed phase is found to be close to that of Group-1 drops. This indicates that in these experimental runs, the numbers of Group-2 drops measured are quite small and that the flows fall into bubbly-to-cap bubbly transition region. The zero relative motion assumption reduces the two-fluid-IATE model into a non-slip two-fluid model, similar to the homogeneous equilibrium model (HEM).

As a summary, based on the experimental observations, the following four assumptions are made:

1. $C_{v,1} \simeq 1.5$;

2. $C_{v,2} = 0.8824 \alpha^{0.747}$;

3. $C_{v,3} = -0.9028 \alpha^2 + 0.0552 \alpha + 1.1555$;
4. The velocities of the different phases can be assumed the same, i.e.,

\[ v_1 = v_2 = v_3 = v. \]

Here, \( \alpha \) stands for the total void fraction of Therminol 59\textsuperscript{®} drops. It should be noted that for a more general analysis, the momentum flux parameters may be better correlated with additional parameters.

Furnishing the above assumptions, the characteristic function \( g(\lambda) \) is simplified to a function of the void fraction of Group-1 \( \alpha_1 \), void fraction of Group-2 \( \alpha_2 \), characteristic root \( \lambda \), and velocity \( v \) only. In addition, if one introduces a new parameter, \( w \), as the dimensionless velocity and defines it as \( w = \lambda / v \), the characteristic equation \( g(\lambda) = 0 \) converts to \( g(w) = 0 \). The roots of \( g(w) = 0 \) have the same mathematical properties as those of \( g(\lambda) = 0 \), i.e., if \( g(w) = 0 \) has four real roots, so does the original equation \( g(\lambda) = 0 \).
Figure 6.2. $g(w)$ for Runs 13, 17, and 18 over: (a) a wide range of $w$ from 0 to 4 and (b) a narrower range of $w$
Figure 6.3. $g(w)$ for Runs 14, 15, and 19 over: (a) a wide range of $w$ from 0 to 3 and (b) a narrower range of $w$
Figure 6.4. $g(w)$ for Runs 16, 21, and 29 over: (a) a wide range of $w$ from 0 to 6 and (b) a narrower range of $w$.
Figure 6.5. $g(w)$ for Runs 20 and 27 over: (a) a wide range of $w$ from 0 to 10 and (b) a narrower range of $w$.
Figure 6.6. $g(w)$ for Runs 22 and 26 over: (a) a wide range of $w$ from 0 to 6 and (b) a narrower range of $w$
Figure 6.7. $g(w)$ for Run 23 over: (a) a wide range of $w$ from 0 to 3.5 and (b) a narrower range of $w$
Figure 6.8. $g(w)$ for Runs 24, 25, and 28 over: (a) a wide range of $w$ from 0 to 8 and (b) a narrower range of $w$

Figures 6.2-6.8 provide plots of $g(w)$ versus $w$ for the 17 flow conditions. In these figures, subplot (a) is a plot for a relatively large range of $w$; while subplot (b) shows a plot in a sufficiently narrow range of $w$ for the benefit of observing the two roots near which $g(w)$ has small variations in the real axis. These plots show clearly that
$g(w)$ has four positive roots, which are consistent with the physics. As illustrated in the plots, the typical shape of $g(w)$ is that $g(w)$ has one pair of roots that are close to each other, approaching a less than-unity $w$ value; whereas the other pair intersects at the values of $w$ on the order of unity.

Close attention should be paid to the first pair of roots, which demonstrates an essential role on the stability. For the flow conditions investigated, it was demonstrated that the modified two-fluid-IATE model satisfies the necessary condition of the well-posedness, which indicates the flows tend to be stable. Therefore, it is mathematically consistent with the HEM, in which the dispersed phase is assumed to have the same velocity as the continuous phase.

The advantage of the model considering the momentum flux parameters over the conventional two-fluid model can be shown if the relative velocity between the phases is considered. Based on a force balance, the magnitude of the relative velocity between a spherical dispersed phase particle and the continuous phase ($U_r$) can be obtained as (Ishii and Zuber, 1979)

$$U_r = \sqrt{\frac{4 D_d \Delta \rho g (1 - \alpha)}{3 C_D \rho_3}},$$

(6.13)

where $D_d$, $g$, $C_D$, and $\rho_3$ are the bubble/drop diameter, gravitational acceleration, drag force coefficient, and density of the continuous phase (Field-3), respectively. The drag force coefficient for distorted bubbles/drops is employed for Field-1 as (Ishii and Mishima, 1984):
\[ C_D = \frac{2D_d}{3(1 - \alpha)} \sqrt{\frac{g \Delta \rho}{\sigma}}, \]  

(6.14)

where \( \sigma \) is the surface tension. Assuming the diameter of the slug bubbles is 80% of the pipe inner diameter, the following drag force coefficient for slug bubbles/drops is used for Field-2 as (Ishii and Mishima, 1984):

\[ C_D = 9.8 \left(1 - \alpha \right)^3. \]  

(6.15)

As a result, the relative velocity is a function of the total void fraction \( \alpha \) as shown in Figure 6.9.

Figure 6.9. \( U_r \) vs. \( \alpha \) for the distorted and slug drops
Our study shows that there is no hyperbolic region for the one-dimensional three-field two-fluid model with the unity momentum flux parameters if the relative velocities given by Eq. (6.13) are taken into account, indicating that the model is ill-posed.

In contrast, if the two-fluid-IATE model with the momentum flux parameters is considered, the stability criteria, which ensures the hyperbolicity of the model, is shown in Figure 6.10 as a map with the continuous phase velocity $v_3$ as the $y$-axis and the Group-1 void fraction $\alpha_1$ as the $x$-axis. When the total void fraction is smaller than 0.45, the model is always hyperbolic no matter what the continuous phase velocity is. When the total void fraction is between 0.45 and 0.65, the continuous phase velocity must increase to ensure the model hyperbolicity as the Group-1 void fraction increases, indicating the hyperbolic region becomes smaller. When the total void fraction is larger than 0.65, the model is unstable, which indicates the same mathematical property of the conventional two-fluid model.
Furthermore, the stability criteria can be represented using the slip ratios for Field-1 and Field-2 dispersed phase with respective to the continuous phase velocity, which are respectively defined as

\[
S_1 = \frac{v_1}{v_3}, \quad (6.16)
\]

and

\[
S_2 = \frac{v_2}{v_3}. \quad (6.17)
\]
The stability criteria for $S_1$ and $S_2$ are plotted in Figure 6.11. In the current case study for the upward liquid-liquid flow, the dispersed phase is slightly lighter than the continuous phase; therefore the slip ratios defined by Eqs. (6.16) and (6.17) are always
larger than unity. It is clearly seen that except for the case when the total void fraction is 0.45, the region of hyperbolicity decreases as the Group-1 void fraction decreases. When the total void fraction reaches 0.65, the slip ratios are slightly larger than 1.0, which is close to the HEM assumption to ensure the model hyperbolicity. When the total void fraction is beyond 0.65, there is no hyperbolic region. Note that to ensure model hyperbolicity, the criteria for $S_1$ and $S_2$ shown in Figure 6.11 should be satisfied simultaneously, and this requirement is met in all the 17 flow conditions examined.

6.5. Conclusions

This study examines the hyperbolicity property of the one-dimensional incompressible three-field two-fluid model with the two-group IATE model. The proposed two-fluid-IATE model can be applied dynamically over a wide range of flow regimes, up to the churn-turbulent flow and including the flow transition regions.

In this study, the momentum flux parameters are adopted to take into account the effect of the void fraction and velocity profiles. These momentum flux parameters have physical meaning based on the local flow distributions and do not introduce any artificial terms. The model’s hyperbolicity depends heavily on local flow parameters, such as the void fraction, phase velocities, etc.

As a case study, a characteristic analysis has been performed to obtain the necessary conditions of the well-posedness of the one-dimensional incompressible two-fluid-IATE model for liquid-liquid slug flows in a circular pipe. Based on the available experimental data, the constitutive correlations of the momentum flux parameters were approximated as functions of the total void fraction of the dispersed phase. It was shown
that the inclusion of the momentum flux parameters in the three-field two-fluid model with the two-group IATE model helps the model maintain hyperbolicity. When the relative velocity is considered, stability criteria pose restrictions on the continuous phase velocity, which is to reduce the effect of the relative velocity, to achieve model hyperbolicity.

This analysis only provides the necessary condition of the well-posedness of the two-fluid-IATE model. The sufficient condition could be provided by using a wake equation with an accompanying infinitesimal perturbation. In addition, it remains questionable as to how to generalize the results of the incompressible model for the applications of gas-liquid two-phase flows, where the gas compressibility needs to be considered in most applications encountered in nuclear reactor safety analysis. The effect of the compressibility of the gas phase is essential for the validity of two-fluid-IATE applications in general two-phase flows. Despite the aforementioned considerations, the introduction of the momentum flux parameters appears promising to the regularization of the one-dimensional two-fluid-IATE model.
Chapter 7. Simulations Using Three-field Two-fluid Model

In this chapter, air-water cap-bubbly and churn-turbulent flows, as well as air-water planar bubble jet flows are chosen to validate the proposed three-field two-fluid model with the two-group IATE model discussed in Chapter 3. The relevant experiments were conducted by Sun (2001), Sun et al. (2004b), and Sun et al. (2005).

7.1. Definition of error

Attention is first paid to the definition of the relative error between the model predictions and experimental data, particularly for the interfacial area concentration parameter. Let \( a_{i1} \) and \( a_{i2} \) be the interfacial area concentration of Group-1 and Group-2 bubbles, respectively. The total interfacial area concentration is then calculated as

\[
a_{it} = a_{i1} + a_{i2}.
\]  

Thus, \( RE_{ait} \), which is the absolute value of the relative error of the total interfacial area concentration between model predictions (with the subscript Model) and experimental values (with the subscript EXP), is given as:

\[
RE_{ait} = \frac{\left| \langle a_t \rangle_{Model} - \langle a_t \rangle_{EXP} \right|}{\langle a_t \rangle_{EXP}} \times 100\% \text{,}
\]  

where the interfacial area concentrations are area averaged.

If the interfacial area concentration of each group is considered, there are two types of the relative error, namely, the relative error with respect to the value of Group-1
or Group-2 bubbles \((RE_{a1} \text{ or } RE_{a2})\), and the relative error with respect to the total value \((RE_{a1t} \text{ or } RE_{a2t})\). They are defined as:

\[
RE_{a1} = \left( \frac{\langle a_{\text{i1}} \rangle_{\text{Model}} - \langle a_{\text{i1}} \rangle_{\text{EXP}}}{\langle a_{\text{i1}} \rangle_{\text{EXP}}} \right) \times 100\% \tag{7.3}
\]

\[
RE_{a1t} = \left( \frac{\langle a_{\text{i1}} \rangle_{\text{Model}} - \langle a_{\text{i1}} \rangle_{\text{EXP}}}{\langle a_{\text{i1}} \rangle_{\text{EXP}}} \right) \times 100\% \tag{7.4}
\]

\[
RE_{a2} = \left( \frac{\langle a_{\text{i2}} \rangle_{\text{Model}} - \langle a_{\text{i2}} \rangle_{\text{EXP}}}{\langle a_{\text{i2}} \rangle_{\text{EXP}}} \right) \times 100\% \tag{7.5}
\]

\[
RE_{a2t} = \left( \frac{\langle a_{\text{i2}} \rangle_{\text{Model}} - \langle a_{\text{i2}} \rangle_{\text{EXP}}}{\langle a_{\text{i2}} \rangle_{\text{EXP}}} \right) \times 100\% \tag{7.6}
\]

As emphasized by Sun (2001), the ones defined by Eqs. (7.4) and (7.6) are more reasonable since small values usually have relatively large measurement errors. For instance, when it is in the transition from bubbly to cap-bubbly flows, the measured values related to the Group-2 bubbles, such as the void fraction, interfacial area concentration, etc., are generally small, resulting in a large value of \(RE_{a2}\), which, however, may not significantly affect the overall prediction.

7.2. Description of experiments

Experiments used for model validations in this study were performed using the same experimental facility, i.e., the facility with the rectangular test section mentioned in Chapter 5. The acrylic test section was confined by two flat walls with 2.95 m in height \((H)\), 200 mm in width \((W)\), and 10 mm in gap thickness \((G)\), as shown in Figure 7.1.
Water and air were the liquid and gas phases, respectively. The two phases flowed concurrently upward along the test section at a constant temperature of 20 °C. Miniaturized four-sensor conductivity probes were mounted at six axial locations, i.e., $z/D_h = 8.0, 34.8, 61.5, 88.2, 115.0,$ and 141.7 from the top of the two-phase mixture injection unit to measure the local two-phase flow data. The measurement errors were evaluated to be within ±7%. In addition, a SONY Hi-8 camcorder or a Kodak high-speed movie camera was used to capture the images and determine the flow regimes.

Figure 7.1. Experimental facility (Sun, 2001; Sun et al., 2004b; Sun et al., 2005)
Six porous sparger units, shown in Figure 7.2, were installed to generate bubbles of near-uniform size. Different types of flows could be generated by controlling the number of the opened sparger units at the inlet of test section. Here, two types of flows at the inlet were produced, namely, a relatively uniform two-phase flow and a planar bubble jet flow. The former was generated by opening all the six sparger units while the latter was produced by using only the center two sparger units (# 2 and 4 in Figure 7.2) in the experiments. For the bubble jet flows, a center-peaked void fraction profile existed at the test section inlet.

![Figure 7.2. Two-phase mixture injection unit (Sun, 2001; Sun et al., 2004b; Sun et al., 2005)](image)

7.3. **Numerical model**

CFD simulations were conducted for two-phase flows in a rectangular duct having dimensions of 200 mm (x) × 10 mm (y) × 2338 mm (z) in a full three-dimensional two-fluid model framework in the Fluent code. As discussed in Chapter 3, three fields
were defined, namely, Group-1 bubbles, Group-2 bubbles, and liquid phase as Field-1, Field-2, and Field-3, respectively. Both Group-1 and Group-2 bubbles were modeled as air following the ideal gas law at a constant temperature of 20 °C while the liquid phase, i.e., water was modeled as an incompressible fluid.

Table 7.1 summarizes the experimental measurements for the four relatively uniform flow conditions (Runs 11, 17, 18, and 20) at the location of $z / D_h = 34.8$ and superficial velocities for the two planar bubble jet conditions flow conditions (Tests 1 and 2). It was observed that Runs 11 and 17 and Tests 1 and 2 belonged to cap-bubbly flows while Runs 18 and 20 were churn-turbulent flows. The wall boundary was set as the non-slip condition with a zero value for the interfacial area concentration.

```markdown
<table>
<thead>
<tr>
<th>Run #*</th>
<th>$\langle j_f \rangle$ (m/s)</th>
<th>$\langle j_{g,0} \rangle$ (m/s)</th>
<th>Group-1</th>
<th>Group-2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$\alpha_1$ (%)</td>
<td>$a_{i1}$ (m$^{-1}$)</td>
<td>$\mu_{g1}$ (m/s)</td>
<td>$\alpha_2$ (%)</td>
</tr>
<tr>
<td>Run 11</td>
<td>0.95</td>
<td>22.5</td>
<td>402</td>
<td>1.45</td>
</tr>
<tr>
<td>Run 17</td>
<td>1.4</td>
<td>12.7</td>
<td>260</td>
<td>1.93</td>
</tr>
<tr>
<td>Run 18</td>
<td>0.95</td>
<td>7.0</td>
<td>132</td>
<td>2.26</td>
</tr>
<tr>
<td>Run 20</td>
<td>0.95</td>
<td>9.5</td>
<td>210</td>
<td>2.63</td>
</tr>
<tr>
<td>Test 1</td>
<td>0.95</td>
<td>0.095</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Test 2</td>
<td>0.95</td>
<td>0.19</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
```

*: The Run #'s are consistent with experiments

Table 7.1 Flow conditions for model validation (Sun, 2001; Sun et al., 2004b; Sun et al., 2005)

### 7.4. Assumptions and coefficients in two-group IATE model

For the unique geometry of this experimental test loop, some assumptions were made. Group-1 bubbles were assumed to have a spherical shape; while Group-2 bubbles, such as cap bubbles, were assumed to be sandwiched by two flat walls with a thickness of
and a wake angle of 100 degree, assuming the liquid films between the cap bubbles and the walls were very thin.

The base width of cap bubbles \((2a)\), shown in Figure 3.1, was considered to be the characteristic length scale that determined the group boundary between the two groups of bubbles (Sun, 2001; Sun et al., 2004b). Based on these assumptions, Sun et al. (2004b) gave the following relationship between \(2a\) and the Group-2 bubble Sauter mean diameter: \(2a = 2.21D_{sm2}\). The maximum radius of curvature for Group-2 bubbles (i.e., cap bubbles) was given as \(R_{m2} \approx 1.915D_{sm2}\) based on a uniform bubble distribution assumption. The critical bubble diameter at the group boundary was given as \(D_{c1} = 1.7(G\sigma / g\Delta\rho)^{1/3}\).

Sun et al. (2004b) further obtained the following correlation for \(\chi\) from the experimental data of the bubble chord length distribution as

\[
\chi = 4.44 \times 10^{-3} \left( \frac{\langle D_{sm1} \rangle^{0.36}}{\langle \alpha_1 \rangle^{1.35}} \right)^{-1.35}.
\]  
(7.7)

Recall \(\chi\) is the coefficient in the two-group IATE, shown in Eqs. (2.18) and (2.19). For the planar bubble jet flow, experimental observations suggested all the Group-1 bubbles be far away from the critical volume at the group boundary, which leads to a small possibility for a Group-1 bubble to become a Group-2 bubble due to volume expansion, therefore, we have

\[
\chi \approx 0.
\]  
(7.8)
The values of model coefficients in the two-group IATE model were determined by Sun (2001). Some of the parameters, such as $C_{RC}^{(1)}$, $C_{WE}^{(1)}$, $C_{TI}^{(1)}$, $C_{RC1}$, and $We_{c,TI1}$, were pre-determined from the previous one-group IATE study. Finally, the model coefficients are summarized as:

**Random collision:**

$$C_{RC}^{(1)} = 0.005, \quad C_{RC}^{(12,2)} = 0.005, \quad C_{RC}^{(2)} = 0.005, \quad C_{RC1} = 3.0, \quad C_{RC2} = 3.0, \quad \alpha_{\text{max}} = 0.75;$$

**Wake entrainment:**

$$C_{WE}^{(1)} = 0.002, \quad C_{WE}^{(12,2)} = 0.002, \quad C_{WE}^{(2)} = 0.005;$$

**Turbulent impact:**

$$C_{TI}^{(1)} = 0.03, \quad C_{TI}^{(2)} = 0.02, \quad We_{c,TI1} = 6.5, \quad We_{c,TI2} = 7.0;$$

**Shearing-off:**

$$C_{SO} = 3.8 \times 10^{-5}, \quad C_d = 4.80, \quad We_{c,SO} = 4500.$$ 

These coefficients were adopted in this study.

### 7.5. Discussion on interfacial forces

Similar to bubbly flows, cap-bubbly and churn-turbulent flows also experience different interfacial forces, such as drag force, lift force, wall lubrication force, etc. The lift force on large bubbles was found in the literature (Lucas et al., 2005) to destabilize the flows. Similar phenomenon was observed in our simulations. Therefore, the lift force is not included in the simulations when the flow regimes are beyond bubbly flows.
It is noted that except for the drag force, other closure laws have been developed in the literature based on potential flow theory, which means the inviscid solution for flow around a sphere is used to approximate the flow around the bubbles in the flow field. The application of these forces in cap-bubbly and churn-turbulent flows remains questionable. Since there are few studies focusing on the development of the wall lubrication and turbulent dispersion forces in cap-bubbly and churn-turbulent flows, the correlations from the potential flow analysis are adopted here, which will inevitably introduce errors. The formulas of the drag, wall lubrication, and turbulent dispersion forces are summarized as follows:

\[
\vec{F}_{d, gn} = -\frac{a_{i,n}}{8} C_{D,n} \rho_f \vec{v}_{r,n} \left| \vec{v}_{r,n} \right| \left( \frac{D_{w,n}}{D_d} \right)_n,
\]

\[
\vec{F}_{w, gn} = \frac{2\sigma_{n} \rho_f}{D_{d,n}} \left| \vec{v}_{\|,n} \right|^2 \left[ C_{w1,n} + C_{w2,n} \left( \frac{D_{d,n}}{2d_{w,n}} \right) \right] \vec{n}_n,
\]

\[
\vec{F}_{TD, gn} = -C_{T,n} \rho_f k_f \nabla \alpha_n,
\]

\[
\vec{F}_{TD, gn}^{BI} = -\frac{3}{4} C_{DB,n} \rho_f C_{T,n} \alpha_n \vec{v}_{r,n} \left| \vec{v}_{r,n} \right| \nabla \alpha_n,
\]

where \( n \) (1 or 2) represents Group-1 or Group-2 bubbles. \( \vec{F}_{TD, gn} \) and \( \vec{F}_{TD, gn}^{BI} \) are the shear- and bubble-induced turbulent dispersion forces, respectively.

The model coefficients for each group that were used in the present simulations are summarized in Table 7.2. More details were discussed in Section 3.3.
Table 7.2 Coefficients of interfacial forces

<table>
<thead>
<tr>
<th>Force</th>
<th>Coefficient</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Drag</strong></td>
<td></td>
</tr>
<tr>
<td>Group-1</td>
<td>$C_{D,1} = \max \left{ \min \left[ \frac{24}{\text{Re}<em>{b,1}} \left( 1 + 0.15 \text{Re}</em>{b,1}^{0.687} \right), \frac{72}{\text{Re}<em>{b,1}^{3/4}} \right] \frac{8Eo</em>{l}}{3(3Eo_{l} + 4)} \right}$</td>
</tr>
<tr>
<td>Group-2</td>
<td>$C_{D,2} \approx \frac{8}{3}(1 - \alpha_1 - \alpha_2)^2$</td>
</tr>
<tr>
<td><strong>Wall lubrication</strong></td>
<td>$C_{w1,n} = -0.104 - 0.06 \left</td>
</tr>
<tr>
<td><strong>Turbulent dispersion</strong></td>
<td></td>
</tr>
<tr>
<td>Group-1</td>
<td>$C_{T,1} = 0.1$, $C_{DB1} = 0.63$, $C_{T,1}^{*} = -C_{D,1} \frac{D_{d,2}}{D_{d,1}} \left</td>
</tr>
<tr>
<td>Group-2</td>
<td>$C_{T,2} = 0.1$, $C_{DB2} = 0.63$, $C_{T,2}^{*} = C_{D,1} \frac{D_{d,2}}{D_{d,1}} \left</td>
</tr>
</tbody>
</table>

7.6. **Numerical scheme**

The 2nd-order upwind scheme estimates the scalar value at a given face based on the central value and gradient of the upstream cell. Compared to the 1st-order upwind scheme, the 2nd-order upwind scheme offers trickier convergence, but weakens the numerical diffusion errors that may significantly influence the physical nature of flow with swirling and rotating.

Figure 7.3 provides the numerical results of the gas velocity and void fraction of Group-1 bubbles at the location of $z / D_{h} = 141.7$ for Test 1 shown in Table 7.1 using the two different schemes, namely, 1st-order upwind and 2nd-order upwind. As we aim at studying the different numerical schemes, the simulations were conducted with the two-fluid model in which the two-group IATE model was incorporated, but the interfacial
forces were not included. A mesh of 400,000 cells (100×10×400) was employed. A more
detailed mesh sensitivity study will be carried out later in Section 7.7.

In Figure 7.3 and in all of the following figures, results that are line-averaged in
the gap direction ($y$-direction) are reported so as to make the comparison clearer. Again,
locations $x = 0.0$ and 100.0 mm represent the wall and centerline of the cross-section of
the duct in the width direction ($x$-direction), respectively.

Figure 7.3 illustrates clearly that there is a sharp drop of gas velocity of Group-1
bubbles when the 1$^{st}$-order upwind scheme is used, which corresponds to the location
where the void fraction of Group-1 bubbles is almost zero: the magnitude of the void
fraction of Group-1 bubbles approaches zero (below $10^{-8}$) as shown in Figure 7.3(b). It is
however not physical according to the experimental observations. Therefore, the 2$^{nd}$-
order upwind scheme, which produces smooth predictions of the gas velocity of Group-1 bubbles, was selected to discretize the momentum equations and IATEs.

7.7. *Mesh sensitivity*

Different numbers of hexahedral meshes ranging from 10,000 cells up to 160,000 cells over the computational domain were created using the GAMBIT software and examined in this mesh sensitivity study.

![Figure 7.4](image_url)

**Figure 7.4.** Predicted void fractions at the location of \( z / D_h = 141.7 \) using different meshes in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.4 provides the predicted void fractions of Group-1 and Group-2 bubbles at the location of \( z / D_h = 141.7 \) in Test 1 using three different meshes, which are coarse mesh (50×10×100), finer mesh (100×10×400), and finest mesh (200×20×400). Again, the simulations were conducted without the interfacial forces. A mesh of 400,000 cells (100×10×400) was determined to be sufficiently fine and computationally affordable, and was therefore used to provide the numerical results shown in the following sections.
7.8. **Test on boundary conditions**

Attention is also paid to the entrance effect due to the inlet geometry of the current experimental loop. It was found out that there was not enough time for the liquid to diffuse, such that a jet was unavoidably formed from each of the auxiliary liquid injection sites, even when attempting to produce a relatively uniform flow condition (Sun et al., 2004b).

To illustrate this impact, both the area-averaged values (given in Table 7.1) and the lateral profiles of the measurements at $z / D_h = 34.8$ were separately employed as uniform and non-uniform inlet boundary conditions in two CFD simulations. A 3rd-order polynomial was used to fit the measured data and the value was set to be 0.0001 if the computed value was below zero. In the results shown in this section, the two-group IATE model was successfully implemented into the two-fluid model, but the drag force was the only interfacial force included in the simulations.

We first study the effects of the inlet profiles for the relatively uniform-inlet flow conditions. Take Run 17, for example. The profiles of the measured void fractions of both bubble groups at $z / D_h = 34.8$ are given in Figure 7.5(a). The predicted void fractions of both groups are presented in Figure 7.5(b) and (c) and compared to the measured data at the location of $z / D_h = 141.7$. 

148
Figure 7.5. Void fractions in Run 17 for: (a) Group-1 and Group 2 bubbles at $z / D_h = 34.8$ (measured), (b) Group-1 bubbles at $z / D_h = 141.7$, and (c) Group-2 bubbles at $z / D_h = 141.7$

Figure 7.5(b) demonstrates that different boundary conditions have a minor impact on the predicted void fraction distribution of Group-1 bubbles, which is consistent with the conclusion drawn by Wang and Sun (2008). It is explained that the upstream flow history could be dissipated significantly by the strong turbulence induced by the inherent complexity of two-phase flow. On the other hand, two different boundary conditions generate some differences in the predicted profiles of the void fraction of Group-2 bubbles, as shown in Figure 7.5(c). It incites us to carefully use non-uniform boundary conditions in all following simulations. It can be seen that the flow fields are
poorly described by the simulations compared to the experimental data as of yet. This misrepresentation of bubble migration, especially in Group-2 bubbles, is further investigated in the subsequent sections.

Figure 7.6. Profiles of Test 1 at the location of $z / D_h = 34.8$ for: (a) interfacial area concentration for Group-1 bubbles, (b) void fraction of Group-1 bubbles, (c) interfacial area concentration for Group-2 bubbles, and (d) void fraction of Group-2 bubbles
Figure 7.7. Profiles of Test 2 at the location of $z / D_h = 34.8$ for: (a) interfacial area concentration for Group-1 bubbles, (b) void fraction of Group-1 bubbles, (c) interfacial area concentration for Group-2 bubbles, and (d) void fraction of Group-2 bubbles.

Figures 7.6 and 7.7 illustrate the curve-fitting of the interfacial area concentration and void fractions of both groups at the location of $z / D_h = 34.8$ for the two planar bubble jet flow conditions. As the profiles show clear variations across the test section, it is more appropriate to use these profiles to provide the inlet profiles as the boundary conditions in the simulations.
7.9. **Test on turbulence models**

Since the void fraction in the cap-bubbly or churn-turbulent flow is usually large, the per-phase turbulence model, which accounts for the gas-phase modalities, is more appropriate than the dispersed model, which was applied in the simulations of bubbly flows discussed in Chapter 5. Concerning the $k - \varepsilon$ per-phase turbulence model, two types were examined here, namely, the standard model and the RNG model.

It was found out that the predicted flow field distributions using the RNG model were similar to those using the standard model through simulations. However, the estimated values of $k$ and $\varepsilon$ using the RNG model were generally higher than those using the standard model. For instance, in the case of Test 1, the volume-averaged values of the predicted $k$ and $\varepsilon$ of the liquid phase were 0.00843 m$^2$/s$^2$ and 0.4884 m$^2$/s$^3$, respectively, when the RNG model was used; while they became 0.00751 m$^2$/s$^2$ and 0.4811 m$^2$/s$^3$, respectively, when the standard model was applied. It is known that the $k - \varepsilon$ turbulence model usually underestimates the values of $k$ and $\varepsilon$. The RNG model takes into account the low-Reynolds-number phenomena and the proximity of walls and is more appropriate for modeling high swirl flows (Fluent 6.3 User’s Guide, 2006). Therefore, the RNG $k - \varepsilon$ turbulence model was employed in the cap-bubbly and churn-turbulent flow simulations.

7.10. **Test on interfacial forces**

Bubbles migrate due to the general interfacial forces, which mainly consist of the drag, lift, wall lubrication, and turbulent dispersion forces in steady-state two-phase flows. The drag force, which is due to the relative motion of flows, is predominant in the
main flow direction (z-direction) with a significantly higher magnitude compared to the other forces. Contributions to the lateral phase predictions are primarily made by forces other than the drag force, among which the lift and wall lubrication forces are generally responsible for the lateral void distribution in the test section. In addition, the turbulent dispersion force tends to flatten the void fraction.

As aforementioned, the lift force is a function of the curl of the liquid velocity and is normal to the bubble relative velocity. Simulations confirmed that the gradient of the liquid velocity is almost zero except in the region fairly adjacent to the wall, where the lift force typically plays an important role. In addition, it was pointed out in the previous work that the lift force caused a severe divergent issue in two-phase flows, particularly when large bubbles existed (Lucas et al., 2005). Nevertheless, the lift force was not included in the present numerical models. Therefore, the wall lubrication force becomes important in predicting the lateral void distribution. As shown in Table 7.2, the wall lubrication force becomes zero out of the region bounded by the wall and at a distance from the wall that is proportional to the bubble size. Since the size of Group-2 bubbles is on the order of centimeters, the wall lubrication force exists in a relatively large region for Group-2 bubbles.

Based on the above discussions, simulations were carried out with non-uniform boundary conditions when the drag and wall lubrication forces were taken into account. The turbulent dispersion force was also included, which reflected the genuine physical feature and helped stabilize the solutions. The void fractions of Group-1 and Group-2 bubbles at the location of $z / D_h = 88.2$ for Run 17 are plotted in Figure 7.8 and
compared to the measured data. The wall lubrication force does not affect the prediction of the lateral phase distribution of small bubbles, as shown in Figure 7.8(a); whereas, it pushes large bubbles to the flow duct center, as shown in Figure 7.8(b). The void fraction peak of Group-2 bubbles is located around \( x = 50.0 \) mm, which is approximately the location at which the wall lubrication force becomes negligible for Group-2 bubbles. These results suggest that the wall lubrication force is indispensible for the simulations of cap-bubbly flows.

Figure 7.8. Void fraction at \( z / D_h = 88.2 \) in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles

7.11. Model validation: cap-bubbly flows

In this section, two simulation models were applied: Fluent without the IATE model (denoted as “Fluent w/o IATE”) and Fluent with the IATE model (denoted as “Fluent with IATE”). The former was the three-field two-fluid model in the conventional Fluent code where the bubble diameters of both groups were initially set individually as a constant. In the latter model, the bubble diameters were evaluated dynamically using the
two-group IATE model. In what follows, the numerical results from both models, together with the experimental data obtained at different elevations are presented and discussed for four cap-bubbly flow conditions, i.e., Runs 11 and 17, and Tests 1 and 2 as described in Table 7.1. In most of the figures in this section, subplots (a) and (b) respectively present the results of Group-1 bubbles and Group-2 bubbles.

Figure 7.9. Velocity at $z / D_h = 141.7$ in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles

The bubble velocity is closely related to the void fraction and interfacial area concentration estimation. As shown in Figure 7.9, the Fluent w/o IATE model provides very biased predictions of the gas velocities for Run 11 while the Fluent with IATE model shows reasonable agreement with the experimental data. It is realized that the drag force coefficient model developed for bubbly flows was employed for both groups in the Fluent w/o IATE model, which underestimates the drag force for Group-2 bubbles and therefore results in the much higher Group-2 bubble velocity.
Remarkable improvements for the predictions of the void fractions are shown in Figure 7.10. As the mixture flowed up adiabatically, the pressure drop along the flow duct reduced the gas density, which led to an increase in the gas phase volumetric flow rate. This increase would in turn result in an increase in the bubble velocity and/or the void fraction. Upon examining the experimental data and the code calculations, it was discovered that the major effect of the gas expansion was reflected in the increase of the void fraction rather than the bubble velocity. However, a relatively large decrease in the void fraction of Group-1 bubbles associated with a significant increase in the void fraction of Group-2 bubbles along the main flow direction was observed in the experiment. This phenomenon was captured by Fluent with the IATE model, as shown in Figure 7.10. In contrast, this flow development was not reflected by the conventional Fluent code, from which the void fraction of Group-2 bubbles remained small and was comparable to the inlet Group-2 void fraction. This is because the conventional Fluent
code does not account for the inter-group mass transfer resulting from bubble interactions.

Figure 7.11. Contours of the void fraction in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles
The bubble interactions modeled in the two-group IATE model include the bubble coalescence due to random collision and wake entrainment, and bubble breakup due to the impact of turbulent eddies, surface instability, and small bubbles shearing off at the rim of large bubbles. In the mechanism of bubble disintegration, turbulent eddies that break up bubbles are assumed equal to or marginally smaller than the bubble size. This mechanism generally plays a role when the velocities of the gas and liquid phases are relatively high and will lead to an increase in the interfacial area concentration values. In Run 11, bubble breakup is not a major contribution as will be shown when we examine the development of the interfacial area concentration. The mass transfer from Group-1 to Group-2 bubbles indicates that the small bubbles tend to coalesce and form large bubbles as the flow develops. This inter-group transport due to Group-1 bubble coalescence is more significant compared to the pressure effect alone, with a net effect of decreasing the void fraction of Group-1 bubbles. This process is illustrated in Figure 7.11, in which the contours of the void fractions of both groups of bubbles at different locations are shown along the flow direction.

The calculated and measured values of the interfacial area concentration for both bubble groups at $z / D_h = 141.7$ are given in Figure 7.12. It is clearly seen that the predicted values of the interfacial area concentration of both groups quantitatively match the measured data and exhibit similar profiles as the void fractions.
Figure 7.12. Interfacial area concentration at $z/D_h = 141.7$ in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Furthermore, contours of the interfacial area concentration at different axial locations are illustrated in Figure 7.13. For the interfacial area concentration of Group-1 bubbles, a slight reduction was observed in the experiment along the flow direction while a small increase was predicted, which was probably caused by the over-estimation of the turbulent impact effect due to relatively high turbulence in the wall region. Figure 7.13(b) shows an increase in the interfacial area concentration of Group-2 bubbles compared to the area-average interfacial area concentration value at $z/D_h = 34.8$. This increase arises mainly in the center region of the flow channel.
Figure 7.13. Contours of the interfacial area concentration in Run 11 for: (a) Group-1 bubbles and (b) Group-2 bubbles

The code results at the location of $z / D_h = 141.7$ for Run 17 are shown in Figures 7.14-7.18. Similarly, the results of the gas velocity and void fraction computed
by the Fluent code without using the IATE model fail to provide satisfactory agreement for Group-2 bubbles with the experimental data. To the contrary, the Fluent with IATE model performs favorably as compared to the experimental data. A wall peak starts to form for the void fraction of small bubbles shown in Figure 7.16(a) while large bubbles tend to accumulate in the center of the duct as shown in Figure 7.16 (b). It is noted that the void fraction and interfacial area concentration of Group-2 bubbles in the center region are under-predicted by the Fluent code with the IATE model, which may be due to the lack of the lift force in our current work. The lift force may become important in this flow condition to transport the cap bubbles to the center region of the flow channel. This will be further studied in the near future.

Figure 7.14. Velocity at $z / D_h = 141.7$ in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figure 7.15. Void fraction at $\frac{z}{D_h} = 141.7$ in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figure 7.16. Contours of the void fraction in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figure 7.17. Interfacial area concentration at $z / D_h = 141.7$ in Run 17 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Before presenting the results for the planar bubble jet flow conditions, we show the relative errors of the interfacial area concentration in Table 7.3 for Test 1. The
relative errors of Group-1 and Group-2 interfacial area concentration with respect to the total interfacial area concentration are 18.7 and 3.3%, respectively, at the location of \( z / D_h = 88.2 \), and 13.1 and 8.0%, respectively, at the location of \( z / D_h = 141.7 \). These acceptable relative errors help validate the three-field two-fluid model with the two-group IATE model.

It is also noted that the relative error of the interfacial area concentration of Group-2 bubbles are quite large with respect to its own values, particularly at the location of \( z / D_h = 141.7 \). As the averaged value of the interfacial area concentration of Group-2 bubbles at \( z / D_h = 141.7 \) is rather small, being less than 10 m\(^{-1}\) and contributing to less than 10% of the total interfacial area concentration, \( RE_{a2} \) is not considered as an appropriate measure to examine the validity of the current simulation.

<table>
<thead>
<tr>
<th>Location</th>
<th>( RE_{a1} )</th>
<th>( RE_{a11} )</th>
<th>( RE_{a2} )</th>
<th>( RE_{a1t} )</th>
<th>( RE_{a2t} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( z / D_h = 88.2 )</td>
<td>15.5%</td>
<td>20.2%</td>
<td>43.9%</td>
<td>18.7%</td>
<td>3.3%</td>
</tr>
<tr>
<td>( z / D_h = 141.7 )</td>
<td>21.1%</td>
<td>13.3%</td>
<td>53.4%</td>
<td>13.1%</td>
<td>8.0%</td>
</tr>
</tbody>
</table>

Table 7.3 Relative errors of the interfacial area concentration for Test 1

Figures 7.19-7.21 show the numerical results of Test 1 compared to the experimental data at two elevations, i.e., \( z / D_h = 88.2 \) and 141.7. Generally speaking, the predictions using the Fluent code with the two-group IATE model are in satisfactory agreement with the experimental data compared to the results using the conventional Fluent code.
Figure 7.19. Velocity at $z / D_h = 88.2$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles

As illustrated in Figure 7.19(a), there is a close-to-zero region in the gas velocity distribution of Group-1 bubbles at the location of $z / D_h = 88.2$ when the conventional Fluent code was applied, which might be due to inappropriate estimation of the interfacial forces. The turbulent diffusion force induced by Group-2 bubbles, turbulent dispersion force, and wall lubrication force are closely related to the bubble size, which is predetermined in the conventional Fluent code and does not change dynamically as the flow develops. The turbulent dispersion force acting on Group-1 bubbles appears not sufficient to flatten the central peak of the void fraction profile of Group-1 bubbles created due to the inlet injections. As few bubbles exist in the close-to-zero region, the gas velocity of Group-1 bubbles is approximately zero. In contrast, the Fluent code with the two-group IATE model predicts a more smooth distribution for the gas velocity of Group-1 bubbles, which matches the experimental data better.
In addition, Figure 7.19(b) shows that the gas velocity of Group-2 bubbles at $z / D_h = 88.2$, especially in the center region, could be predicted well by the Fluent code with the two-group IATE model. Furthermore, Figure 7.21 illustrates that the proposed numerical model is capable of predicting the interfacial area concentrations for both bubble groups reasonably well.

Figure 7.20. Void fraction at $z / D_h = 88.2$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figure 7.21. Interfacial area concentration at $z / D_h = 88.2$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.22. Velocity at $z / D_h = 141.7$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Similarly, the comparisons between the numerical results and experimental data of the gas velocity, void fraction, and interfacial area concentration for both groups in Test 1 at a higher elevation, namely, $z / D_h = 141.7$, are given in Figures 7.22-7.24, respectively.

It is shown in Figure 7.23(b) that the computed void fraction of Group-2 bubbles is overestimated compared to the measurements. However, a mass balance of the gas phase is obtained in the simulations. On the contrary, the mass flow rates calculated from the measured data are about $2.6 \times 10^{-1}$ kg/s at the location of $z / D_h = 34.8$ and $1.5 \times 10^{-1}$ kg/s at $z / D_h = 141.7$. This inconsistency in the measurements may be attributed to the face that Test 1 is at the flow regime transition from bubbly to cap-bubbly flows. As a result, the value of the void fraction of Group-2 bubbles is quite small, resulting in relatively large measurement uncertainties. In this respect, the code predictions may be considered more reliable.
Figure 7.24. Interfacial area concentration at $z / D_h = 141.7$ in Test 1 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.25. Contours of the void fraction in Test 1 from experimental observations (left), predicted Group-1 bubbles (middle), and predicted Group-2 bubbles (right)
Figure 7.25 compares the developments of the void fractions for both bubble groups from the experimental observations and code predictions. Here, the code predictions are from the Fluent code with the two-group IATE model. Ports 2, 3, 4, and 6 respectively refer to the location at $z / D_b = 34.8$, $61.5$, $88.2$, and $141.7$. It is observed experimentally that as the flow develops from Port 2 to Port 6, Group-1 bubbles are diffused to the whole flow channel, which can be also captured qualitatively by the code. Furthermore, Group-2 bubbles tend to remain concentrated in the center region.

Similar to the discussions for Test 1, Figures 7.26-7.28 show the comparisons between the measured and predicted distributions of the bubble velocity, void fraction, and interfacial area concentration for both groups at location of $z / D_b = 141.7$ for Test 2. The advantage of using the Fluent code with the two-group IATE model can be appreciated here. For instance, a relatively uniform phase distribution of Group-1 bubbles is captured by both the experiment and Fluent code with the two-group IATE model; whereas the conventional Fluent code provides a significant core peak for the void fraction of Group-1 bubbles, as demonstrated in Figure 7.27.
Figure 7.26. Bubble velocity at $z / D_h = 141.7$ in Test-2 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.27. Void fraction at $z / D_h = 141.7$ in Test 2 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figure 7.28. Interfacial area concentration at $z / D_h = 141.7$ in Test 2 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.29. Drag force coefficient in different flow regimes

When the Fluent code with IATE model was used, the bubble velocity of Group-2 bubbles is under-predicted, as shown in Figure 7.26. The under-prediction of the gas velocity of Group-2 bubbles implies that the drag force coefficient of the Group-2 bubbles (i.e., cap bubbles) employed in the simulations, shown in Table 7.2, is too large. As observed by Sun et al. (2005), a flow regime transition from cap-bubbly to churn-turbulent flows occurred in Test 2, which indicated that the drag force coefficient...
applicable to churn-turbulent flow rather than slug flow would be more appropriate. The drag force coefficient in different flow regimes is plotted in Figure 7.29. It is shown that the drag force coefficients for churn-turbulent bubbles are always smaller than those for cap-bubbly flows. If we adopt the drag force coefficient for churn-turbulent flows in the simulations, an increase in the velocity of Group-2 bubbles would be obtained.

![Figure 7.30](image)

Figure 7.30. Contours of the void fraction in Test 2 from experimental observations (left), predicted Group-1 bubbles (middle), and predicted Group-2 bubbles (right)

Furthermore, Figure 7.30 demonstrates the development of the measured and predicted void fractions for both groups at Ports 2, 3, 4, and 6. Similar to the observation in Test 1, Group-2 bubbles remain in the center region while Group-1 bubbles tend to spread in the lateral direction as to provide a uniform distribution.
7.12. Model validation: churn-turbulent flows

7.12.1. Study on unsteady solver

Due to its intrinsic unsteady feature, churn-turbulent flow is usually modeled with the time marching approach using the unsteady solver. The pseudo-steady-state is reached when the fluctuations in the whole flow field are stabilized.

First, an appropriate time step is investigated using the conventional Fluent code, in which the two-group IATE model is not implemented. Figure 7.31 shows the void fractions of both groups predicted by the code at \( t = 13 \) s using different time steps for Run 20, which has relatively high gas velocity and void fraction of Group-2 bubbles. The experimental experiments are also plotted in Figure 7.31 for comparisons. The flow is considered to reach the pseudo-steady state at \( t = 13 \) s, for which the reason will be discussed later. In Figure 7.31, simulations using the larger time step, namely, 0.01 s, give different results from the predictions using a smaller time step; whereas simulations with the two relatively small time steps, i.e., 0.001 and 0.0005 s, predict similar phase distributions. This discussion is consistent with the conclusion drawn by Laborde-Boutet et al. (2009), who suggested that a time step should be equal to or less than 0.001 s for churn-turbulent flow simulations. They also claimed that a time step no greater than 0.001 s not only captured the transient instabilities, but also provided the converged solution for churn-turbulence flows. As a result, a time step of 0.001 s is applied in the following simulations. It is, however, noteworthy that the numerical results presented here do not match the experimental data well. The application of the two-group IATE
might be helpful to improve the capabilities of the Fluent code, which will be investigated later.

Figure 7.31. Void fraction at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.32. Bubble velocity at $z / D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figures 7.32-7.35 show the predicted gas velocities and void fractions for both groups in Runs 18 and 20 at the location of $z / D_h = 141.7$ at different computing times. Again, the simulations were performed with the conventional Fluent code without the two-group IATE model. It is observed that a time lapse of 13 s is sufficient for the flows to approach a pseudo steady state. The numerical results, particularly those of the void fractions, fail to agree with the experimental measurements.

Figure 7.34. Velocity at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figure 7.35. Void fraction at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles

7.12.2. Comparison of results

This section shows the model comparisons for the two churn-turbulent flow conditions, i.e., Runs 18 and 20, when the two-group IATE model was incorporated into the two-fluid model. It can be seen that neither of the numerical models, namely, the conventional Fluent code and the Fluent code with the two-group IATE model, provides satisfactory predictions of phase distributions for these two churn-turbulent flow conditions, as shown in Figures 7.36-7.41. However, the values provided by the Fluent code with the two-group IATE model qualitatively match the measured interfacial area concentrations, as shown in Figures 7.38 and 7.41. Future work is however required for churn-turbulent flows, perhaps with a focus on the turbulence model and interfacial forces in the momentum equations.
Figure 7.36. Bubble velocity at $z / D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.37. Void fraction at $z / D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figure 7.38. Interfacial area concentration at $z / D_h = 141.7$ in Run 18 for: (a) Group-1 bubbles and (b) Group-2 bubbles

Figure 7.39. Bubble velocity at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles
Figure 7.40. Void fraction at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles.

Figure 7.41. Interfacial area concentration at $z / D_h = 141.7$ in Run 20 for: (a) Group-1 bubbles and (b) Group-2 bubbles.

7.13. Test on inlet effect

The final study performed is to examine the effects of the inlet boundary condition profiles on the development of the downstream flow structure. We use Run 17 as an example. Simulations were conducted in two test sections with different heights, one being 2338 mm high (named “short section”) and the other 3338 mm (named “long section”). Contours of the void fraction of Group-2 bubbles at the center plane (i.e.,
$y = 5$ mm) show similarities up to 2338 mm high, as illustrated in Figure 7.42. The effect from the inlet profile gradually diminishes as the flow develops. At the top-most part of the long test section, it is found out that the bubble velocity distributions for both bubble groups are similar to that in single-phase turbulent flow and that the flow is supposed to be nearly fully developed.

Figure 7.42. Contours of the void fraction of Group-2 bubbles at center-plane in Run 17 for: (a) short section and (b) long section
Chapter 8. Conclusions and Future Work

8.1. Conclusions

In summary, the current work built the groundwork of implementing the one-group interfacial area transport equation model and two-group IATE model into the two-fluid model in the Fluent code and provided a more reliable computational tool to simulate gas-liquid and liquid-liquid two-phase flows. A technical approach was presented to implement the two-group IATE model into the two-fluid model and a three-field two-fluid model was proposed. The modified governing equations of mass, momentum, and energy were introduced, along with discussions on the interfacial forces including the drag, lift, wall lubrication, and turbulent dispersion forces.

Furthermore, the two-fluid model incorporated with the one-group IATE model was validated by performing extensive simulations. Various scenarios were simulated including air-water bubbly flows in a circular pipe and a confined rectangular duct. In addition, liquid-liquid two-component flows in a circular pipe were simulated. A set of coefficients in the one-group IATE model was suggested for three-dimensional simulations instead of using the coefficients that were calibrated from the one-dimensional model. It was shown from comparisons with the experimental data that the one-group IATE model appreciably improved the predictive capabilities of the Fluent code in bubbly flows.
Before validating the three-field two-fluid model with the two-group IATE model, the well-posedness of the proposed model was studied for one-dimensional applications using characteristic analysis. The analysis demonstrated that the momentum flux parameters, as well as local flow variables, such as the void fraction, phasic velocities, etc., contributed to the model stability. The introduction of the momentum flux parameters helps achieve the hyperbolicity of the numerical model.

Finally, the three-field two-fluid model with the two-group IATE model was applied to simulate cap-bubbly and churn-turbulent flows in a confined flow channel. The simulations showed that the overall predictive capabilities could be reasonably improved, but additional work is needed for churn-turbulent flow simulations.

8.2. Future work

First, additional work to examine the model capability to churn-turbulent flows and two-phase flows in different flow channel configurations is recommended. It is also recommended to further evaluate the proposed numerical model in accordance with a more detailed study on the wall conditions and interfacial forces including the drag, lift, wall lubrication, and turbulent dispersion forces. For instance, the lift force was excluded in the current simulations of cap-bubbly and churn-turbulent flows, but appeared to be essential for a certain flow conditions.

Secondly, an area of future study is to simulate the processes involving the phase change since boiling and condensation are significant in the safety analysis of nuclear power reactors (Hibiki and Ishii, 2003; Yao and Morel, 2004; Situ et al., 2005; Park et al., 2007; Situ et al., 2008; Lee et al., 2009). A study is recommended to incorporate the
phase change terms into the IATE model such that the proposed numerical model is able to simulate the phase change phenomena.

Thirdly, the well-posedness of the three-field two-fluid model with the two-group IATE model needs to be further studied. The current analysis presented in this dissertation only provides the necessary condition. The question remains whether the instability growth rate due to a perturbation is unbounded as the amplitude of the perturbation decreases to zero. This requires a study of the dynamic behavior using the linear stability theory, from which the sufficient condition could be provided by using a wake equation with an accompanying infinitesimal perturbation (Jones and Prosperetti, 1985; Pokharna et al., 1997; Song, 2003). In addition, it is still undetermined as to how to generalize the results of the current incompressible model for application to gas-liquid two-phase flows, considering the gas compressibility. The effect of the compressibility of the gas phase is essential to the validity of the proposed model in applications of general two-phase flows (Song and Ishii, 2001).


Clebsch, H., 1856. Über die Bewegung eines Ellipsoid in einer tropfbaren Flüssigkeit. Journal für die reine und angewandte Mathematik 52, 103-121.


Fu, X., 2001. Interfacial area measurement and transport modeling in air-water two-phase flow. Ph.D. Thesis of Purdue University, West Lafayette, IN, USA.


189


Kim, S., 1999. Interfacial area transport equation and measurement of local interfacial characteristics. Ph.D. Thesis of Purdue University, West Lafayette, IN, USA.


Miller, J.W., Ishii, M., and Revankar, S.T., 1993. An experimental analysis of large spherical cap bubbles rising in an extended liquid. Report of School of Nuclear Engineering (PU NE-93/5), Purdue University, West Lafayette, IN, USA.


Smith, T.R., 2002. Two-group interfacial area transport equation in larger diameter pipes. Ph.D. Thesis, School of Nuclear Engineering, Purdue University, West Lafayette, IN, USA.


Sun, X., 2001. Two-group interfacial area transport equation for a confined test section, Ph. D Thesis of Purdue University, West Lafayette, IN, USA.


Wang, X., 2007. Computational fluid dynamics simulations of phase distribution in adiabatic upward bubbly flows using interfacial area transport equation. Master Thesis of The Ohio State University, Columbus, OH, USA.


Vasavada, S., 2008. Interfacial area transport equation for reduced-gravity two-phase flows. Ph.D. Thesis, School of Nuclear Engineering, Purdue University, West Lafayette, IN, USA.


