
Dissertation

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ABSTRACT

Multiphase flows involving bubbles and droplets are ubiquitous in nature and in many industrial processes. Detailed information of such flows can be acquired from direct numerical simulations that directly resolve the flow on the bubble or droplet scale. In recent years, the lattice Boltzmann method (LBM) has emerged as a novel numerical method for multiphase flow simulation. While having many favorable features such as incorporation of physics on the more fundamental level and efficient algorithm for fast computation, the current multiphase LBM still faces challenges in issues such as numerical instability and narrow parameter window, which severely restrict its application in a broad range of real world engineering problems.

This dissertation presents the development of a novel multiphase LBM which significantly expands the application of the method in various flow problems. Specifically, three techniques are developed to achieve enhanced performance in three aspects: First, new interaction potential functions are developed for multi-component LBM model to improve numerical stability at high density ratios between the liquid and gas phase. Second, an adaptive mesh refinement (AMR) scheme is developed to provide sufficient resolution of the gas-liquid interface. Third, the multi-relaxation time
(MRT) scheme is incorporated into the interaction potential model to enhance the numerical stability at low viscosities. The above new techniques are presented in detail, and simulations are performed in both 2D and 3D to evaluate their performance. It is demonstrated that the new interaction potential model is able to raise the stable density ratio from below 50 to over 1000. The AMR can provide accurate predictions of the interface, while reduce the computation cost by about 50% in real computations. In addition, with the MRT algorithm the maximum Reynolds number in bubble simulations can be increased from 100 to about 1000.

The performance of the newly developed LBM technique is further illustrated in different applications. In the study of the buoyant rise of a gas bubble in a viscous liquid, simulations are carried out to investigate the shape and rise velocity of the bubble. Particularly, both bubbles with large deformation and bubbles with high Reynolds number are studied. Good agreement is found between the model predictions and experimental results in the literature. Then the collision between a liquid droplet and a porous surface is investigated. Using the adaptive mesh approach, the flows on both the droplet scale and the pore scale are direct resolved simultaneously. The deformation of the droplet on the porous surfaces is compared to that on impermeable surfaces. Finally, the LBM simulation is performed for bubble formation in microchannels. The bubble shape and formation mechanism are discussed in different regimes and compared with experimental results.
In summary, a systematic investigation is conducted to improve the stability and accuracy of the LBM for multiphase simulations. A novel LBM model is developed and its performance is studied in various test problems. The application of the new model in the simulation of bubble rise, droplet collision, and microchannel bubble formation further illustrates the enhanced capability of the current LBM model.
DEDICATION

Dedicated to my family
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**FIELDS OF STUDY**

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# TABLE OF CONTENTS

ABSTRACT....................................................................................................................... iii  
DEDICATION................................................................................................................... vi  
ACKNOWLEDGEMENTS.............................................................................................. vii  
VITA ................................................................................................................................ viii  
TABLE OF CONTENTS.................................................................................................... x  
LIST OF TABLES........................................................................................................... xiii  
LIST OF FIGURES.......................................................................................................... xiv  
NOMENCLATURE ...................................................................................................... xviii  

CHAPTER 1  
INTRODUCTION .............................................................................................................. 1  
1.1. Multiphase flow ................................................................................................... 1  
1.2. Numerical simulation of multiphase flow............................................................ 2  
1.3. Direct numerical simulation (DNS) techniques for dynamic interfaces ............. 4  
1.4. Scope of current work......................................................................................... 6  

CHAPTER 2  
OVERVIEW OF LATTICE BOLTZMANN METHOD ................................................... 9  
Abstract ........................................................................................................................... 9  
2.1. Kinetic theory and Boltzmann equation ............................................................... 9  
2.2. Lattice Boltzmann method.................................................................................. 12  
2.3. Boundary conditions ....................................................................................... 15  
   2.3.1. Periodic condition ....................................................................................... 15  
   2.3.2. Bounce back condition .............................................................................. 15  
   2.3.3. Velocity condition ..................................................................................... 16  
   2.3.4. Pressure condition .................................................................................... 17  
2.4. Force term ......................................................................................................... 18  
2.5. LBM for multiphase flow ................................................................................. 20  
2.6. Advantages and technical barriers .................................................................. 22  
2.7. Conclusions....................................................................................................... 24  

CHAPTER 3  
MULTICOMPONENT-MULTIPHASE LBM WITH HIGH DENSITY RATIO ........... 26  
Abstract ......................................................................................................................... 26  
3.1. Introduction ........................................................................................................ 26  
3.2. Interaction potential model for multiphase flow ............................................... 28  
   3.2.1. Model for single component ...................................................................... 29  
   3.2.2. Model for binary mixture ....................................................................... 31  
3.3. High density ratio in single component model .............................................. 32
LIST OF TABLES

Table 3.1 Equilibrium properties of C-S EOS (a=1, b=4, R=1) ............................................. 41

Table 3.2 Equilibrium properties of binary mixture .................................................................. 41

Table 4.1 Comparison of equilibrium densities and pressure obtained by forcing schemes
developed by Guo et al and by Shan and Chen. ............................................................... 70

Table 4.2 Equilibrium properties for different interaction strength $G$.................................... 70

Table 5.1 Simulated equilibrium densities and pressure at different viscosities ............... 103
LIST OF FIGURES

Figure 2.1 Typical lattice structures in 2D and 3D........................................................... 25

Figure 3.1 Comparison of ideal EOS \((c_s^2 = 1/3)\) and C-S EOS \((a=1, b=4, R=1)\)......... 41

Figure 3.2 Binary mixture with flat interface after 10^5 steps........................................ 42

Figure 3.3 Binary mixture with flat interface using modified model under the same condition as in Figure 3.2........................................................................................................ 42

Figure 3.4 Flat interface, \(T/T_c=0.58\), (case 4 in Table 3.2)........................................ 43

Figure 3.5 Equilibrium distributions in a binary mixture ........................................ 44

Figure 3.6 Droplet falling into a liquid pool................................................................. 45

Figure 4.1 Schematic illustration of the change of particle distributions in the cells near the refinement jump in a 2D computation. ......................................................... 71

Figure 4.2 Flowchart of the computation procedure during one time step for two refinement levels................................................................................................................................. 71

Figure 4.3 Results of single phase flow obtained using LBM-AMR. .............................. 72

Figure 4.4 Comparison of simulated and theoretical density profiles under different interaction strength................................................................................................................................. 73

Figure 4.5 Relation between surface tension and parameter \(k_0, T\)........................................ 73

Figure 4.6 Change of surface tension as a function of the grid size............................... 74

Figure 4.7 Buoyant rise of a 2-D ellipsoidal cap bubble with \(Eo=43.4, Mo=27.1\)............. 75

Figure 4.8 Adaptive grid used for simulation shown in Figure 4.7................................. 76

Figure 4.9 Coalescence of two bubbles. \(Mo=1.5*10^{-4}, Eo=8.3\). ................................. 77

Figure 5.1 Effect of relaxation time \(\tau\) on the gas phase density in original Shan-Chen pseudo potential model (SC), Shan-Chen model with Guo’s forcing scheme (SC-Guo), and current MRT scheme................................................................. 103
Figure 5.2 Phase diagram obtained from the SC-Guo (BGK) scheme and current MRT scheme. .......................................................... 104

Figure 5.3 Laplace law tests for the SC-Guo model with BGK collision and the MRT model. .......................................................... 104

Figure 5.4 Effects of $s_2$ and $s_5$ on the magnitude of the spurious velocity in MRT model. .......................................................... 105

Figure 5.5 Magnitude of the spurious velocity as a function of viscosity. ............... 105

Figure 5.6 Spurious velocities at the gas-liquid interface in 2D. .............................. 106

Figure 5.7 Simulation of 2D bubble rise, $Eo=1.16$, $Mo=6.18 \times 10^{-9}$, $Re=148.5$ .......... 107

Figure 6.1 Bubble regime diagram (Bhaga and Weber, 1981). ................................. 126

Figure 6.2 Grid arrangements for 2D simulation of an ellipsoidal cap bubble with $Eo=49.8$ and $Mo=137.4$. .......................................................... 126

Figure 6.3 Time sequence of a 3D bubble rise with $Eo=9.81$ and $Mo=1.19 \times 10^{-4}$ .... 127

Figure 6.4 Simulated shapes of oblate ellipsoidal cap bubbles. .............................. 128

Figure 6.5 Streamlines of relative velocity ................................................................. 128

Figure 6.6 3D ellipsoidal cap bubble. $Eo=31.4$, $Mo=0.21$ ........................................ 129

Figure 6.7 Skirted bubble. $Eo=86.8$, $Mo=54.3$ ....................................................... 129

Figure 6.8 Spherical cap bubble in 2D. .............................................................. 130

Figure 6.9 2D ellipsoidal bubbles with $Mo=2.3 \times 10^{-5}$ ........................................ 131

Figure 6.10 Reynolds number of bubbles rising in silicon oil DMST-05 ($Mo=6.2 \times 10^{-7}$) and DMST-01 ($Mo=1.6 \times 10^{-8}$) ......................................................... 132

Figure 6.11 Aspect ratio of ellipsoidal bubble in silicon oil DMST-05 ....................... 132

Figure 6.12 Simulated shape and streamlines of ellipsoidal bubbles with $Mo=4.4 \times 10^{-7}$ 133

Figure 6.13 Simulated shape and flow field of ellipsoidal bubbles ............................... 133

Figure 6.14 Path and streamlines of 2D ellipsoidal bubbles ................................. 134
Figure 6.15 Simulation results for millimeter air bubbles in water. ......................... 135
Figure 6.16 Drag coefficients for spherical and ellipsoidal bubbles ......................... 135
Figure 6.17 Summary of typical simulation conditions in the current work on the regime map ......................................................................................................................... 136
Figure 7.1 Schematic illustration of the model system with a droplet and a porous surface. ......................................................................................................................... 156
Figure 7.2 Generation of the porous surface with 3000 particle using Monte-Carlo deposition .................................................................................................................. 156
Figure 7.3 Single phase flow in a porosity medium made up of ordered particle array. 157
Figure 7.4 Single phase flow in a porosity medium made up of randomly packed particles ......................................................................................................................... 158
Figure 7.5 Equilibrium contact angles of a droplet on a surface ................................. 159
Figure 7.6 Snapshots of the collision of a droplet with a non-porous superhydrophobic surface .................................................................................................................. 160
Figure 7.7 Spreading factor and dimensionless height of the droplet ......................... 161
Figure 7.8 Snapshots of a droplet colliding with a surface with $We=6.14$ and equilibrium contact angle of $60^\circ$ ........................................................................................................ 161
Figure 7.9 Spreading dynamics of the droplet on the surface ..................................... 161
Figure 7.10 Collision of a droplet on a porous substrate. ......................................... 163
Figure 7.11 A slice of the mesh and phase distribution at $t=1920$. ............................. 163
Figure 7.12 Velocity field in a cross section at $t=1920$. .......................................... 164
Figure 7.13 Droplet deformation on the porous substrate. ........................................ 164
Figure 7.14 Droplet collisions on superhydrophobic porous surface. ........................ 165
Figure 8.1 Experimental setup .................................................................................. 184
Figure 8.2 Simulation results for $Ca=0.2$. .............................................................. 185

xvi
Figure 8.3 Experimental results for air-silicon oil in 125 µm channel. ......................... 186

Figure 8.4 Simulation results for Ca=0.03. Q_g:Q_l =1:2 .................................................. 186

Figure 8.5 Air bubble formation in sugar solution in 250µm channel. Ca=0.04. Q_g:Q_l =1:2
......................................................................................................................................... 187

Figure 8.6 Simulation results for Ca=0.04, Q_g:Q_l =1:2 .................................................. 187

Figure 8.7 Experimental and simulation results for slug regime .................................... 188

Figure 8.8 Simulation results for Ca=0.006, Q_g:Q_l =1:2. ............................................... 189

Figure 8.9 Comparison of simulation results in “cross” and “converging” channels..... 190

Figure 8.10 Comparison of bubble formation process in different geometries with
Ca=0.07 Q_g:Q_l =1:4 ........................................................................................................ 191

Figure 8.11 Simulation results for Ca=0.017, Q_g:Q_l =1:1, µ_g:µ_l=1:26......................... 192

Figure 8.12 Pressure and velocity field........................................................................... 193
## NOMENCLATURE

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Meaning</th>
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<tbody>
<tr>
<td>$a$</td>
<td>Acceleration</td>
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<tr>
<td>$Cd$</td>
<td>Drag coefficient</td>
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<tr>
<td>$d$</td>
<td>Diameter</td>
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<td>Darcy number</td>
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<td>Morton number</td>
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<td>$u$</td>
<td>Velocity</td>
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</table>
**Greek letters**

ε Porosity

φ Cross interaction potential

μ Dynamic viscosity

ν Kinematic viscosity

ρ Density

σ surface tension

τ Relaxation constant

ψ Self interaction potential

Ω Collision integral

**Superscript and subscripts**

eq Equilibrium

g Gas phase

i Lattice direction

l Liquid phase

p Particle

σ Component index
CHAPTER 1

INTRODUCTION

1.1. Multiphase flow

Bubbles and droplets are ubiquitous in both nature and industrial systems. Particularly, they are of fundamental importance to many chemical engineering operations, such as floatation, fermentation, and spray drying. For example, in gas-liquid-solid fluidization systems, bubble dynamics significantly affects the flow pattern and mass transfer rates in the reactor and ultimately influences the overall reaction rates. In FCC riser reactors, oil injected from feed nozzles forms sprays of droplets that come into contact with high-temperature catalyst particles. Different droplet-particle contact modes, such as rebound, breakup, and penetration, have great effect on the transport processes and reaction kinetics, which are crucial to the hydrocarbon product distributions from the catalytic and thermal cracking reactions in the riser. Therefore, understanding of the dynamics of these fluid particles is necessary for the design and optimization of multiphase chemical reactors.
1.2. Numerical simulation of multiphase flow

Numerical simulation is becoming an important approach in the design of chemical reactors and the study of their operations. One important factor in modeling multiphase reactors is the disparate scales that are involved. While industrial multiphase chemical reactors usually have dimensions of several meters and contain a huge number of solid and/or fluid particles, the individual particle size is often on the scale of millimeters or less. Naturally, different models have been developed to predict the multiphase flow behavior depending on the scope of the problem, the required level of details, and the time and cost to be spent on the simulation.

On the reactor scale, most simulations are carried out using the Eulerian-Eulerian (E-E) two-fluid model, in which both the continuous phases and the dispersed phase are considered to be interpenetrating fluids. The two phases each has their own mass, momentum, and energy transport equations, and are coupled to each other through the inter-phase transport terms. Such models have been widely applied in various types of reactor simulations. In gas-liquid systems such as bubble columns, the bubbles are modeled as a continuous gas phase and coupled with population balance to account for the change of bubble size distribution. In gas-solid system such as fluidized beds, the pseudo fluid made up of the solid particles is usually described by the kinetic theory for granular material. On the other hand, when the fraction of the dispersed phases is small compared to the continuous phase, the dispersed particles are usually tracked individually by their equation of motion, while the flow of the continuous phase is still governed by
the Navier-Stokes equation. Such models are referred to as the Eulerian-Lagrangian (E-L) model, since the continuous and dispersed phases are treated in the Eulerian and Lagrangian coordinates, respectively. In both E-E and E-L models, the set of equations are not closed without proper model for the interaction between the two phases, which is represented by a series of forces, including drag, lift, virtual mass, etc. In fact, the closure for inter-phase interactions has become the most critical issue in determining the reliability of the simulation. Since the grid size in these simulations are usually much larger than the particle size, the models for such interactions are sometimes known as sub-grid models. In the past most closure relations are obtained from experimental correlations. However, with the rapid progress in computation techniques, direct numerical simulation (DNS) is becoming an increasingly useful tool in obtaining such closure relations due to its versatility and low cost.

Direct numerical simulation directly resolves the flow field around each individual particle by using a very fine mesh whose size is much smaller than the particle size. The momentum exchange between the two phases is accounted for by employing proper boundary conditions on the interface. Direct numerical simulation can provide the detailed information of the motion of individual particles, the deformation of the bubble or droplet surface, and the evolution of the configuration of particle clusters. Simulation results also provide pressure and velocity fields in the entire computational domain, including the vicinity of the interface. Therefore, closure relations for interaction between two phases can be obtained by gathering the hydrodynamic force on each particle.
1.3. Direct numerical simulation (DNS) techniques for dynamic interfaces

A distinct feature of the DNS for bubbles or droplets is that it involves the simulation of deformable interfaces which divide the entire simulation domain into regions occupied by either gas or liquid phase. Currently, there are a number of numerical techniques for the direct simulation of the flows involving bubbles or droplets. Depending on the type of mesh they use, these techniques can be divided into two large categories: the method based on body-fitted mesh, and that based on Cartesian mesh. In the method with body-fitted mesh, the interface is represented by the mesh boundary, and the mesh must be regenerated as the interface moves or deforms with time. Representative technique in this category is the Arbitrary- Lagrangian-Eulerian (ALE) method. The other category of methods is based on the Cartesian mesh in which the phase boundary is immersed in a fixed set of rectangular (2D) or cubic (3D) grids. The flow in the entire domain is solved using a “single-filed” approach in which both phases are calculated using a unified set of equations, with smooth change of material properties across a finite thickness of the interface.

The approaches based on a fixed Cartesian mesh can be further divided into sharp interface modes, including the front tracking method, the volume of fluid method (VOF), and the level set method; and the diffused interface models, such as the phase field model. In the sharp interface model, the two fluid phase domains are jointed conceptually by an infinitesimally thin boundary with jump conditions across the interface, and this approach
can be further divided into the front-tracking method and the front-capturing method. In the front-tracking method, the interface is explicitly represented by a surface mesh, which is made up of Lagrangian particles that are convected by the local flow field in each time step to update the location of the interface. In the front-capturing approaches the interface is represented implicitly by the contour of a scalar function. The most popular front-capturing techniques include the volume of fluid (VOF) method, and the level-set method (LSM). The scalar field in these cases is either the volume fraction of the gas phase in the computational cell (in VOF), or the distance to the interface (in LSM). On the other hand, in the diffused interface model, the interface has a finite width, and fluid properties are allowed to vary smoothly across the interface according to thermodynamic principles. A typical technique involving this approach is the phase-field model. In actual computation, however, the interfaces in both the physically sharp interface model and the diffused interface model are numerically smeared out. The difference between them is that, for the sharp interface method the properties are merely numerically interpolated across the interface, while the distributions of the properties in the diffused interface method are determined by the thermodynamic laws. At the same time, the interface width in the sharp interface is usually smaller than that in the diffused interface model.

The dynamics of the interface is closely coupled with the flow field, which is solved by the flow solver. While most DNS today employs the Navier-Stokes (N-S) equation for incompressible flow, other models has emerged, such as the Lattice Boltzmann method (LBM). Different from the N-S equation, which is the momentum conservation on the
continuum level, the LBM focuses on the discrete particles that comprise the fluid, and calculates the evolution of the particle distribution function. While it is formally related to the classic Boltzmann equation in non-equilibrium statistical mechanics, it can also be proved that the lattice Boltzmann equation recovers the N-S equation for the macroscopic flow in the incompressible limit. This makes LBM a mesoscopic method and therefore can simulate problems on a more fundamental level than the N-S equation based methods. In addition, the algorithm in LBM is much simpler than that in traditional CFD methods, and parallel computation can be implemented with ease. This gives the LBM significant advantage in computation efficiency as compared to traditional CFD methods. In practice, the LBM has been accepted as a reliable tool in the simulation of incompressible single phase flows, and commercial CFD software based on LBM algorithm has emerged. At the same time, a number of LBM models for multiphase flows have also been proposed. However, although some promising results for non-traditional multi-component or multiphase flow problems have been demonstrated, the application of LBM under realistic multiphase flow conditions that are relevant to industrial processes is still limited. Numerical issues such as stability and accuracy have placed severe restrictions to the range of conditions accessible to LBM, and therefore seriously affect its application in multiphase flow simulation.

1.4. Scope of current work

The purpose of this study is to develop an advanced LBM technique which can overcome the inadequacy of current LBM in simulation of multiphase flow problems. Specifically,
this study focuses on a type of multiphase LBM which is based on the interaction
potential approach, and addresses the improvements in three aspects. In chapter 3, the
maximum stable density ratio between the gas and liquid phase in the multicomponent
LBM model is increased from about 50 to over 1000 by introducing a new potential
function. In addition to the use of proper equation of state for the non-ideal component,
special attention is paid to the cross interaction between the two components to ensure
their correct distribution in each phase. In chapter 4, the adaptive mesh refinement
technique is developed to significantly enhance the accuracy of multiphase LBM and to
reduce the computation cost. Care has been taken to maintain consistent physical
properties over different mesh sizes. The adaptive mesh is especially useful for modeling
multiphase flows with moving interfaces such as bubble’s surface, where the interface
motion has significant effect on the entire flow field. In chapter 5, the multi-relaxation
time algorithm is employed to stabilize the computation at low fluid viscosities. As the
result, high Reynolds number two-phase flows can now be simulated. The second half of
the dissertation switches the attention to the applications of the newly developed LBM.
The buoyant rise of a gas bubble in a viscous liquid is discussed in Chapter 6. The shape
and rise velocity of the bubble under various conditions are simulated and compared with
experimental results. With the adaptive mesh and multi-relaxation time scheme, both
bubbles with large deformation and with high Reynolds numbers are successfully
simulated. Chapter 7 studies the impingement of a liquid droplet on a porous surface.
Thanks to the adaptive mesh, flows on the droplet scale and on the pore scale can be both
simulated simultaneously. Deformation of the droplet on the surface is analyzed under
different conditions and compared to the collision on an impermeable surface. Chapter 8 investigates the bubble formation in microchannels. Different flow regimes are observed in the simulation as a function of the Capillary number. Bubble formation mechanism in each regime is also analyzed. Finally, a summary of the research and recommendations for future study are provided in Chapter 9.
CHAPTER 2

OVERVIEW OF LATTICE BOLTZMANN METHOD

Abstract

This chapter presents a brief overview of the lattice Boltzmann method (LBM). The general background of the LBM is related to the kinetic theory and Boltzmann equation, which describe the dynamics of gas molecules. Operating in a discrete velocity space, the LBM can be regarded as a simplified kinetic scheme that models the macroscopic flow behavior. The basic algorithm and boundary conditions are both easy to implement. In addition, several versions of multiphase LBM models have been developed, and they are briefly described in this chapter. Finally the advantages and disadvantage of LBM are discussed in comparison to other traditional computational fluid dynamics (CFD) techniques.

2.1. Kinetic theory and Boltzmann equation

In the kinetic theory, a fluid is described as a set of classic particles which travel in space and collide with each other. These particles have different velocities which change through the collision process. The collective behavior of the microscopic states of
the particles, such as their location and velocity, is reflected on the macroscopic level by
the hydrodynamic quantities such as density, flow velocity, and pressure. In non-
equilibrium statistic mechanics, the transport of the particles is described by the well-
known Boltzmann equation:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \mathbf{a} \cdot \nabla_v f = \Omega, \quad (2.1)$$

where $f(x, v, t)$ is the particle distribution function that represents the number density of
particles with velocity $v$ at location $x$ and time $t$. $a$ is the force per unit mass on the
particle. The operators $\nabla_x$ and $\nabla_v$ are the gradient with respect to the spatial coordinates
and the gradient in the velocity space, respectively. The right hand side, $\Omega$, is the
collision integral that accounts for the change of particle distributions due to collision.
The Boltzmann equation is an integral-differential equation whose solution would seem
an impossible task, thanks to the complicated nature of the collision integral. Several
models have been proposed to simplify the collision integral, and the Bhatnagar-Gross-
Krook (BGK) model is the most commonly used model due to its simple form. The BGK
collision term approximates the change of distribution function due to collision by a
relaxation process towards the local equilibrium with a single relaxation time scale $\tau$:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f + \mathbf{a} \cdot \nabla_v f = -\frac{f - f^{eq}}{\tau} \quad (2.2)$$

The local equilibrium distribution $f^{eq}$ is the Maxwell-Boltzmann distribution that
depends on the local hydrodynamic variables at $(x, t)$:
The macroscopic transport equations for mass, momentum and energy as well as the transport coefficients can be systematically derived from the Boltzmann equation under the condition of small Knudsen number ($Kn$), which is the ratio between the mean free length of the fluid and the characteristic length scale of the system. The derivation procedure is known as the Chapman-Enskog expansion. By applying this expansion up to the $2^{nd}$ order for the momentum equation, the Navier-Stokes equation can be obtained, with the kinematic shear and bulk viscosities

$$\nu = \xi = \frac{\pi k_B T}{m}$$  \hspace{1cm} (2.7)

And the pressure is given by

$$p = nk_B T$$  \hspace{1cm} (2.8)

which is essentially the equation of state (EOS) for an ideal gas.
2.2. Lattice Boltzmann method

The lattice Boltzmann equation (LBE) can be regarded as a special discretization of the continuous Boltzmann equation with BGK approximation (Equation 2.2). For the sake of simplicity, in the following discussion of the discretization procedure in this section, only the Boltzmann equation without force term \( \mathbf{a} = \mathbf{0} \) will be considered. The particle distribution function \( f(x,v,t) \) is first discretized in the velocity space, where a finite set of velocities \( \{v_i\} (i = 1 \cdots q) \) is used to replace the continuous spectrum of velocities. Correspondingly, the distribution function associated with \( v_i \) is written as \( f_i(x,t) \). Then the discrete Boltzmann equations

\[
\frac{\partial f_i}{\partial t} + v_i \cdot \nabla_x f_i = -\frac{f_i - f_i^{eq}}{\tau} \tag{2.9}
\]

is further discretized in space and time

\[
f_i(x,t + \Delta t) - f_i(x,t) + \frac{\Delta v_i}{\Delta x_i} [f_i(x + \Delta x_i, t + \Delta t) - f_i(x,t + \Delta t)] = -\frac{\Delta t}{\tau} (f_i - f_i^{eq}) \tag{2.10}
\]

By choosing \( \Delta x_i = v_i \Delta t \), the above equation is simplified to

\[
f_i(x + \Delta v_i \cdot t + \Delta t) - f_i(x,t) = -\frac{\Delta t}{\tau} (f_i - f_i^{eq}) \tag{2.11}
\]

The relation \( \Delta x_i = v_i \Delta t \) establishes the link between the discrete velocity set \( \{v_i\} \) and the discretization of the space, which is represented by the lattice (grid). One of the most commonly used lattice structures is the D2Q9 lattice, which has 9 lattice directions in 2-dimensional space, is shown in Figure 2.1(a). With the dimensionless lattice speed \( c = \Delta x / \Delta t \), the 9 dimensionless lattice velocities \( \hat{c}_i = c_i / c \) can be written as.
Similarly, the D3Q19 lattice has 19 lattice velocities in 3-dimensional space, and the lattice velocities are

\[
\mathbf{c}_i = \begin{cases} 
(0,0) & i = 0 \\
(\pm 1,0),(0,\pm 1) & i = 1 ~ 4 \\
(\pm 1,1),(\mp 1,-1) & i = 5 ~ 8
\end{cases}
\]  

(2.12)

as shown in Figure 2.1(b). The D2Q9 and D3Q19 lattice are the lattice structure that will be used in this study for 2-D and 3-D computations, respectively. Since the velocity set \( \{ \mathbf{c}_i \} \) consists of only a very limited number of velocities, it is insufficient to describe the temperature variation due to velocity fluctuation in the same way as used in the gas kinetic theory. Therefore, the LBE discussed here is restricted to isothermal conditions.

After replacing \( \{ \mathbf{v}_i \} \) with lattice velocities \( \{ \mathbf{c}_i \} \), the working equation in LBM is derived as

\[
f_i(x + \Delta \mathbf{c}_i, t + \Delta t) - f_i(x, t) = -\frac{\Delta t}{\tau_f} (f_i - f_i^{eq})
\]  

(2.14)

The equilibrium distribution function \( f_i^{eq} \) is a truncated Maxwell-Boltzmann distribution

\[
f_i^{eq}(\rho, \mathbf{u}) = \rho \sqrt{\frac{m_i}{2\pi}} \exp \left[ -\frac{\mathbf{u} \cdot \mathbf{u}}{2m_i} \right] 
\]  

(2.15)

where \( \mathbf{w}_i \) is the weight coefficient associated with the lattice. For a D2Q9 lattice, the weight coefficients are
\[ w_i = \begin{cases} 
4/9 & i = 0 \\
1/9 & i = 1 \sim 4 \\
1/36 & i = 5 \sim 8 
\end{cases} \quad (2.16) \]

And for a D3Q9 lattice, the weight coefficients are

\[ w_i = \begin{cases} 
1/3 & i = 0 \\
1/18 & i = 1 \sim 6 \\
1/36 & i = 7 \sim 18 
\end{cases} \quad (2.17) \]

In general, all quantities in LBM are nondimensionalized in a way such that

\[ c = \Delta x = \Delta t = 1 \quad \text{and} \quad m = 1. \]

The macroscopic hydrodynamic quantities are calculated from the summation of the discrete particle distribution functions:

\[ \rho(x,t) = \sum_i f_i(x,t) \quad (2.18) \]

\[ \rho u(x,t) = \sum_i e_i f_i(x,t) \quad (2.19) \]

Which are the lattice version of Equations (2.4) and (2.5). Fluid viscosity is related to the relaxation time by

\[ \nu = \Delta t e_s^2 (\tau - \frac{1}{2}) \quad (2.20) \]

The pressure is given by the equation of state for ideal gas

\[ p = \rho c_s^2 \quad (2.21) \]

In which the constant \( c_s = \sqrt{\frac{\partial p}{\partial \rho}} \) corresponds to the speed of sound in LBM. The value of \( c_s \) depends on the lattice structure, and on the D2Q9 or D3Q19 lattice \( c_s = \frac{1}{\sqrt{3}} c \).
2.3. Boundary conditions

Unlike common CFD techniques that directly specify conditions for different hydrodynamic quantities on the domain boundaries, the LBE is based on particle distributions functions and therefore the boundary conditions for macroscopic hydrodynamic quantities needs to be translated to the boundary conditions for particle distributions. This section briefly describes a few of the boundary conditions that are relevant to this study.

2.3.1. Periodic condition

The simplest boundary condition is the periodic condition, which only requires copying the distribution functions from the opposite boundary.

2.3.2. Bounce back condition

The bounce back condition corresponds to the no-slip condition that is usually employed at fluid-solid interfaces. In such situations, at a lattice site adjacent to the solid boundary, the distributions propagating into the fluid domain can not be obtained from the neighboring solid site, and need to be specified through the boundary condition. In the bounce back condition, the distributions propagating towards the solid boundary are simply scattered back into the fluid domain along their incoming directions. In the example of the bottom boundary of a D2Q9 lattice, the incoming distributions $f_2, f_5, f_6$ are calculated from the outgoing distributions $f_4, f_7, f_8$: 
\[ f_2 = f_4 \quad f_5 = f_7 \quad f_6 = f_8 \] (2.22)

It is well known that the bounce back condition gives only 1st order accuracy when the lattice site is placed on the solid boundary (referred to as “node bounce back” or “complete bounce back”), but 2nd order accuracy is achieved when the lattice site is placed half lattice spacing away from the solid boundary (referred to as “link bounce back” or “half way bounce back”).

### 2.3.3. Velocity condition

The velocity condition employed in this study follows the concept of bounce-back of the non-equilibrium part of the distribution function, which was originally developed by Zou and He (1997). Its implementation on the D2Q9 lattice is illustrated as follows. If velocity \( u_x \) and \( u_y \) are to be specified at the lattice site on the bottom boundary, distributions \( f_5, f_2, f_6 \) need to be calculated from \( u_x, u_y \) and the rest of the distributions which are known after propagation:

\[
f_2 + f_5 + f_6 = \rho - (f_0 + f_1 + f_3 + f_4 + f_7 + f_8)
\] (2.23)

\[
f_5 - f_6 = \rho u_x - (f_1 - f_3 - f_7 + f_8)
\] (2.24)

\[
f_2 + f_5 + f_6 = \rho u_y + (f_4 + f_7 + f_8)
\] (2.25)

Comparison between Equations 2.23 and 2.25 leads to

\[
\rho = \frac{1}{1-u_y} \left[ f_0 + f_1 + f_3 + 2(f_4 + f_7 + f_8) \right]
\] (2.26)

It is assumed that the bounce-back rule can be applied to the non-equilibrium part of the distribution normal to the boundary, so that
\[ f_2 = f_4 + (f_2^{eq} - f_4^{eq}) \]  

(2.27)

With Equations 2.26 and 2.28, the three unknown distributions can be solved from Equations 2.23-2.25, leading to:

\[ f_2 = f_4 + \frac{2}{3} \rho u_y \]  

(2.28)

\[ f_5 = f_7 - \frac{1}{2} (f_1 - f_3) + \frac{1}{2} \rho u_x + \frac{1}{6} \rho u_y \]  

(2.29)

\[ f_6 = f_8 + \frac{1}{2} (f_1 - f_3) - \frac{1}{2} \rho u_x + \frac{1}{6} \rho u_y \]  

(2.30)

2.3.4. Pressure condition

Since the pressure and density are related by the equation of state in LBM, specifying the pressure value at boundaries is equivalent to imposing density condition. Zou and He (1997) also developed the pressure (or density) condition using bounce-back of the non-equilibrium part of the distribution. Taking the left boundary of a D2Q9 lattice for example, the distributions to be specified are \( f_1, f_5, f_8 \). Using the condition of constant density (\( \rho = \rho_{in} \)) and no cross flow (\( u_y = 0 \)), the following equations can be obtained:

\[ f_1 + f_5 + f_8 = \rho_{in} - (f_0 + f_2 + f_3 + f_4 + f_6 + f_7) \]  

(2.31)

\[ f_1 + f_5 + f_8 = \rho_{in} u_x + (f_3 + f_6 + f_7) \]  

(2.32)

\[ f_5 - f_8 = -f_2 + f_4 - f_6 + f_7 \]  

(2.33)

Combing (2.31) and (2.32) gives

\[ u_x = 1 - \left[ \frac{f_0 + f_2 + f_4 + 2(f_3 + f_6 + f_7)}{\rho_{in}} \right] \]  

(2.34)
And applying bounce-back for the non-equilibrium part of the distribution normal to the boundary

\[ f_1 = f_3 + \left( f_{1}^{eq} - f_{3}^{eq} \right) \]  \hspace{1cm} (2.35)

The distributions to be specified can be calculated from

\[ f_1 = f_3 + \frac{2}{3} \rho_m u_x \]  \hspace{1cm} (2.36)

\[ f_5 = f_7 - \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho_m u_x \]  \hspace{1cm} (2.37)

\[ f_8 = f_6 + \frac{1}{2} (f_2 - f_4) + \frac{1}{6} \rho_m u_x \]  \hspace{1cm} (2.38)

It should be mentioned that since the lattice involves diagonal directions, the boundary conditions at the corners of the domain need to be specified in a way slightly different from the edges (In 3-D cases, the boundary conditions for face, edge, and corners need to be address differently). It should also be noted that both the velocity and pressure conditions described above can be easily extended to 3-D LBM.

### 2.4. Force term

In Section 2.3 the LBE is introduced without the force term. However, in most applications either interactions between particles or an external field such as gravity or electric field are present, and therefore a force term has to be included. In general, when a body force \( \mathbf{F} \) is applied to the particles, the force term needs to be added to the LBE, so Equation (2.14) is replaced by
\[
    f_i(x + \Delta x, t + \Delta t) - f_i(x, t) = -\frac{\Delta t}{\tau}\left(f_i - f_i^{eq}(\rho, v)\right) + \Delta t K_i
\]

Compared to Equation (2.14), two changes are made in Equation (2.39). Firstly, when calculating the equilibrium distribution \( f_i^{eq} \) using Equation (2.15), a new equilibrium velocity \( v \) is used instead of the macroscopic flow velocity \( u \) calculated from Equation (2.19). Secondly, an additional term \( \Delta t K_i \) is included at the end of the equation.

Determination of the value of \( v \) and \( K_i \) can be either approached from the kinetic theory on the continuous Boltzmann equation level (Martys, et al, 1998, Shan, et al, 2006), or by matching the corresponding macroscopic equation of Equation 2.38 to the Navier-Stokes equation using the Chapman-Enskog expansion (Guo, et al, 2002).

Various forms have been proposed to specify the force terms, and systematic studies are conducted to summarize and compare their accuracy (Buick and Greated, 2000, Guo, et al, 2002). The two most commonly used force terms are both related to the method employed in the current study. The first one is the Shan-Chen force scheme, which only shifted the equilibrium velocity (Shan and Chen, 1993):

\[
    v = \tilde{u} + \frac{\mathbf{F}}{\rho} \quad \text{and} \quad K_i = 0
\]

in which \( \tilde{u} \) is an intermediate velocity value given by

\[
    \rho \tilde{u} = \sum_i c_i f_i
\]

The other one is the Guo’s force scheme (Guo, et al, 2002):
\begin{align*}
\mathbf{v} &= \mathbf{\bar{u}} + \frac{\Delta t \mathbf{F}}{2\rho} \\
K_i &= \left(1 - \frac{1}{2\tau}\right) w_i \left[ \frac{c_i - \mathbf{v}}{c_i \cdot c_i} + \frac{(c_i \cdot \mathbf{v})}{c_i^2} \mathbf{c}_i \right] \cdot \mathbf{F}
\end{align*}

(2.42)  
(2.43)

When the force term is included, the macroscopic fluid velocity \( \mathbf{u} \) will no longer be the same as the one calculated from Equation (2.19). Instead, it is computed from the average momentum before and after the force is added:

\[
\rho \mathbf{u} = \sum_i c_i f_i + \frac{\Delta t}{2} \mathbf{F}
\]

(2.44)

### 2.5. LBM for multiphase flow

The LBM is a promising technique in modeling multiphase flow problems, particularly for flows with complex topological changes of the interface or in complex geometries. A number of models have been developed to model multiphase flows in LBM. The most widely used ones are the color function model, the interaction potential model, and the free energy model.

The color function model (Gunstensen et al, 1991) is the first multiphase model in LBM. Two components are used in this model to represent two types of fluids. The red and blue particle distributions each follow its own LB equation. The collision term in the equation includes both the self-interactions for particles of the same type, and the cross-interactions for particles with different colors. The latter one is used to generate a surface tension between the two phases, and is calculated using the gradient of the color function.
In order to maintain phase segregation, the particle density near the interface needs to be redistributed to minimize mixing. In practice, the redistribution is a time-consuming step, and can be replaced by an evolution equation for the color function in a way similar to the level set type of methods. Another drawback of the color function method is the limited numerical stability for high density ratio or large surface tension value.

The interaction potential or pseudo potential model developed by Shan and Chen (1993) is the most widely used multiphase LBM model due to its simplicity and versatility. An interaction force between the particles is introduced to account for the molecular interactions in non-ideal fluids. Consequently the fluid spontaneously segregates into dense and dilute phases under proper condition according to the equation of state of the fluid. The automatic phase separation is an attractive feature in this model, since it does not require the interface-tracking or interface-capturing step that is often necessary in other models. The implementation of the model is also straightforward since the interaction force can be simply calculated from the pair-wise interaction potential. In recent years many researches have been conducted to discuss the properties and the improvements of the interaction potential model (Shan, 2008; Sbragaglia et al, 2007).

The free energy approach (Swift et al, 1996) is based on the thermodynamic equilibrium of fluid phases. The free energy functional at a fixed temperature includes both the bulk part and the interface part. The former introduces equilibrium between two phases, while the latter introduces surface tension. The model is incorporated into LBE by adding a
term to the equilibrium distribution to ensure the correct stress tensor condition. The free energy model is also capable for automatic phase separation, and it is easier to specify density and surface tension values in free energy model than in interaction potential model. However, a major criticism of the free energy model is that it lacks Galilean invariance, i.e. the physical properties in the model are dependent upon the velocity (Swift et al, 1996).

2.6. Advantages and technical barriers

Due to its kinetic nature, the LBM has many advantages over the traditional CFD methods. It has a clearer physical picture in modeling fluid flow by taking into account the collision, propagation, and interactions between fluid molecules. On one hand, it describes the particle kinetics, and is therefore easy to be linked to molecular dynamics (MD) for microscopic flows. On the other hand, it recovers the Navier-Stokes equation for macroscopic flows under the incompressible limit. Therefore, it can be viewed as a mesoscopic approach that is versatile in multiscale simulations. The better physical background also exhibits itself in multiphase problems. By employing the concepts of particle interaction or free energy, it models the phase segregation in accordance with the thermodynamics, rather than depending on mathematical interfaces that is used in other CFD techniques to divide the domain into different phases. Moreover, by using simple implementation of the bounce back condition, the LBM is capable of simulating flows in extremely complex geometries, such as flow in the porous medium which is extremely challenging for other CFD techniques.
Computationally, the LBM is an efficient method. The propagation of the particle distribution functions is linear in LBM, as compared to the nonlinear convective term in the Navier-Stokes equation. Most importantly, by using the equation of state, the LBM avoids solving the pressure Poisson equation, which is the most time-consuming step in traditional incompressible CFD algorithms. This not only gives the LBM fast computation speed, but also results in an algorithm that only needs local information rather than global information. Consequently, the LBM is intrinsically suitable for parallel computation. Finally, the LBM algorithm is easy to implement, and the resulted code is often much simpler than the traditional CFD code with the same function.

In spite of the many attractive features of LBM, there are still a number of issues that restrict its application in many real flow problems. The method is only valid for incompressible and isothermal flows, due to the small set of discrete velocities. Especially, since an equation of state is used, the pressure variation in the flow field needs to be small to satisfy the incompressible condition. In addition, the numerical instability becomes a concern when the fluid viscosity is small. This often limits the application of LBM in high Reynolds number flows. For gas-liquid flows, the numerical instability is often triggered at high density ratio between the phases. Although new methods are being developed to improve the performance of LBM in the above aspects, the LBM has not been widely used in industrial multiphase simulations or commercial multiphase CFD software packages. Currently the only commercial LBM software is the
POWERFLOW®, which is mostly used in automobile industry for aerodynamic simulation of vehicles.

2.7. Conclusions

The LBM is distinguished from other traditional CFD techniques by its kinetic nature which gives it a clear physical picture on a more fundamental level. The theoretical background of LBM is the kinetic theory and Boltzmann equation, which are connected with the macroscopic Navier-Stokes equation by the Chapman-Enskog expansion. The LBM can be regarded as a simplified kinetic scheme by using a finite set of discrete velocities and a simplified collision integral. Both the algorithm and the boundary conditions are easy to implement in LBM. It also has lots of promising features in multiphase flow modeling. When compared to the traditional CFD techniques, the advantages of LBM are mostly in its clear physics and simple algorithm, while the major disadvantages lie in its numerical instability and over predicted compressibility. It is worth noting that some of the numerical features of LBM are also found in other CFD techniques. For example, the counterpart of the LBM in traditional CFD is the artificial compressibility method (Chorin, 1967), which also replaces the pressure Poisson equation by an artificial equation of state. In the treatment of the interface between two phases, both the interaction potential model and the free energy model employ the idea of a diffused interface, which is also used in the phase field model that is coupled with Navier-Stokes equation (Anderson, et al, 1998; Jacqmin, 1999).
Figure 2.1 Typical lattice structures in 2D and 3D
(a) D2Q9 lattice; (b) D3Q19 lattice
CHAPTER 3

MULTICOMPONENT-MULTIPHASE LBM WITH HIGH DENSITY RATIO

Abstract

The original interaction potential LBM model for multi-component multiphase systems can only reach density ratios below 50. This severely restricts its application for many real gas-liquid two-phase flows. In this study, the effect of the interaction potentials in the two-component two-phase LBM simulation is analyzed. By using appropriate equations of state for each component and modified interaction between the two components, the improved model can reach density ratios over 1000 between two phases. This capability of reaching high density ratio is important for the simulation of many real two-component gas-liquid flow systems, such as air and water.

3.1. Introduction

Although the LBM has proved to be an effective approach to simulate a number of multiphase flow problems that are difficult for the traditional Navier-Stokes equation
based CFD techniques, its use in realistic engineering applications is severely restricted by some well-known weaknesses. One of such limitations is that the LBM algorithm tends to become numerically unstable when the density ratio between the two phases becomes large. The instability is mainly caused by the source terms in the LB equation, which is the force that needs to be applied at the interface between two phases. This force accounts for the phase segregation behavior in LBM as well as the interfacial tension, and its magnitude increases with the density ratio and surface tension. When the density ratio becomes large, this force becomes so large that it eventually destabilizes the computation. The discontinuity at the interface for various properties such as density and viscosity may also attribute to the instability problem, and a certain width of the interface must be maintained in simulation to allow a smooth transition of the properties from one phase to the other. Although different multiphase LBM models use very different techniques to represent the segregation between phases, they all suffer from the density ratio problem. For example, the color function model and the free energy model are often limited by density ratios less than 10, and the interaction potential model can reach a higher density ratio of 50. However, in real gas-liquid systems, the density ratio can be easily over 1000. Therefore, in order to accurately model the physical properties of real two-phase flow systems, it is necessary to develop new robust LBM models for high density ratio multiphase flows.

Several attempts have already been made to enhance the stability of LBM at high density ratios. Inamuro et al. (2004) simulated two-phase flows with large density differences by
solving the pressure Poisson equation with the free energy based LBM. They were able to obtain stable results at the density ratio of 1000. However, the solution of the pressure Poisson equation is a very time-consuming procedure that is often used in traditional CFD techniques for incompressible flows. The use of pressure Poisson equation in LBM causes the loss of thermodynamic meaning of the interface and the advantage in computation speed. Lee and Lin (2005) developed a pressure evolution equation and simulated two-phase flows at density ratio of 1000. In their model, the discretization of the collision step was different before and after the streaming step, which also added to the computation expense. Recently, it has been shown by Yuan and Schaefer (2006) that the formulation of the interaction potential in the pseudo-potential based LBM has important effects on the density ratio range in a single-component system. By employing the appropriate interaction potential, which is related to the equation of state of the fluid, they were able to reach density ratio of 1000, without the need for complicated discretization or solving the Poisson equation. However, their study is restricted to single component model and equilibrium conditions. To study many real two-phase flows, however, a multicomponent model for dynamic flow conditions is required.

3.2. Interaction potential model for multiphase flow

The interaction potential model, also known as the pseudo potential or Shan-Chen (SC) model, is widely used in LBM multiphase simulations due to its simplicity and versatility. The model is based on the fact that in real fluids the separation of phases is caused by
intermolecular interactions. In single phase BLM, the particle dynamics only includes inter-particle collision and free propagation in space, which describes the behavior of ideal gas molecules. In order to include other long-range interactions that cause the attractive or repulsive forces between particles, Shan and Chen (1993) proposed to add into LBM an interactive force term that is calculated from the interaction potential $\psi$.

For a single component fluid, this additional interaction modifies the equation of state (EOS) to a non-ideal gas EOS, which allows the fluid to separate into dense and dilute phases when the fluid is at subcritical condition. For a binary fluid mixture, the additional force also causes repulsion between the two components and controls the degree of immiscibility of the two phases.

### 3.2.1. Model for single component

In the single component model, the interaction force is given by

$$
\mathbf{F}(\mathbf{x}) = -\rho(\mathbf{x}) G \sum_{i} w_i \psi(\mathbf{x} + \mathbf{c}_i) \mathbf{c}_i
$$

(3.1)

where $\psi = \psi(\rho(\mathbf{x}))$ is the interaction potential that depends on the local fluid density. $w_i$ is the weight factor associated with lattice directions, as given in Equation 2.16 and 2.17. The negative scalar $G$ denotes the strength of the interaction. The summation is performed for all lattice directions ($i = 1 \cdots q$), and represents the pair-wise interaction between particles at location $\mathbf{x}$ and those at neighboring sites $\mathbf{x} + \mathbf{c}_i$. Mathematically, by expanding the terms $\psi(\mathbf{x} + \mathbf{c}_i)$ at $\mathbf{x}$, the interaction force can be shown to be

$$
\mathbf{F} = -c_i^2 G \nabla \psi + o(\Delta x^2)
$$

(3.2)
And on the macroscopic level (i.e., the N-S equation), this force can be combined with the pressure gradient term so that the modified pressure becomes

\[ p(\rho) = \rho c_i^2 + \frac{1}{2} G c_i^2 \psi(\rho) \]  

(3.3)

which is essentially a non-ideal equation of state for the fluid.

Shan and Chen suggested the form of the interaction potential to be

\[ \psi(\rho) = 1 - \exp(-\rho) \]  

(3.4)

It can be shown that with this potential, the \( p - \rho \) relation becomes subcritical when the interaction strength falls below the critical value of -4, and consequently two stable phases with different densities can co-exist. With the help of Equation 3.3, other types of EOS can also be easily implemented.

The interaction force is included in the LBE by shifting the velocity used in the calculation of equilibrium distribution

\[ f_i^{eq} = f_i^{eq}(\rho, v) \]  

(3.5)

\[ \bar{u} = \frac{1}{\rho} \sum_i c_i f_i \]  

(3.6)

\[ \dot{v} = \bar{u} + \frac{\tau}{\rho} F \]  

(3.7)

The macroscopic fluid velocity is calculated from the average momentum before and after the force is applied:
\[ u = \tilde{u} + \frac{1}{2\rho} F \]  

(3.8)

### 3.2.2. Model for binary mixture

The interaction potential model can also be applied to simulate a binary mixture (Shan and Chen, 1993). In this case, each component \( \sigma \) (\( \sigma = 1 \ or \ 2 \)) has its own distribution functions \( f_i^\sigma \) that are governed by their own evolution equations:

\[ f_i^\sigma (x + c_i, t+1) - f_i^\sigma (x, t) = -\frac{1}{\epsilon^\sigma} \left[ \left( f_i^\sigma (x, t) - f_i^{\sigma (eq)} (\rho_\sigma, v_\sigma) \right) \right] \]  

(3.9)

As in the case of single component interaction potential model, the equilibrium velocity is shifted by the interacting force \( F_\sigma \), which accounts for the interactions among particles of the same component (self interaction) as well as the interactions between the two components (cross interaction). The interaction force is again calculated from the interaction potential \( \psi_\sigma (x) \).

\[ F_\sigma = -\psi_\sigma (x) \sum_\sigma G_{\sigma \sigma} \sum_i w_i \psi_\sigma (x + c_i) c_i \quad (\sigma, \bar{\sigma} = 1 \ or \ 2) \]  

(3.10)

For example, the force acting on component 1 is made up of two parts:

\[ -G_11 \psi_1 (x) \sum_i w_i \psi_1 (x + c_i) c_i \]  

for self interaction among particles in component 1, and

\[ -G_12 \psi_1 (x) \sum_i w_i \psi_2 (x + c_i) c_i \]  

for cross interactions between components 1 and 2.

In the multicomponent model proposed by Martys and Chen (1996), the force is again added by shifting the equilibrium velocity:

\[ v_\sigma = \tilde{u} + \frac{\tau_\sigma}{\rho_\sigma} F_\sigma \]  

(3.11)
where the intermediate velocity $\tilde{u}$ is calculated by

$$
\tilde{u} = \frac{\sum_{\sigma=1}^{2} \frac{1}{\tau_\sigma} \sum_{i=1}^{q} c_{i,\rho} \rho}{\rho}
$$  \hfill (3.12)

Finally, the macroscopic densities and velocity are calculated from the distribution functions

$$
\rho_\sigma = \sum_i f_i^\rho
$$  \hfill (3.14)

$$
\rho = \rho_1 + \rho_2
$$  \hfill (3.15)

$$
u = \frac{1}{\rho} \sum_\sigma \left[ \sum_i c_{i,\rho} \rho + \frac{1}{2} F_\sigma \right]
$$  \hfill (3.16)

In the following simulation for binary mixtures for gas-liquid systems, component 1 is set to be a non-ideal fluid, while component 2 is assumed to be ideal gas so that $G_{22}=0$.

### 3.3. High density ratio in single component model

In thermodynamics, the density of the two co-existent phases of a non-ideal gas at a certain subcritical temperature can be found by applying the Maxwell equal area construction technique to its equation of state:

$$
\int_{v_x}^{v_1} (p - p_o) dv = -\int_{\rho_x}^{\rho_1} \frac{1}{\rho^2} (p - p_o) \frac{1}{\rho^2} d\rho = 0
$$  \hfill (3.17)

which requires that the two shaded regions under the $p - \nu$ curve shown in Figure 3.1 are equal in size. Therefore, once the EOS is known, the densities of the two phases are determined. In the interaction potential model for a non-ideal fluid, the densities of two
phases in equilibrium can be found from the balance of the pressure tensor, as described by Shan (2008). The results indicate that the densities of the co-existing phases in a fluid whose EOS follows Equation 3.3 are determined by

\[
\int_{\rho_0}^{\rho} [p(\rho) - p_0] \frac{\psi'}{\psi^{1+\epsilon}} d\rho = 0
\]  

(3.18)

where \( \epsilon \) is a constant which depends on the lattice. The Equations 3.17 and 3.18 have slightly different forms. However, studies indicate that the difference of the densities predicted by these two equations is very small (Yuan and Schaefer, 2006).

Yuan and Schaefer (2006) compared several types of EOS, and found that EOS has important effect on the density ratio that the interaction model is able to achieve. Particularly, they demonstrated that under the equilibrium condition, the Peng-Robinson (P-R) and Carnahan-Starling (C-S) EOS are stable when the density ration is over 1000. Closer examination of the parameters used in their EOS shows that those parameters made the fluid much more compressible than the original model, and the enhanced stability is in fact the result of the reduced sound speed. The effect of sound speed on the numerical stability of multiphase LBM is also discussed by Wagner and Pooley (2007) in a similar situation for deeply quenched liquid-gas systems.

To test the effect of EOS on density ratio, a 2-D simulation is performed for the equilibrium condition of a non-ideal fluid with C-S EOS, which is given by

\[
p(\rho) = \rho RT \left( \frac{1 + b\rho/4 + (b\rho/4)^2 - (b\rho/4)^3}{(1 - b\rho/4)^3} - a\rho^2 \right) 
\]  

(3.19)
where the constants used in the simulation are: a=1, b=4, R=1. The C-S EOS is plotted in Figure 3.1, together with the ideal gas EOS in LBM. The combination of LBM EOS (Equation 3.3) and C-S EOS (Equation 3.19) gives the form of the interaction potential

$$
\psi(\rho) = \sqrt{\frac{2(\rho(\rho) - \rho c_s^2)}{c_s^2 G}} \quad (3.20)
$$

The two phases are the initially distributed in a periodic computation domain with a 50*200 mesh and are separated by flat interfaces. The simulation runs for a sufficiently long period of time until the fluid velocity falls below O(10^{-16}), at which point it is assumed that equilibrium has been reached. Table 3.1 lists the equilibrium densities and pressures at different reduced temperatures (\(T/T_c\)). When \(T/T_c = 0.58\), the density ratio of 2249.76 is obtained, which is considered to be sufficiently large for practical gas-liquid systems.

### 3.4. High density ratio in multicomponent model

In order to simulate two-component gas-liquid flow systems such as water-air, it is required that the model can lead to two stable phases, with liquid phase mainly made up of the non-ideal component, and the gas phase that contains reasonable amount of the ideal component. And the non-ideal and ideal component will preferably stay in the liquid and gas phase, respectively. These requirements can be realized by employing appropriate interactions between the two components.
As mentioned before in Equation 3.10, in the original pseudo-potential LBM model, the same potential function was used to account for both the interactions between same type of molecules, and interactions between molecules of different components. Once the potential functions are determined by the equations of state of each individual component, the strength of the cross interaction could only be adjusted by changing the value of $G_{12}$. In practice, in order to achieve high density ratio between the liquid and gas phase, a high-density-ratio EOS such as the C-S EOS needs to be used for the non-ideal component. Then it is found that with zero or positive $G_{12}$, the mutual diffusivity is often very small so that it is difficult to reach equilibrium even after long time of simulation. On the other hand, negative $G_{12}$, which results in an attractive force between the two components, would make the ideal component preferably stay in the liquid phase, which is also not desired.

Shan and Doolen (1995) mentioned that both attraction between the same species and repulsion between different species decreases the mutual diffusivity. Since at high density ratios the attractive force in C-S EOS is very strong, it might be the reason for the low diffusivity problem.

In order to solve this problem, the inter-species interaction force needs to be attractive in the gas phase to enhance the diffusivity, and slightly repulsive in the liquid phase to keep the two components separated. It is realized that the form of the inter-component
interaction potential \( \varphi_1, \varphi_2 \) can be different from that for the same component \( \psi_1, \psi_2 \), and the interaction potential between two components can be devised as follows:

\[
\varphi_1(\rho_2(x)) = 1 - \exp(-\rho_2 / \rho_20) \tag{3.21}
\]

\[
\varphi_2(\rho_1(x)) = a_0 - \exp(-\rho_1 / \rho_{10}) \tag{3.22}
\]

where \( 0 < a_0 < 1 \), \( \rho_{10}, \rho_{20} \) are parameters depending on the simulation condition (mainly \( T/T_c \)). In practice, the parameters \( a_0, \rho_{10}, \rho_{20} \) often have a small value. For example, the values \( a_0=0.005; \rho_{10}=-0.0008/\log(a_0); \rho_{20}=0.0003 \) are used in the current study.

This interaction potential has following properties:

1) Attractive for \( 0 < \rho_1 < -\rho_{10} \ln a_0 \), repulsive for \( \rho_1 > -\rho_{10} \ln a_0 \). Therefore, the value of \( a_0, \rho_{10} \) should be chosen such that \( -\rho_{10} \ln a_0 \) is between the gas density and the liquid density.

2) As the densities increase, the potential approaches a finite value \( a_0 \). Therefore, to maintain a slightly repulsive interactive force in the dense phase, \( a_0 \) should be chosen as a small number between 0 and 1.

3) The potential is mainly affected by \( \rho_1 \), since it varies in a much larger range across the interface than \( \rho_2 \).

The new total interaction force is

\[
F^\sigma = -\psi^\sigma G^\sigma \sum_i T_i \psi^\sigma(x + e_i) c_i - \varphi^\sigma G^\sigma \sum_i T_i \varphi^\sigma(x + e_i) c_i \tag{3.23}
\]
Or explicitly:

\[
\mathbf{F}^1(x) = -G_{11} \sum_i T_i \psi_1(x) \psi_1(x + \mathbf{e}_i) \mathbf{e}_i - G_{12} \sum_i T_i \varphi_1(x) \varphi_2(x + \mathbf{e}_i) \mathbf{e}_i
\]

\[
\mathbf{F}^2(x) = -G_{22} \sum_i T_i \psi_2(x) \psi_2(x + \mathbf{e}_i) \mathbf{e}_i - G_{12} \sum_i T_i \varphi_2(x) \varphi_1(x + \mathbf{e}_i) \mathbf{e}_i
\]

(3.24)

It can be proved that the interaction force conserves mass for each component. The momentum is not conserved for each component, and the total momentum is not conserved locally. But the total momentum of two components in the entire computation domain is conserved.

3.5. Discussion

A typical result obtained using original pseudo-potential model with \( G_{12} = 0 \) is shown in Figure 3.2. The C-S EOS is used for component 1, while the ideal EOS is specified for component 2. After \( 10^5 \) time steps, the liquid phase is almost uniform and mainly consists of component 1 (non-ideal), with negligible amount of component 2 (ideal). In contrast, the density profiles of the two components in the gas phase show alternating patterns. The non-uniform distributions indicate that the two components in the gas phase cannot reach equilibrium even after a long period of simulation time. Physically, the two components in the gas phase should be miscible. The simulated slow mutual diffusion of the two components in gas phase is against physical reality and the consequently the model needs to be modified.
Using the modified interaction potential in Equation 3.2-3.3, simulation is carried out under the same conditions as in Figure 3.2. The result is shown in Figure 3.3. No alternating pattern is found in the distribution of component 2 from Figure 3.3(a). The density profiles in Figure 3.3(b) further prove that the densities of the two components in gas phase are both uniform. Evidently, the newly designed cross-interaction potential outperforms the original model in reaching equilibrium in the gas phase.

In order to test the model’s ability to reach high density ratio, the simulation is also run at different temperatures. The results are summarized in Table 3.2. As the reduced temperature $T/T_c$ drops from 0.7 to 0.58, the density ratio between the liquid phase and the gas phase increases from 18.75 to 1239.37. The density profiles, pressure profile, and the velocity profile for at $T/T_c=0.58$ are shown in Figure 3.4. The liquid phase is mainly occupied by component 1, while the gas phase is mostly made up of component 2. It is clear from Figure 3.4(a) that the densities in the liquid phase and in the gas phase differ by three orders of magnitude. The pressures inside the bulk gas phase and bulk liquid phase are identical, which is consistent with the equilibrium condition. The change of the pressure at the interface is caused by neglecting the stress due to density gradient. In the velocity profile, the maximum velocity is found to be on the order of $10^{-11}$, which means that there is negligibly small flow velocity when equilibrium is reached.

The new interaction potential’s capability to simulate curved interfaces is tested by simulating the equilibrium of a droplet with surrounding gas in a 2D domain with
100*100 grids. Periodic conditions are used for all boundaries. The two components with uniform distributions are placed in the domain initially, with small disturbance of the densities. The mixture then automatically goes through a phase separation process and finally evolves into two distinct phases. With proper initial densities, a circular bubble/droplet will form at the final state. A typical result is shown in Figure 3.5. The density ratio between the droplet and the surrounding gas in this case is 1360. Both phases are uniform. The circular shape of droplet indicates the isotropic property of the model. The difference in pressure inside and outside the droplet is caused by the Laplace pressure due to the surface tension.

Finally, to show the model’s performance under flow conditions, a droplet falling into a liquid pool was simulated. The liquid droplet has a density of 0.42, while the gas density is 0.0004. The initial distributions are allowed to equilibrate for 100000 steps in order to reach stable densities. Then the droplet is released with a downward initial velocity of 0.1. The Reynolds number and Weber number in this case are:

\[
Re = \frac{ud}{\nu} = 13.2 
\]  
(3.25)

\[
We = \frac{\rho_i u^2 d}{\sigma} = 4.17 
\]  
(3.26)

The initial densities of each species as well as the time sequence for the total density field are shown in Figure 3.6. Due to the small Reynolds and Weber numbers, the droplet only makes a dimple after its collision with the free surface, without splashing. The free surface oscillates a few times and then goes back to flat surface at a level higher than the
initial state. The density field keeps a sharp interface throughout the simulation, showing the stability of the algorithm for dynamic flow conditions.

3.6. Conclusions

A new potential function is designed for multi-component interaction potential LBM model. It significantly improves the numerical stability of the interaction potential model at high density ratios, and successfully raises the stable density ratio between the two phases from below 50 to over 1000. In the new model, the self-interaction in the non-ideal component is based on the Carnahan-Starling equation of state, which has been proven to reach high density ratios in the single component model. For the cross-interaction between the two components, separate potential functions are designed to introduce a small attraction in the gas phase to ensure proper distribution of the two component at equilibrium. The new model is tested under equilibrium conditions with flat and curved interfaces, and stable density ratios of over 1000 are achieved. The model is also able to maintain a stable sharp interface even when the interface is under motion or deformation. The newly developed model is expected to extend the application of LBM to many realistic gas-liquid flows that often has high density ratios.
Table 3.1 Equilibrium properties of C-S EOS (a=1, b=4, R=1)

<table>
<thead>
<tr>
<th>T/Tc</th>
<th>rhoL</th>
<th>rhoG</th>
<th>pressure</th>
<th>Density ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.8</td>
<td>0.30642</td>
<td>0.01855</td>
<td>0.001165</td>
<td>16.51</td>
</tr>
<tr>
<td>0.7</td>
<td>0.35754</td>
<td>0.004585</td>
<td>0.00034</td>
<td>77.99</td>
</tr>
<tr>
<td>0.6</td>
<td>0.40595</td>
<td>0.000457</td>
<td>2.57E-05</td>
<td>889.07</td>
</tr>
<tr>
<td>0.58</td>
<td>0.41553</td>
<td>0.000185</td>
<td>1.01E-05</td>
<td>2249.76</td>
</tr>
</tbody>
</table>

Table 3.2 Equilibrium properties of binary mixture

<table>
<thead>
<tr>
<th>T/Tc</th>
<th>rho1g</th>
<th>rho2g</th>
<th>rho1l</th>
<th>rho2l</th>
<th>rhoG</th>
<th>rhoL</th>
<th>Pressure</th>
<th>rho1 / rhoG</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.7</td>
<td>0.005766</td>
<td>0.01351</td>
<td>0.36127</td>
<td>0.00017</td>
<td>0.01927</td>
<td>0.3614</td>
<td>0.00179</td>
<td>18.75</td>
</tr>
<tr>
<td>0.65</td>
<td>0.000856</td>
<td>0.00117</td>
<td>0.38208</td>
<td>1.80E-06</td>
<td>0.00202</td>
<td>0.3821</td>
<td>0.00021</td>
<td>188.90</td>
</tr>
<tr>
<td>0.6</td>
<td>0.000273</td>
<td>0.00087</td>
<td>0.4061</td>
<td>6.68E-07</td>
<td>0.00114</td>
<td>0.4061</td>
<td>0.00014</td>
<td>355.98</td>
</tr>
<tr>
<td>0.58</td>
<td>0.000108</td>
<td>0.00023</td>
<td>0.41556</td>
<td>4.58E-08</td>
<td>0.00034</td>
<td>0.4156</td>
<td>3.28E-05</td>
<td>1239.37</td>
</tr>
</tbody>
</table>

Figure 3.1 Comparison of ideal EOS ($c_i^2 = 1/3$) and C-S EOS (a=1, b=4, R=1)
Figure 3.2 Binary mixture with flat interface after $10^5$ steps.
(component 1 C-S EOS, $a=0.09926$; $b=0.18727$; $R=0.20$; $\tau=1.0$, $T/T_c=0.65$, $G_{12}=0$)

(a) Density profile in y direction
(b) Enlarged density profile of each component in gas phase.
(c) Density distribution of component 2 in 2D

Figure 3.3 Binary mixture with flat interface using modified model under the same condition as in Figure 3.2

(a) Density of component 2
(b) Enlarged density profile of each component in gas phase.
Figure 3.4 Flat interface, T/Tc=0.58, (case 4 in Table 3.2)
(a) Density of each component
(b) Density of the mixture
(c) Pressure
(d) Velocity
Figure 3.5 Equilibrium distributions in a binary mixture
(a) Distribution of component 1
(b) Distribution of component 2
(c) $\rho_1$ and $\rho_2$ profile across the center of the droplet
(d) Pressure profile across the center of the droplet
Figure 3.6 Droplet falling into a liquid pool
(a) Initial densities of the two components
(b) Time evolution of the total density field.
CHAPTER 4

ADAPTIVE MESH REFINEMENT FOR TWO-PHASE LBM

Abstract

The lattice Boltzmann method (LBM) for two-phase flow simulation is often hindered by insufficient resolution at the interface. As a result, the LBM simulation of bubbles in bubbling flows is commonly limited to spherical or slightly deformed bubble shapes. In this chapter, the adaptive mesh refinement (AMR) method for the LBM is developed to overcome such a problem. The approach for this new method is based on the improved interaction potential model, which is able to maintain grid-independent fluid properties in the two fluid phases and at the interface. The LBM-AMR algorithm is described, especially concerning the LBM operation on a non-uniform mesh and the improved interaction potential model. Numerical simulations have been performed to validate the method in both single phase and multiphase flows. Integration of LBM with AMR can significantly improve the accuracy and reduce the computation cost. The method developed in this chapter may appreciably enhance the capability of LBM in the simulation of multiphase flows with complex deformation of the interface.
4.1. Introduction

In direct simulation of two-phase flows, the essential problem is the accurate representation of the interface between two phases. On one hand, in all numerical methods in which the flow field is solved on a fixed Eulerian mesh (VOF, Level-Set, Front tracking, LBM, etc.), the interface is numerically diffused and usually requires a minimum spatial resolution which spans typically to a thickness of 3~5 grid spacing. On the other hand, the size of a well-defined bubble or droplet in the simulation must be much larger than the width of the interface. Taking the buoyant rise of a single bubble in a quiescent liquid as an example, the simulated bubble size must be significantly larger than the interface thickness so that the region inside the bubble can have well-defined physical properties. For bubbles with small deformation, at least 16 grid points across the diameter are usually required to faithfully represent the bubble. This minimum grid number increases when the bubble undergoes larger deformation, for example, in higher Reynolds number flows. In addition, the simulation domain needs to be significantly larger than the bubble size in order to avoid unwanted boundary effects, and the computation time and memory usage increase rapidly with the increasing mesh resolution and domain size. Therefore, it would require enormous computation resource in order to satisfy the resolution requirement for all three scales: the interface, the bubble/droplet, and the entire domain. However, under current computation capability, this resolution requirement often has to be compromised. As the result, most simulations to date consider only small bubbles with spherical or ellipsoidal shapes, while simulations for large spherical cap and skirted bubbles that frequently appear in engineering applications
are scarcely reported. Moreover, in numerical studies which explore the bubble interactions, the number of bubbles that can be put into the simulation domain is also restricted due to the computation power. Consequently, there is a demand for a simulation technique that can simultaneously achieve sufficient mesh resolution near the bubble surface, while maintaining the total computation cost under control.

Adaptive Mesh Refinement (AMR) technique is a natural candidate to meet such requirement in both resolution and computation cost. Using AMR technique, the mesh resolution varies in the computation domain. Fine mesh resolution is used near the bubble surface to ensure the accuracy, while coarse mesh is applied in the bulk fluid faraway from the interface to reduce computation cost. The mesh resolution is updated dynamically during the simulation in accordance with the motion of the interfaces. There have been a few studies that integrate AMR into incompressible fluid-phase flow models based on N-S equation. Ginzburg and Wittum (2001) performed 2D simulation of bubbles using VOF approach with AMR. The mesh near the interface is further split, and unstructured mesh that is aligned with the interface is used to solve the VOF equation, while the flow equations are solved on a separate regular mesh. The level-set technique has been coupled with AMR by Sussman et al. (1999) and Olsson et al. (2007). Two and three-dimensional simulations were performed in example problems involving droplets and bubbles. Recently, Hua et al (2008) combined the front-tracking method with AMR and successfully simulated a wide range of bubble regimes which compare well with
well-known experimental results. In particular, large deformation of the bubble surface in spherical cap regime and skirted regime can be accurately reproduced.

In LBM, although the original algorithm is closely coupled with a uniform mesh, some recent research has been conducted to extend the method to non-uniform grids, mainly for the modeling of single phase flows. In those works, the computation domain consists of multiple blocks with variable grid sizes, but within each block the mesh remains uniform and structured. Communication between blocks with different grid size depends on the exact location of the particle distributions. If the distributions reside on the grid nodes, usually a special interpolation procedure will be necessary to rescale the non-equilibrium part of the distribution (Filippova and Hanel, 1998; Dupuis and Chopard, 2003; Yu, et al., 2002; Peng et al, 2006). If a volumetric formulation is used and the distributions are located at cell center, however, no such rescaling is required (Rohde, et al, 2006; Chen, et al, 2006; Fares, 2006). In such simulations, fine mesh is often applied near the irregular solid boundary to enhance the accuracy of the boundary condition, or near the high-vorticity region to resolve the complex flow field. Since they do not involve moving objects, the mesh resolution is specified in the beginning of the simulation, without being dynamically updated. Despite the promising results obtained for single phase flows, there is no straightforward extension of the non-uniform grid LBM algorithm to two-phase flow problems. There seems to be only one publication concerning the multiphase LBM-AMR (Tolke, et al, 2006). In that study, the interface algorithm was based on the color function model, and therefore was similar to the
interface capturing methods. Only a single condition of bubble rising was demonstrated in the result, without experiment comparison for broader regimes.

In this study, a new LBM-AMR approach is developed for the gas-liquid flows. The two-phase LBM is based on the interaction potential model developed by Shan and Chen (1993). Due to its diffuse-interface nature, the properties across the interface are determined by the thermodynamics. Therefore, it is essential to have consistent fluid properties on different sized grids, which is different from the LBM-AMR with sharp interface model developed by Tolke et al. (2006). The LBM algorithm on a non-uniform grid for single phase flows will be introduced first. Then the relationship between interface properties in the interaction potential model and the grid size is discussed, followed by the adaptive mesh refinement algorithm for two-phase LBM. Finally, numerical results for the buoyant rise of bubbles in a viscous liquid will be compared with experimental results to prove the validity of the newly developed method.

4.2. Single phase LBM with non-uniform mesh

When applying different mesh resolutions inside the computation domain, it is crucial to determine which variables change with the mesh size and which variables are independent of the grid. In LBM, in order to achieve the same lattice speed of sound

\[ c_s = \frac{1}{\sqrt{3}} \frac{\Delta x}{\Delta t} \]

across the entire domain, the time step needs to be proportional to the mesh size. Following the convention of LBM, both space and time are non-dimensionalized in
such a way that $\Delta \hat{t} = \Delta \hat{t} = 1$, so the non-dimensional lattice speed of sound is kept to be

$$\hat{c}_s = \frac{1}{\sqrt{3}}$$

throughout the entire domain.

The fact that the time step $\Delta t$ scales with $\Delta x$ has two important consequences. Firstly, according to Equation (2.20), to keep the fluid kinematic viscosity $\nu$ independent of grid size, the relaxation factor $\tau$ also has to be adjusted with $\Delta x$ and must be calculated from Equation (2.20). Explicitly, this requires

$$\tau_f - \frac{1}{2} = \left( \tau_c - \frac{1}{2} \right) \frac{\Delta x_c}{\Delta x_f}$$

(4.1)

Secondly, the LBM algorithm performs more steps on the fine mesh since it requires a smaller $\Delta t$ than on the coarse mesh. Therefore, interpolation/average operations need to be performed at the coarse/fine resolution interface in both space and time.

The LBM-AMR approach developed here is based on the multi-block structured grid. The entire computation domain is divided into a number of blocks that have identical grid structure but may have different grid sizes. The blocks are categorized into different refinement levels, and grid resolutions in each two consecutive levels differ by a factor of 2. In order to have a smooth transition of the grid size, at most one refinement level difference is allowed at the boundary between two neighboring blocks. Inside each block, uniform structured grid is used as in the traditional LBM simulation. In this way, the original LBM algorithm can be applied within each individual block without any modification, therefore the simplicity and efficiency of LBM algorithm is maintained in
the computation inside each block. In this study, the classical D2Q9 lattice is employed for the 2D computations, and the D3Q19 lattice is used for the 3D simulations.

When a refinement level jump is present between two neighboring blocks, a special algorithm is devised to communicate information across block boundaries. Similar to the volumetric formulation of Rohde et al. (2006), the particle distributions in the current method are located at the center of each computational cell, so that rescaling of the non-equilibrium part of the distribution at coarse/fine grid interface is not necessary. The inter-block communication process is shown schematically in Figure 4.1. The computational cells at the boundary between the coarse and fine grid are referred to as the “interface” cells, as shown in the shaded zones in Figure 4.1. They act as the transition layer between two blocks, and alternate between coarse and fine levels during a computation step through splitting and merging. Two specially designed operations take place in these interface cells, and they are named “explosion” and “coalescence” after the terminology used by Chen et al. (2006). In the 2D example illustrated in Figure 4.1, a coarse interface cell is uniformly divided into four smaller cells during the explosion step (step 2-3 in Figure 4.1), and its particle population is either evenly distributed or linearly interpolated in these new cells. In the coalescence step (step 6-7 in Figure 4.1), the four fine interface cells again merge into a single coarse level cell, whose particle population is the summation of those in the four fine cells.
The original “collision-propagation” algorithm is now complicated by the additional “explosion” and “coalescence” operations. The flowchart of the computation procedure on a mesh with two refinement levels is shown in Figure 4.2. As noted previously, the computation on coarse level uses $dt$ as its time step, while the fine grid has the time step of $0.5dt$. Therefore, the “collision-propagation” operations happen twice on the fine level in each $dt$, but only once on the coarse level. The “explosion” and “coalescence” steps each operates once during $dt$. The “explosion” takes place after the first collision step at $0.5dt$, which transfers the information from coarse level to the fine level. And the “coalescence” happens at the end of the time step so as to pass the information back from the fine level to the coarse level.

The change of particle distributions in each sub-step is illustrated graphically in Figure 4.1, in which only one pair of opposing lattice velocities are shown for clarity. The first collision step operates on both fine and coarse levels as in ordinary LBM, but with different relaxation parameters. The interface cells, which are originally on the coarse level, are then divided into 4 fine cells in the “explosion” step. The distribution functions $f_i$ can be either uniformly distributed or interpolated linearly in the new fine cells.

Propagation step then occurs on both coarse and fine level, including the interface cells. Up to this point, the coarse level has completed a time step $dt$, while the fine level only completes a half $dt$. Therefore, the second collision and propagation process only occurs on the fine level, and distribution functions only change on the fine and interface cells while the information on the coarse level is unaffected. Finally, the four fine interface
cells again merged into a coarse level cell, and the distribution functions in the new
coarse interface cell is just the sum of those in the four fine cells. This finishes the entire
computation loop and both levels come back to the pre-collision status before step 1.

The generation and refinement of the mesh are performed with the open-source code
PARAMESH (MacNeice, et al, 2000), which use a tree data structure to manage the
hierarchy of block-structured grid with different refinement levels. It has been integrated
with the non-uniform grid LBM algorithm described above.

The above LBM algorithm for non-uniform mesh is validated by simulating two simple
flow conditions: the Couette flow driven by shear force and the Poiseuille flow driven by
pressure gradient. Both cases use two levels of grid refinement, as shown in Figure 4.3 (a)
and (c). For the simple shear flow, the fine grids are applied in the lower half of the
domain near the stationary wall, and in the pressure driven flow the fine grids are applied
near both top and bottom walls. Periodic conditions are used in the horizontal direction,
and bounce-back conditions are used at the wall boundaries. The velocity profiles are
shown in Figure 4.3 (b) and (d). The simulated profiles are in good agreement with the
analytical results. Especially, both the velocity and the stress are continuous at the
interface between coarse and fine grids. In addition to the conditions where the
coarse/fine grid interface is parallel to the flow direction, Figures 4.3(e) and (f) present
the Poiseuille flow simulation with grid interface perpendicular to the flow direction. In
this simulation, 80*80 grid is used in the region 0<x<40, while 40*40 resolution is
applied in the region $40 < x < 80$. Velocity profiles across the channel extracted at $x=10$ for the fine resolution region and $x=60$ for the coarse grid region are compared against the analytical curve. The two numerically obtained profiles are both in good agreement with the analytical profile. While the coarse grid give the maximum velocity $u_m=0.001965$ at $y=20$, the fine grid results in $u_m=0.00199$. Since the theoretical maximum velocity is 0.002, numerical errors with both the coarse and fine grids are within 2%. The result obtained with the fine grid is closer to the theoretical value, due to the fact that the current LBM algorithm with link bounce-back boundary condition has second order spatial accuracy.

4.3. Two-phase interaction potential model with non-uniform mesh

4.3.1. Equilibrium and surface properties in interaction potential model

The interaction potential model developed by Shan and Chen (1993) is employed for the two-phase flow simulation in this study. In this model the interaction forces between fluid molecules are accounted for base upon the inter-molecular interactions. In a single component fluid, the interaction forces convert the original ideal gas equation of state (EOS) in LBM into a non-ideal EOS, and therefore phase separation takes place spontaneously when the temperature falls below the critical temperature of the fluid. In a
binary fluid mixture, both intra-species and inter-species interactions are incorporated into the model, which result in different distributions of the two components in two immiscible phases. For simplicity, only the single component interaction model will be discussed in this section in order to illustrate how the interaction model can be integrated with the AMR algorithm.

As previously described in Chapter 3, the Shan-Chen model defines an interaction potential as a function of the local density of the fluid.

\[ \psi = \psi(\rho(x)) \]  

(4.2)

The interaction force on the fluid at grid location \( x \) is the sum of its pair-wise interactions with the nearest neighbors in each lattice direction:

\[ \mathbf{F} = -G\psi \sum_i w_i \psi(x + \mathbf{e}_i) \mathbf{e}_i / \Delta x \]  

(4.3)

Mathematically, the following equation can be obtained by expanding Equation 4.3 to the 2\(^{nd}\) order:

\[ \mathbf{F} = -\nabla \left( \frac{1}{2} c_s^2 G \psi^2 \right) - \frac{1}{2} \Delta x^2 c_s^2 G \psi \nabla^2 \psi + o(\Delta x^3) \]  

(4.4)

The first term can be absorbed into the pressure term in the momentum equation and it results in a non-ideal EOS with the following expression:

\[ p = \rho c_s^2 + \frac{1}{2} c_s^2 G \psi^2(\rho) \]  

(4.5)

The second term in Equation (4.4) represents the interface stresses corresponding to the gradient free energy, which has been used in both LBM and other types of diffuse
interface models (Jacqmin, 1999; He and Doolen, 2002). It is responsible for the structure of the interface as well as the surface tension. It should be noted that this force has a dependency of $\Delta x^2$, and is therefore dependent on the mesh resolution.

In thermodynamic theory, the EOS determines the bulk property of the fluid phase, and the equilibrium densities at a particular temperature can be located using techniques such as Maxwell construction (Rowlinson and Widom, 1982). The interface structure can be found by applying the mechanical equilibrium condition on the stress tensor across the interface, and the surface tension can be calculated from the stress profile

$$\sigma = \int_{-\infty}^{\infty} (P_{zz} - P_{xx}) dz$$ (4.6)

In the above equation, the interface is assumed to lie in the x-y plane, and $P_{zz}$ and $P_{xx}$ are the stresses normal and parallel to the interface, respectively.

Due to the discrete lattice effects, the pressure tensor in LBM is slightly different from its counterpart in the macroscopic thermodynamics. The analytical solution of the interface structure and the value of surface tension in the interaction potential model have been reported recently by Shan (2008):

$$\left( \frac{d\rho}{dz} \right)^2 = \frac{8(1-\varepsilon)\psi^e}{3Gc_s^4(\psi^e)^2\Delta x^2} \int_{\rho_s}(p(\rho) - \rho c_s^2 + \frac{1}{2}Gc_s^2\psi^e) \frac{\psi'}{\psi_1+\varepsilon} d\rho$$ (4.7)

$$\sigma = -\frac{3Gc_s^4\varepsilon \Delta x^2}{2} \int_{-\infty}^{+\infty} \left( \frac{d\psi}{dz} \right)^2 dz$$ (4.8)
where \( c \) and \( e_4 \) are constants depending on the lattice. With further analysis, it can be shown that in the original interaction potential model, both the interface width and the surface tension are proportional to the grid spacing \( \Delta x \). Therefore, in order to have a consistent surface tension value, an additional term is necessary to compensate for the grid effect. In this study, the following additional term is introduced with a variable coefficient \( k \), which is a function of grid size \( \Delta x \).

\[
F' = k \psi \nabla^2 \psi
\]  

Equation (4.9)

The above equation can be implemented using the pair-wise interaction between lattice sites in a similar way to the original Shan-Chen model:

\[
F'(x) = k \psi(x) \sum_y \lambda_{xy} \psi(y) r_{xy} / \Delta x^3,
\]  

Equation (4.10)

where \( r_{xy} \) is the vector pointing from \( x \) to \( y \), and \( \lambda_{xy} \) is the coefficient depending on \( r_{xy} \). However, since the numerical evaluation of Equation (4.9) requires a higher order difference operator for the interaction potential \( \psi \), the summation in Equation (4.10) needs to involve a larger set of lattice sites in addition to the nearest neighbors. There is a certain degree of freedom in choosing the set of the lattice sites and coefficients, and one example used in the 2D simulations in this study takes the form

\[
F'_{x,ij} = \frac{k \psi_{i,j}}{\Delta x^3} \left[ -\frac{5}{6} (\psi_{i+1,j} - \psi_{i-1,j}) + \frac{1}{6} (\psi_{i+2,j} - \psi_{i-2,j}) 
\right.
\]

\[
\left. -\frac{1}{9} (\psi_{i+1,j+1} + \psi_{i+1,j-1} - \psi_{i-1,j+1} - \psi_{i-1,j-1}) + \frac{5}{36} (\psi_{i+2,j+1} + \psi_{i+2,j-1} - \psi_{i-2,j+1} - \psi_{i-2,j-1}) 
\right.
\]

\[
\left. + \frac{1}{36} (\psi_{i+1,j+2} + \psi_{i+1,j-2} - \psi_{i-1,j+2} - \psi_{i-1,j-2}) + \frac{1}{36} (\psi_{i+2,j+2} + \psi_{i+2,j-2} - \psi_{i-2,j+2} - \psi_{i-2,j-2}) \right]
\]
It can be seen from Equation (4.11) that the force exerted on fluid particles at location $x$ due to their interaction with the fluid particles at $y$ can be written as

$$k \lambda_{xy} \psi(x) \psi(y) r_{xy} / \Delta x^3,$$

which has the same magnitude but opposite direction with the force on location $y$ exerted by the particles at $x$. Therefore, the total momentum of the entire domain is exactly conserved, which has been confirmed by the numerical simulations in this study.

As a result, the total interaction force is now

$$F = F^0 + F^s = -\nabla \left( \frac{1}{2} c_s^2 G \psi^2 \right) + \left( k - \frac{1}{2} \Delta x^2 c_s^2 G \right) \psi \nabla \nabla^2 \psi$$

(4.12)

By using different value of $k$ on different sized grids, the sum $k_0 = k - \frac{1}{2} \Delta x^2 c_s^2 G$ can be kept constant, and therefore a constant surface tension force can be achieved. In addition, compared to the original Shan-Chen model with only one parameter $G$, another parameter $k$ is introduced, and therefore the surface tension can be tuned independent of the EOS, while bulk fluid properties at equilibrium are determined by $G$ only. This is in fact similar to the concept of tuning the surface tension with two-parameter multi-range pseudo-potential (Sbragaglia, et al, 2007).
Equation (4.7) can be used to obtain the theoretical density profile across a flat interface at equilibrium. With the condition that the density gradient vanishes in both bulk phases, and that the equilibrium pressure is identical in both phases, Equation (4.7) can be integrated numerically to find $\rho(z)$. Once the density profile is obtained, it can be used in Equation (4.8) to find the theoretical value of the surface tension.

### 4.3.2. Forcing scheme

There are various ways to incorporate the interaction force into the LBM model. In the original Shan-Chen model, the force is incorporated by shifting the equilibrium velocity in the collision step.

$$\mathbf{u}^{\text{eq}} = \mathbf{v} + \frac{\tau \Delta t \mathbf{F}}{\rho} \quad (4.13)$$

The macroscopic fluid velocity is given by averaging the momentum before and after the collision:

$$\mathbf{u} = \mathbf{v} + \frac{\Delta t \mathbf{F}}{2\rho} \quad (4.14)$$

In practice, it is found that with this forcing scheme the equilibrium pressure and densities vary when the relaxation parameter $\tau$ changes. As shown in the previous section, for a constant fluid kinematic viscosity, the value of the relaxation parameter $\tau$ is dependent on the grid resolution. Thus, the equilibrium properties of the same fluid will be different in sub-domains with different mesh sizes if the original Shan-Chen forcing scheme is used. This not only causes conceptual problems about inconsistent fluid property, but also leads to numerical instabilities due to the property mismatch at fine-
coarse grid interface. Fortunately, by using some other forcing schemes, constant
equilibrium properties can be maintained regardless of the value of $\tau$. In this study, the
forcing method of Guo et al. (2002) is used, which has the form

$$f_i (x + \Delta t c_i, t + \Delta t) - f_i (x, t) = -\frac{1}{\tau} [f_i (x, t) - f_i^{(eq)} (\rho, u^{eq})] + K_i \quad (4.15)$$

The last term $K_i$ is given by

$$K_i = \left(1 - \frac{1}{2\tau}\right) w_i \left[\frac{c_i - u_i^{eq}}{c_i^2} + \frac{c_i \cdot u_i^{eq}}{c_i^4} c_i\right] \cdot \Delta t F \quad (4.16)$$

And both the macroscopic fluid velocity and the equilibrium velocity are expressed in the
same form:

$$u = u^{eq} = v + \frac{\Delta t F}{2\rho} \quad (4.17)$$

**4.3.3. Numerical results for non-uniform grid Shan-Chen model**

A few numerical tests have been performed in order to demonstrate the above properties
of the original Shan-Chen model and our improved interaction potential model. The
original Shan-Chen model is made up of Equations (4.1), (4.2), (4.3), (4.5), (4.13), and
(4.14). In the improved model, Equations (4.11) and (4.12) are used instead of Equation
(4.3) to introduce adjustments of the interaction force, and Equations (4.15), (4.16) and
(4.17) replace Equations (4.1), (4.3), (4.13), and (4.14) to implement Guo’s forcing
scheme.
Table 4.1 shows an example of the different equilibrium properties obtained by using Guo’s forcing scheme and the original Shan-Chen forcing scheme. The interaction potential is chosen to be

$$\psi(\rho) = \exp(-1/\rho)$$

(4.18)

The simulation was performed in a periodic domain with flat interfaces between the two phases. With a fixed interaction strength $G = -10$, the simulation was conducted for different the grid size $\Delta x$, which leads to a varying $\tau$ according to Equation (4.1). Ideally, the equilibrium properties of the fluid should be independent of the grid size, which is the case in the results obtained from Guo’s forcing scheme. However, with the original forcing scheme in Shan-Chen model, the equilibrium densities and pressure are found to be changing with grid size and consequently with $\tau$. Through extensive investigation, it is found that this unfavorable feature of Shan-Chen forcing scheme exists for all equations of state, and the resulted density ratio $\rho_l/\rho_v$ decreases with the increase of $\tau$. The calculated equilibrium densities and pressure only approaches the theoretical value with a vanishing viscosity, which is equivalent to $\tau = 0.5$. The deviation is mainly in the gas phase density, which changes about 20% in this case when $\tau$ changes from 0.548 to 1.268. The deviation could be much more severe in the case of a low quench temperature ($T/T_c$), or a high density ratio. For example, if Carnahan-Starling equation of state is used at $T/T_c=0.76$, the equilibrium gas density will change from 0.0122 to 0.00043 when $\tau$ changes from 1 to 0.506. As the result, the equilibrium pressure will drop from $7.7 \times 10^{-4}$ to $3.1 \times 10^{-5}$, and the density ratio will increase dramatically from 26.8 to 747.8. The independence of equilibrium properties from $\tau$ in Guo’s forcing scheme makes it a
superior choice to the Shan-Chen forcing scheme, and the difference of the two schemes can be shown to be on the order of $O(F^2)$. The dependence of equilibrium properties on $\tau$ in Shan-Chen model has not been discussed extensively in the literature, since in most two-phase simulations both viscosity and mesh size are fixed, and therefore $\tau$ is a constant. However, if grid size is allowed to change, it is inevitable to yield different values of $\tau$ in the same computational domain. Therefore, in order to achieve consistent equilibrium properties in the entire domain, Guo’s forcing scheme is used for all the results presented in the following sections.

Table 4.2 compares the numerical and theoretical equilibrium properties at various values of $G$. The density ratio between the two phases increases with an increasing magnitude of $G$, and the difference between the numerical and theoretical values are very small in all cases. A good agreement between theoretical and numerical results can also be found in Figure 4.4, which shows the density profiles for three cases with different values of $G$. Table 4.2 and Figure 4.4 indicate that the equilibrium properties as well as the density profile can be accurately predicted using Equation (4.7).

The relation between $k_0$ and surface tension is presented in Figure 4.5. Theoretical values of the surface tension are calculated from Equation (4.8). The numerical results of the surface tension are in good agreement with the theoretical prediction. It is noted that the form of the interface stress in Equation (4.9) is also employed in other diffuse interface methods to specify the gradient energy at the interface (Jacqmin, 1999). From the
analysis in those studies, the surface tension is roughly proportional to the square root of $k_0$. This trend is also observed in this study by investigating the slopes in Figure 4.5. The LBM simulation gives $\sigma \propto k_0^{0.55}$, while the prediction by Equation (4.8) gives a slightly different relationship, which is $\sigma \propto k_0^{0.37}$. This indicates that the parameter $k_0$ provides a predictable way to adjust the surface tension.

When non-uniform grid size is used, the surface tension in the original interaction force specified in Equation (4.3) may change with the grid size, as shown in Figure 4.6. The slope in the log-log plot in Figure 4.6 is found to be 1.03, which indicates the relation $\sigma \propto \Delta x$ in the original interaction force model. In fact, the same linear relationship can be found analytically by combining Equations (4.7) and (4.8). By introducing the correction term $F_s$ in Equation (4.12), the surface tension value can be tuned to stay constant as grid size changes.

The analysis and simulations above emphasize the relationship between grid sizes and fluid properties such as phase equilibrium and surface tension in the interaction potential model. In the original Shan-Chen model, fluid properties cannot remain constant on different mesh size. However, consistent fluid properties can be achieved by applying Guo’s (2002) forcing scheme and by introducing correction terms in the interaction force. It is also demonstrated that the theoretical analysis by Shan (2008) gives accurate prediction of the properties in the interaction potential model, and thus, can be used as a guide to adjust simulation parameters and to assign initial conditions for the simulation.
4.3.4. **Integration of multiphase LBM with AMR**

The computation procedure of multiphase LBM on a non-uniform mesh is essentially the same as the single phase algorithm described in Section 4.2, and the only additional step is incorporation of the interaction force. Calculation of the force involves taking the gradient of the potential, which requires information from neighboring cells. When this occurs at the coarse-fine grid interface, the potential on the other side of the interface can be easily averaged/interpolated and then communicated across the block boundary. Once the force is obtained, the forcing scheme itself is a local operation and can be performed at the same time as the collision step.

The adaptive refinement of the mesh takes place every few steps in the simulation. For multiphase flows which involve two fluid phases with different densities, it is natural to use the magnitude of density gradient as the criterion for mesh refinement. The interface between two phases is located by finding the blocks whose density gradient is above a critical value, and these blocks are assigned to be at the highest refinement level. Regions away from the interface have successively larger grid size. It is important that the highest and lowest refinement levels are specified to avoid infinite refinement or excessive coarsening during the simulation.
4.4. LBM-AMR for a rising bubble

4.4.1. Bubble shape and velocity

To demonstrate the capability of the LBM-AMR technique, simulations are carried out for the buoyant rise of a single bubble in an otherwise quiescent viscous liquid under different conditions. Firstly, 2D simulation of an ellipsoidal cal bubble with \( E_o = 43.4 \), \( M_o = 27.2 \), and \( R_e = 2.5 \) is performed with the single component model. The equivalent diameter of the bubble is set to be 2.8. The computation domain has a non-dimensional width of 16 and a non-dimensional height of 32. Since the domain width is more than 5 times larger, and the domain height is more than 10 times larger than the bubble size, the boundary effect is considered to be negligible, and the simulation essentially predicts the rise behavior of the bubble in an infinite domain. Seven refinement levels are used in the entire domain, with a minimum grid size of 0.0078125 near the bubble surface, and a maximum grid size of 0.5 in the far field. The mesh adaption process during the rise of the bubble is shown in Figure 4.7. And an enlarge view of the refined mesh near the bubble surface is shown in Figure 4.8.

The capability of LBM in modeling complex topology changes such as bubble breakage and coalescence is maintained in the LBM-AMR technique. Figure 4.9 shows the coalescence of two equal sized bubbles with \( E_o = 8.3 \) and \( M_o = 1.52 \times 10^{-4} \). The two bubbles are initially placed with a separation distance of 1.6D between their centers. Time sequences of the bubbles shape as well as the mesh refinement are provided in Figure 4.9.
The shape of the lower bubble is affected by hydrodynamic interaction between the two bubbles as it approaches the upper bubble. Squeezing of the thin liquid film between bubbles in their collision is seen at $t=400$, and the rupture of the film leads to the coalescence shown in subsequent time frames.

### 4.4.2. Computational efficiency

In the simulations performed in this study, the gain in computation efficiency as a result of the adaptive mesh scheme relies on the number and size of the bubbles as well as the number of refinement levels, and is therefore case-dependent. As a typical example, for a 2D single-component simulation of a bubble with diameter of 128 lattice units in a 1024*1024 domain, 4 levels of grid refinement can reduce the memory usage by about 78%, and reduce the computation time by about 95% compared to the uniform mesh with the finest resolution. Such comparison is based on the numerical experiments using the same computation code which utilizes the PARAMESH package for mesh management. It is noted that the PARAMESH package is not specifically built for LBM algorithms and it causes some redundancy in memory usage and sacrifice in efficiency. However, even compared to a separate program with straightforward implementation of LBM algorithm on a uniform mesh, the current LBM-AMR code (integrated with PARAMESH) with 4 levels can still reduce the computation time by about 50%.
4.5. Conclusions

A lattice Boltzmann method with adaptive mesh refinement is developed for the simulation of two-phase flows. The traditional LBM algorithm based on uniform grids is extended to be able to operate on a non-uniform mesh by introducing special operations to communicate information between blocks with different grid sizes. The interaction potential model is adopted to generate two fluid phases in equilibrium. Theoretical analysis and numerical tests have been performed to investigate the properties of the interaction potential model. It is demonstrated that the original Shan-Chen model cannot maintain consistent fluid properties when the grid size changes. To overcome this problem, the improved interaction potential model is introduced, which has the benefit of grid-independent equilibrium properties and adjustable surface tension. The newly developed LBM-AMR technique is validated through both single phase and two-phase flow simulations. The 2D and 3D bubble rising in viscous liquids are simulated under various conditions, and both bubble shape and rise velocity are found to be in good agreement with experimental data in literature. The bubble shape and the flow field can be adequately resolved even under the condition of large bubble deformation. The advantage of original LBM in simulating large topology changes is maintained in the LBM-AMR algorithm, as demonstrated in the simulation of coalescence between two bubbles. This new LBM-AMR method greatly extends the capability of LBM in multiphase flow simulation by improving the accuracy at the interface between two phases, and reducing the computation cost for the entire computation domain. It is expected that together with other advanced techniques in LBM, the adaptive scheme
developed in this work will enable the application of LBM in a broad range of complex multiphase flow problems that are relevant to real-world engineering practice.
**Table 4.1** Comparison of equilibrium densities and pressure obtained by forcing schemes developed by Guo et al and by Shan and Chen. Simulation is conducted under constant interaction strength \( G = -10 \) and constant viscosity \( \nu = 0.00025 \), while \( \tau \) changes as a function of \( dx \). The analytical results from Equation (3.18) are: \( \rho_g = 0.3675 \), \( \rho_l = 2.7828 \), \( p = 0.1153 \).

<table>
<thead>
<tr>
<th>( \Delta x )</th>
<th>( \tau )</th>
<th>Guo’s forcing scheme</th>
<th>Shan-Chen forcing scheme</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>( \rho_g )</td>
<td>( \rho_l )</td>
</tr>
<tr>
<td>1/64</td>
<td>0.548</td>
<td>0.3677</td>
<td>2.783</td>
</tr>
<tr>
<td>1/128</td>
<td>0.596</td>
<td>0.3667</td>
<td>2.781</td>
</tr>
<tr>
<td>1/256</td>
<td>0.692</td>
<td>0.3673</td>
<td>2.782</td>
</tr>
<tr>
<td>1/512</td>
<td>0.884</td>
<td>0.3663</td>
<td>2.782</td>
</tr>
<tr>
<td>1/1024</td>
<td>1.268</td>
<td>0.3667</td>
<td>2.781</td>
</tr>
</tbody>
</table>

**Table 4.2** Equilibrium properties for different interaction strength \( G \)

<table>
<thead>
<tr>
<th>( G )</th>
<th>LBM Simulation</th>
<th>Theoretical</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>gas density</td>
<td>liquid density</td>
</tr>
<tr>
<td>-8.5</td>
<td>0.5198</td>
<td>1.9651</td>
</tr>
<tr>
<td>-9</td>
<td>0.4557</td>
<td>2.2494</td>
</tr>
<tr>
<td>-10</td>
<td>0.3670</td>
<td>2.7802</td>
</tr>
<tr>
<td>-11</td>
<td>0.3048</td>
<td>3.2938</td>
</tr>
<tr>
<td>-12</td>
<td>0.2601</td>
<td>3.7930</td>
</tr>
</tbody>
</table>
Figure 4.1 Schematic illustration of the change of particle distributions in the cells near the refinement jump in a 2D computation. For simplicity, only a single pair of particle distributions is shown. The arrows pointing towards the cell center represent the “pre-collision” distributions, while the arrows pointing away from the cell center represent the “post-collision” distributions.

Figure 4.2 Flowchart of the computation procedure during one time step for two refinement levels. The sequence of sub-steps (1-6) is in accordance with those in Figure 4.1.
Figure 4.3 Results of single phase flow obtained using LBM-AMR.
(a) Grid arrangement and velocity field for Couette flow
(b) Comparison of simulated and analytical velocity profiles in Couette flow
(c) Grid for Poiseuille flow with grid interface parallel to the flow direction
(d) Velocity profiles in Poiseuille flow with grid interface parallel to the flow direction
(e) Grid for Poiseuille flow with grid interface perpendicular to the flow direction
(f) Velocity profiles in Poiseuille flow with grid interface perpendicular to the flow direction
Figure 4.4 Comparison of simulated and theoretical density profiles under different interaction strength.

Figure 4.5 Relation between surface tension and parameter $k_0$. Theoretical values are obtained from Equation (4.8).
Figure 4.6 Change of surface tension as a function of the grid size
Two series of simulations are performed using interaction force in Equation (4.3) (without $F_s$), and in Equation (4.11) and (4.12) (with $F_s$), respectively.
Figure 4.7 Buoyant rise of a 2-D ellipsoidal cap bubble with $Eo=43.4$, $Mo=27.1$
Figure 4.8 Adaptive grid used for simulation shown in Figure 4.7. Grid refinement level 1-7 are marked in corresponding regions of the grid. Each square represents a block of 8*8 uniform mesh.

(a) Grid of the entire computation domain
(b) Closed-up view of the grid near the bubble
Figure 4.9 Coalescence of two bubbles. $Mo=1.5\times10^{-4}$, $Eo=8.3$. The adaptive refinement of the mesh is shown in the background. Each square represents a block with 8*8 uniform mesh.
CHAPTER 5

MULTI-RELAXATION TIME LBM FOR TWO-PHASE FLOW

Abstract

This chapter introduces a numerical technique that is able to improve the stability of the interaction potential based multiphase LBM at low fluid viscosities. The technique is based on the multi-relaxation time (MRT) scheme, which transforms the collision step into the moment space, while keeps the propagation step in the velocity space. The extra freely adjustable parameters provide a way to fine-tune the stability of the algorithm. The MRT algorithm is incorporated into the interaction potential based LBM. Numerical tests are performed for both the equilibrium conditions and the flow conditions, and show significant improvement in the numerical stability in simulating low viscosity fluids.

5.1. Introduction

The lattice Boltzmann method (LBM) has proven to be a powerful tool in direct numerical simulation of multiphase flows. However, one of the unfavorable properties of LBM is that it tends to become numerically unstable when the fluid viscosity is small. This deficiency put severe restrictions on the application of LBM in high Reynolds
number flows. Moreover, the problem becomes even worse in multiphase flow LBM. As the viscosity decreases, the magnitude of the spurious velocity at the interface often increases and eventually destabilizes the gas-liquid interface and cause the computation to diverge.

The numerical instability of LBM at low viscosities has received considerable attention in recent studies, and a number of techniques have been proposed to overcome this problem. Some researchers attribute the instability of LBM to the absence of the H theorem, which ensures the compliance with the second law of thermodynamics in the continuous Boltzmann equation. Accordingly, they developed the entropic LBM by introducing the entropy function and a variable relaxation time (Ansumali and Karlin, 2002). The entropic LBM has shown better stability in several single phase flow simulations, especially in gas flow with shocks. However, its extension to multiphase flow problems has not been discussed so far. Using an entirely different approach, an implicit formulation of the LBM has been developed (Sankaranarayanan et al. 2002), in which the collision term is treated using a central difference in space and time. Due to its implicitness, this scheme requires iterative calculations, which is more time-consuming than the explicit algorithm usually employed in LBM. However, the increase in computation cost is reported to be only moderate. This implicit scheme has been applied to investigate the drag and virtual mass forces in bubbly suspensions, and is able to simulate bubbles with Reynolds number up to 400. The third class of techniques is based on the multiple-relaxation-time (MRT) scheme for the collision step, which replaces the
Bhatnagar-Gross-Krook (BGK) approximation that employs a single relaxation time. Instead of treating the population distributions functions directly, the MRT approach employs a moment representation that corresponds to various hydrodynamic quantities and their fluxes. The fact that these quantities can relax on different time scales introduces additional adjustable parameters that can be tuned for improved stability. Besides the enhanced numerical stability, the MRT approach has a number of other advantages, including the ability to model complex fluids such as viscoelastic flows (Lallemand, d’Humieres, and Luo, 2003), and ability to model thermo-hydrodynamics with adjustable Prandtl numbers (Lallemand and Luo, 2003). A number of the two-phase models which are originally developed using BGK collision term have also been reformulated with the MRT algorithm. Tolke et al. (2006) used an MRT version of the Gunstensen model (Gunstensen and Rothman, 1991) together with mesh adaption to simulate the buoyant rise of a bubble in liquid. The incompressible two-phase flow model based on the index function (He, Chen, Zhang, 1999) has been recast with MRT in both 2D (McCrachen and Abraham, 2005) and 3D (Premnath and Abraham, 2007). The MRT pressure-evolution model for high density ratio two-phase flows has also been developed (Mukherjee and Abraham, 2007). It was able to increase the maximum accessible Reynolds number by 50% compared to the original BGK version developed by Lee and Lin (2005). The pseudo potential model for non-ideal gas (Shan and Chen, 1993) has also been recently extended with MRT algorithm (Kuzmin, et al, 2008), and was reported to achieve moderate improvement in stability. However, only simple flow conditions such as static droplets in equilibrium and capillary waves were simulated.
From the application point of view, in spite of the numerous studies on the development of LBM techniques, the successful use of LBM for real-world gas-liquid two-phase flow problems is still quite limited. One of the important reasons for such situation is that many typical gas-liquid flows lie in the parameter range that is inaccessible to traditional LBM models. Even the most common air-water system, for example, has been in fact a difficult object for many numerical techniques due to both high interface tension and low viscosity. Millimeter sized air bubbles rising in water under buoyancy force usually have a Reynolds number on the order of $10^2 \sim 10^3$, which is beyond the reach of traditional LBM. For bubbly flows, the ratio between the viscosity and surface tension is often represented by the Morton number $Mo = \frac{g\rho^3 \nu^4}{\sigma^3}$, where $g$ is the gravitational acceleration, $\rho$ and $\nu$ are the density and kinematic viscosity of the liquid, and $\sigma$ is the surface tension. Air-water system has a Morton number of $O(10^{-11})$. However, most LBM models for gas-liquid system can only simulate the conditions where the Morton number is greater than $10^{-5}$, which would correspond to a much more viscous liquid. For instance, Frank et al (2006) used the free energy LBM approach to simulate millimeter bubbles in 99.5% glycerol, which gave a Moron number of $O(10^1)$ and $0.033<Re<1.8$. The free energy model with pressure Poisson equation was used to simulated bubbles with $Mo=10^{-5}$, although at a high density ratio of 1000 (Inamuro, et al, 2004). A phase filed LBM for immiscible fluids used applied for bubbles with $10^{-5}<Mo<10$, and $10^{-1}<Re<10^2$ (Kurtoglu and Lin, 2006). The pseudo-potential type of LBM has the similar applicable
range, as shown in the coarse bifurcation studies (Mo~10^{-4}) (Theodoropoulos, et al, 2004) and multiple bubble dynamics studies (10^{-6}<\text{Mo}<10^2, 10^{-1}<\text{Re}<10^2) \quad \text{(Gupta and Kumar, 2008)}. To the best of the authors’ knowledge, the closest LBM simulation for air bubbles in water to date was based on the implicit LBM formulation (Sankaranarayanan et al. 2002), which achieved the Morton number of 10^{-10}, and Reynolds number up to 400. Even that does not match the conditions of the air-water system exactly. Therefore, an apparent gap exists between the capability of current two-phase LBM models and the real flow conditions in many low-viscosity liquids. There is a demand to further improve the LBM model so as to enable its application in broader flow conditions that are relevant to real-world engineering problems.

The motivation of the current work is to address the LBM simulation of high-Reynolds number gas-liquid flows. In this chapter, a new pseudo potential based two-phase LBM model is developed using the MRT scheme. By using a special way to incorporate the interaction force, the pseudo potential model is integrated into the MRT algorithm in a straightforward manner. To further improve the performance, novel formulation of the interaction force using the midrange potential has also been adapted in the newly developed model. The flexibility gained from the MRT algorithm and the midrange interaction potential is shown to result in significant improvement of numerical stability and reduction of spurious velocity.
The rest of the chapter is organized as follows. The new MRT-LBM will be described in section 5.2. The general framework of LBM and the original pseudo-potential model for a non-ideal gas with BGK collision will be briefly introduced first, followed by a discussion on the role of the interaction force and its novel formulation using the midrange potential. Then the newly developed MRT pseudo-potential model will be described in detail, including the incorporation of the interaction force and the presentation of the collision term in the moment space. The performance of the new model will be demonstrated Section 5.3 with a discussion on the simulation results. The fluid properties at equilibrium in MRT model will be first analyzed with comparison to those in the BGK model. The improvement of the new MRT model will be evaluated regarding to both the stability and spurious velocity. To test the model’s performance in dynamic flow problems, the buoyant rise of bubbles in both 2D and 3D will then be simulated at high Reynolds numbers. Finally, summary of the model and the results will be provided in section 5.4.

5.2. MRT Interaction Potential Model

5.2.1. General framework of LBM

As introduced in Chapter 2, the LBM is based on the Boltzmann equation, which can be written as

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{F}{\rho} \frac{\partial f}{\partial \mathbf{v}} = \Omega,
\]  

(5.1)
where $f(x,v,t)$ is the particle distribution function, and $x, v, t, \rho, F$ are the spatial coordinates, particle velocity, time, fluid density, and force term, respectively. The right hand side of Equation 5.1, $\Omega$, is the collision term that describes the change of particle distribution function due to particle collisions. In traditional LBM, this term is calculated using the BGK approximation that describes the collision as a relaxation process towards local equilibrium with a single relaxation time scale $\tau$:

$$\Omega = \frac{f - f^{eq}}{\tau} \quad (5.2)$$

The lattice Boltzmann equation (LBE) with MRT can be obtained in a similar manner to its BGK counterpart as described in Chapter 2, except that the collision term is treated using a constant matrix $\Lambda$ instead of a single time scale $\tau$:

$$\Omega_i = -\sum_j \Lambda_{ij} (f_j - f_j^{eq}) \quad (5.3)$$

As the result, the LBE in the general form is written as:

$$f_i(x_i + c_i\Delta t, t + \Delta t) - f_i(x_i, t) = -\sum_j \Lambda_{ij} (f_j - f_j^{eq})_{(x,i)} + \Delta tS_i, \quad (5.4)$$

where $c_i$ is the discrete velocity in the $i$th lattice direction, $f_i$ is the particle distribution associated with the velocity $c_i$. The last term $S_i$ in Equation 5.4 represents the force term $\frac{F}{\rho} \frac{\partial f}{\partial v}$ in Equation 5.1, and its detailed implementation will be discussed in more detail in later sections. As in the BGK-LBM, the left hand side of Equation 5.4 is often referred to as the streaming or propagation step, and the right hand side is referred to as the collision step. By convention, the lattice spacing and the time step are both normalized, so that
\[ \Delta t = 1 \quad \text{and} \quad \Delta x = c\Delta t = 1. \] This convention is also adopted in this work.

In general, the collision matrix \( \Lambda \) is a full matrix with constant elements that characterize different relaxation time scales. Traditional LBM with BGK collision can be regarded as a special case in which the collision matrix is a diagonal matrix with identical diagonal elements of \( 1/\tau \):

\[
\Lambda_{ij} = \frac{1}{\tau} \delta_{ij}
\]  

(5.5)

The equilibrium distributions \( f_{i}^{eq} \) in Equation 5.3 and 5.4 are the truncated Maxwell-Boltzmann distribution, as defined in the BGK-LBM in Chapter 2, Equation 2.15. The local hydrodynamic variables such as density and velocity are also calculated in the same way as in the BGK model, following Equation 2.18, 2.19

Rather than solving Equation 5.4 directly in its matrix form, a transformation technique has been established to greatly simplify the computation. However, before proceeding with the solution procedure in Section 5.2.4, it is necessary to review the evaluation and incorporation of the interaction force used in the pseudo potential model.

### 5.2.2. Evaluation of the interaction force

The pseudo-potential model, also called the Shan-Chen model (Shan and Chen, 1993), employs a mean-filed interaction force to mimic the molecular interactions that cause the
segregation of the gas and liquid phases. Two versions of interaction model have been developed. One version models a non-ideal fluid which separates into vapor and liquid at subcritical temperatures according to its Equation of State (EOS). The other version models the mixture of multiple components which are segregated into different phases by repulsive forces. In the following section, only the algorithm for a single component two-phase model will be discussed for its simplicity. The extension of the algorithm to multicomponent case is straightforward.

As described in Chapter 3, the interaction force in the pseudo-potential model is given as the summation of the pair-wise interactions between particles at a given lattice site and their neighbors, and can be written as

\[ F = -G \psi \sum_i w_i \psi(x + c_i)c_i \]  \hspace{1cm} (5.6)

In the above equation, \( G \) is a scalar constant that represents the strength of the interaction. And the interaction potential \( \psi \) is a local quantity that depends on the fluid density. In this study, the following form of the potential is employed (Shan, Chen 1993):

\[ \psi(\rho) = 1 - \exp(-\rho) \]  \hspace{1cm} (5.7)

Upon Taylor expansion of Equation 5.6, the force can be written as

\[ F = -\nabla \left( \frac{1}{2} c_i^2 G \psi^2 \right) - \frac{1}{2} c_i^2 G \psi \nabla \psi + o(\Delta t^3) \]  \hspace{1cm} (5.8)

where the first term on the right hand side corresponds to the non-ideal part of the EOS, while the second term contributes to the surface tension.
Despite its simple form, the implication of the interaction force calculated from Equation 5.6 on the thermodynamic properties of the gas-liquid interface in the pseudo potential model is not well understood. The most in-depth analysis of the interaction model to date is provided in a recent work by Shan (2008) by considering the discrete lattice effect. Using the approach developed in that study, the properties of the interaction model can be found analytically, including the equilibrium densities, stress tensor, density profile across the interface, and the surface tension coefficient.

Recent progress in the study of the pseudo potential model also leads to the development of the midrange potential. In contrast to the original model (Shan and Chen, 1993) that employs only the nearest neighbor sites in the calculation of the interaction force, the generalized midrange potential model includes an enlarged set of grid points in the calculation of the potential gradient (Sbragaglia, 2007, Shan, 2006). Manipulating the formulation of the midrange potential brings extra flexibility to the generalized model, which results in several favorable features. First, the surface tension can now be adjusted independently from the equation of state. Second, the magnitude of the spurious velocity can be reduced by either enlarging the interface thickness, or by employing a higher-order isotropic discretization. Since it is only involved in the calculation of the interaction force, the midrange potential can be readily integrated with other advance algorithms, such as MRT and adaptive mesh scheme.
5.2.3. Incorporation of force into LBM

As described in chapter 3, the original pseudo-potential model is formulated using the BGK collision. The force term $\Delta S_i$ in equation 5.4 has been absorbed into the modified equilibrium distribution $\tilde{f}_i^{eq}(\rho, u^{eq})$, therefore the governing equation is written as:

$$ f_i(x_i + c_i \Delta t, t + \Delta t) - f_i(x_i, t) = -\frac{1}{\tau} \left( f_i - \tilde{f}_i^{eq} \right) $$

(5.9)

The force is added by simply shifting the equilibrium velocity

$$ u^{eq} = v + \frac{\tau F}{\rho} $$

(5.10)

where $v$ is the velocity before the force is added:

$$ \rho v = \sum_i f_i c_i $$

(5.11)

It can be shown that the additional term in the equilibrium velocity introduces a momentum change proportional to $F$ during the collision step. Incorporating the force by shifting the equilibrium velocity, or the Shan-Chen forcing scheme, is a simple and unique feature of the original pseudo-potential model. However, although the Shan-Chen forcing scheme is easy to implement with the BGK collision, its extension to the MRT framework is not straightforward.

On the other hand, the force term in the continuous Boltzmann equation can be approximated using the gradient of the equilibrium distribution (He, 1998):

$$ -\frac{F}{\rho} \frac{\partial f}{\partial v} \approx -\frac{F}{\rho} \frac{\partial f^{eq}}{\partial v} = \frac{(v - u) \cdot F}{\rho RT} f^{eq} $$

(5.12)
With a finite set of discrete velocities, the forcing term in the LBM becomes

\[ S_i = \frac{(c_i - u) \cdot F}{\rho c_i^2} f_{i}^{eq} \]  \hspace{1cm} (5.13)

Then, following the derivation given by Premnath and Abraham (2007), the general LBE with a central difference for the force term is written as

\[ f_i(x + c_i \Delta t, t + \Delta t) - f_i(x, t) = -\sum_j \Lambda_{ij} \left( f_j - f_j^{eq} \right) \bigg|_{(x,t)} + \frac{1}{2} \left[ S_i(x, t) + S_i(x + c_i \Delta t, t + \Delta t) \right] \Delta t \] \hspace{1cm} (5.14)

The above equation has an implicit force term which usually requires complex solution techniques in practice. However, by using a transformation \( \tilde{f}_i = f_i - \frac{1}{2} S_i \Delta t \), equation (5.14) can be converted into an explicit scheme

\[ \tilde{f}_i(x + c_i \Delta t, t + \Delta t) - \tilde{f}_i(x, t) = -\sum_j \Lambda_{ij} \left( \tilde{f}_j - f_j^{eq} \right) \bigg|_{(x,t)} + \sum_j \left( I_{ij} - \frac{1}{2} \Lambda_{ij} \right) S_j \big|_{(x,t)} \Delta t \] \hspace{1cm} (5.15)

in which \( I_{ij} \) is the components of the identity matrix. Since Equation 5.15 applies to both single and multiple relaxation time algorithms, incorporation of the interaction force into the MRT approach becomes straightforward. It is also noted that, when using a single relaxation time, Equation 5.14 reduces to the forcing scheme proposed by Guo (2002).

5.2.4. Solution of MRT-LBE

After incorporating the force term, Equation 5.15 is the governing equation that dictates the evolution of the distribution functions in MRT-LBM. Since the collision matrix \( \Lambda \) is
in general a full matrix, the solution of Equation 5.15 involves complex matrix manipulations. However, in practice, the solution of MRT-LBE takes advantage of a special linear transformation to diagonalize the collision matrix. The transformation matrix \( T \) transforms the distribution functions \( \tilde{f}_i \), which lie in the velocity space, to their moments \( \tilde{f} \), which correspond to macroscopic physical quantities such as density, momentum, energy, and their fluxes in the moment space.

\[
\tilde{f} = T \tilde{f}
\]  

(5.16)

The specific form of the transformation matrix depends on the lattice structure. The procedure presented in this section corresponds to the D2Q9 lattice in 2D. The 3D cases using D3Q19 lattice is given in the Appendix. With D2Q9 lattice, the transformed vector \( \tilde{f} \) in the moment space is given explicitly by:

\[
\tilde{f} = [\rho, e, e^2, j_x, q_x, j_y, q_y, p_{xx}, p_{xy}]^T
\]  

(5.17)

Where \( \rho \) is the density; \( e \) is the energy, \( e^2 \) is the energy squared; \( j_x \) and \( j_y \) are the momentum in x and y direction; \( q_x \) and \( q_y \) are the energy fluxes; \( p_{xx} \) and \( p_{xy} \) are the diagonal and off-diagonal components of the stress tensor. The transformation matrix is expressed explicitly as (Lallemand and Luo, 2000)
The equilibrium moments are obtained by applying the transformation to the equilibrium distributions originally in the velocity space, and can be computed directly from hydrodynamic quantities.

\[
\begin{pmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-4 & -1 & -1 & -1 & 2 & 2 & 2 & 2 \\
4 & -2 & -2 & -2 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\
0 & -2 & 0 & 2 & 0 & 1 & -1 & -1 & 1 \\
0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\
0 & 0 & -2 & 0 & 2 & 1 & 1 & -1 & -1 \\
0 & 1 & -1 & 1 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\
\end{pmatrix}
\]

(5.18)

\[
\tilde{f}^{eq} = T f^{eq} =
\begin{pmatrix}
\rho \\
-2\rho + (j_x^2 + j_y^2)/9\rho \\
\rho - (j_x^2 + j_y^2)/9\rho \\
j_x \\
-j_x \\
j_y \\
-j_y \\
(j_x^2 - j_y^2)/\rho \\
(j_x j_y)/\rho \\
\end{pmatrix}
\]

(5.19)

In the same way, the forcing term is also transformed into the moment space.
By multiplying the transformation matrix $T$, the right hand side (RHS) of equation 5.15 can be entirely transformed into the momentum space:

$$
T(RHS) = -\sum_{\beta} \hat{\Lambda}_{a\beta}(\hat{f}_{\beta} - \hat{f}_{\beta}^{(eq)}) + \sum_{\beta} \left( I_{a\beta} - \frac{1}{2} \hat{\Lambda}_{a\beta} \right) \hat{S}_{\beta}(x,t) \Delta t
$$

(5.21)

The transformed collision matrix $\hat{\Lambda} = T \Lambda T^{-1}$ is now diagonal in momentum space:

$$
\hat{\Lambda} = diag[s_1, s_2, s_3, s_4, s_5, s_6, s_7, s_8, s_9]
$$

(5.22)

The diagonal elements $s_1$ through $s_9$ are the new relaxation parameters associated with each components of $\hat{f}^{eq}$. Since the collision matrix is now diagonal, the relaxations of different physical quantities to $\hat{f}^{eq}$ are now uncoupled, and different time scales determined by $s_1$ through $s_9$ can be adjusted independently, although a few constraints still apply. To be consistent with the macroscopic hydrodynamic equation, it is required that $s_1 = s_4 = s_6 = 1$. Meanwhile, $s_8$ and $s_9$ are related to the kinematic viscosity $\nu$,

$$
s_8 = s_9 = 1/\tau, \quad \text{and} \quad \nu = \left( \tau - \frac{1}{2} \right) c_s^2 \Delta t
$$

(5.23)
And $s_2$ is related to the bulk viscosity of the fluid by

$$\zeta = \left(\frac{1}{s_2} - \frac{1}{2}\right)c_s^2\Delta t$$

(5.24)

Further, symmetry requires that $s_5 = s_7$. As the results, three of the relaxation parameters $s_2, s_3, s_5 (= s_7)$ remain to be independently adjustable, and they can be used to tune the stability of the MRT model.

In practice, the MRT-LBM algorithm is often realized in a way such that the collision step takes place in the moment space, while the propagation step operates in the velocity space. In the actual computation procedure, transformed quantities $\hat{f}, \hat{f}^{eq}$ and $\hat{S}$ are first calculated using Equations 5.16, 5.19 and 5.20, followed by the collision step as described by Equation 5.21. Then the RHS is transformed back to the velocity space to perform the propagation step:

$$\tilde{f}_i(x + c_i\Delta t, t + \Delta t) - \tilde{f}_i(x, t) = T^{-1}[T(RHS)]$$

(5.25)

The hydrodynamic quantities such as density, momentum, potential and force are calculated in the velocity space in the usual way as discussed for the BGK algorithm in Chapter 2.

In summary, the quantities to be involved in the collision operation in MRT algorithm are the moments of the particle distributions and they have distinct physical meanings.

93
relaxation time scales are uncoupled and can be adjusted independently with the parameters s1~s9. Since the transformation between velocity space and momentum space is a local operation, the transformed moments \( \hat{f} \) do not need to be stored. Therefore, the MRT algorithm only requires a small amount of additional computation time compared to conventional LBM, without significant increase in memory usage.

5.3. Numerical results

5.3.1. Phase Equilibrium Properties

A unique feature of the pseudo potential model is that the phase segregation is induced by particle interaction forces. Many properties such as the density, pressure, and surface tension are directly related to the way the interaction force is evaluated and incorporated into the LBE. Current MRT algorithm maintains this physical basis of the pseudo potential model. In order to examine the equilibrium properties in the current MRT model, simulations are carried out in a 2D periodic domain, with 20 and 200 grids in the horizontal and vertical directions, respectively. The computation is initialized with a slab of gas phase in the middle of the domain and liquid phase in other regions, and runs until the macroscopic velocity in the whole field becomes negligibly small, which characterizes the arrival of equilibrium. Density and pressure in each phase are then extracted for analysis.
It has been discussed in Chapter 4 that the way to incorporate the interaction force could affect the equilibrium densities predicted by the pseudo potential model. The original model (Shan and Chen, 1993) uses a shifted equilibrium velocity to incorporate the force term, and introduces a non-linear error term that scales with $F^2$. This causes the equilibrium to depend on the viscosity (or equivalently, the relaxation parameter $\tau$). In addition, the predicted density ratio between the liquid and gas also decreases as the viscosity increases. The artificial effect of viscosity on equilibrium density makes it not only inconvenient to specify fluid properties, but also difficult to reach high density ratio between two phases with high viscosities. Such unfavorable features, however, can be eliminated using a different approach to incorporate of the force, such as Guo’s forcing method (Yu and Fan, 2009).

To illustrate the effect of viscosity on the equilibrium properties predicted by different forcing schemes, the results are compared for three different versions of interaction potential models, including the Shan-Chen (SC) model with BGK collision and shifted velocity, the SC-Guo model with BGK collision and Guo’s forcing, and the MRT model. The interaction force is calculated in the same way in all three models, by summation of interactions among only the nearest neighbors. As shown in Table 5.1, the equilibrium properties predicted by both the SC-Guo model and the MRT model remain nearly constant regardless of the change in viscosity. However, the results from the original Shan-Chen model show clear variation as viscosity changes. The quantity that shows most significant change is the gas phase density, which reduces about 60% as viscosity
changes from 0.4 to 0.01. Comparison of the gas phase density in three models is also plotted in Figure 5.1. It is noted that the gas density in Shan-Chen model tends to converge to the value predicted by two other models only when the viscosity becomes very small.

The phase diagram of the model fluid can be obtained by carrying out the simulation for different values of $G$ used in calculation of the interaction force in Equation (5.6). The critical value of $G$ corresponding to the potential given in Equation (5.7) is -4, which can be calculated from the equitation of state. The phase diagrams simulated using the SC-Guo model and the MRT model are presented in Figure 5.2. The two models predict almost identical equilibrium densities at various values of $G$, indicating that the MRT model does not alter the equilibrium properties of the original pseudo-potential model. The density ratio between the liquid and the gas phase ranges from 3 to 170 when $G$ changes from -4.2 to -6.0. Although the two models predict the same equilibrium properties, the MRT model usually reaches equilibrium much faster than the SC-Guo model, especially at low viscosities. This faster convergence is probably related to the larger value of the bulk viscosity, which can be specified independently from the shear viscosity in the MRT model.

5.3.2. Surface tension

Surface tension in the pseudo-potential model comes from the third order term in the Taylor expansion of the interaction force, and its theoretical value can be calculated from the stress profile across the interface (Shan, 2008). In practice, the value of the surface
tension is computed from the pressure difference across a circular interface according to the Laplace law:

$$\Delta p = \sigma \left( \frac{1}{R_1} + \frac{1}{R_2} \right)$$

(5.27)

In the above equation, $\Delta p$, $\sigma$, $R_1$, and $R_2$ are the pressure difference, surface tension coefficient, and the principal radii of curvature of the interface. Simulations using both the SC-Guo model and the MRT model are performed for a number of circular bubbles with varying radii at equilibrium. In both models, the interaction force is computed from nearest neighbors, and the interaction strength has the value $G=-5.0$. The simulation results plotted in Figure show a linear relationship between the pressure drop and the curvature for both models, and the data obtained from the two models fall on a single line, indicating that the MRT approach does not change the surface tension value in the original pseudo-potential model under the same conditions.

5.3.3. Spurious velocity

The spurious velocity, also referred to as the parasite current, is the small circulating velocity that exists near the interface in the numerical results. This spurious velocity is unphysical, and its presence not only degrades the accuracy of the simulation, but also causes stability problems. This numerical artifact is a common problem for many two-phase flow simulation techniques, such as VOF and LBM. The magnitude of the spurious velocity is found to increase with the increase of surface tension, and decrease with the increase of interface width. In particular, the pseudo-potential model is reported to have a larger spurious velocity, which is probably related to the fact that it often uses a higher
surface tension value. In practice, the spurious velocity results in a serious limitation of the LBM in two-phase flow simulations, especially at high density ratios or low viscosities (Yuan, 2006). The original of the spurious velocity has been identified to be the insufficient isotropy in evaluating the gradient terms for force calculation (Shan, 2008).

Since the MRT scheme involves additional freely adjustable relaxation parameters, it may benefit from the extra flexibility in reducing the spurious velocity. The effect of the adjustable relaxation parameters in the current MRT model is demonstrated in Figure 5.4. The numerical tests are carried out for 2D bubbles with $G=-5.0$ and $\nu = 0.02$. Under such condition, the BGK algorithm is unstable due to severe spurious velocity. In the MRT simulation, two sets of numerical tests are conducted with $s_3 = 1.2$ and $s_3 = 0.8$, respectively. In each of the tests, the value of $s_2$ is varied from 0.3 to 1.2. While the magnitude of the spurious velocity increase monotonically with $s_2$ when $s_3 = 1.2$, it has a minimum value of 0.0062 at $s_2 = 0.7$ when $s_3 = 0.8$. These tests demonstrate that adjusting the free relaxation parameters can effectively decrease the spurious velocity and make the simulation numerically stable. However, the effect of each parameter on the spurious velocity is found to be case dependent. In addition, the free parameters in 2D (D2Q9 lattice) and 3D (D3Q19 lattice) simulations also show different effects. Therefore, no universal rule to reduce the spurious velocity has been established at this moment. It should also be noted that the physical properties of the fluid is not affected by adjusting these free parameters. For example, all the simulations in Figure 5.4 give an almost
identical surface tension value of 0.0378, with the largest deviation to be within 2%. This consistency in physical properties makes it convenient to use these adjustable relaxation parameters for tuning the stability of the computation.

Figure 5.5 presents the magnitude of the spurious velocity as a function of the viscosity. The spurious velocity shown is the maximum value measured from the numerical results for a 2D circular bubble at equilibrium. The spurious velocity increases as the viscosity decreases in all models. Especially, a sharp increase is found in the SC-Guo model when viscosity approaches 0.025. The spurious velocity ultimately becomes so large that no stable results could be obtained for viscosity lower than 0.025 in the SC-Guo model. The MRT model with the same force evaluation gives consistently smaller spurious velocity compared to the BGK model. As a result, fluid with viscosity as low as 0.002 can be easily simulated using the MRT model.

It has been shown that the multi-range potential can be used to reduce the spurious velocity in the pseudo-potential model. By utilizing more neighboring lattices in the calculation of the potential gradient, two approaches have been proposed to mitigate the spurious velocity, including using high-order isotropic discretization (shan, 2006, Sbragalia et al, 2007), and increasing the width of the interface (Sbragalia et al, 2007). It should be noted that adjustments in the multi-range potential may have the effect of changing the surface tension (Sbragalia et al, 2007). This effect can be understood from Equation 5.8, in which the coefficient in front of the term $\psi \nabla \nabla^2 \psi$ is proportional to the
square of the surface tension. A larger value of this coefficient corresponds to both higher surface tension, and wider interface. These two factors actually have opposite effects on the amplitude of the spurious velocity, but numerical results show that their combined effect is to decrease the spurious velocity.

The spurious velocity in the MRT scheme with multirange potential is also plotted in Figure 5.5. The multirange potential model uses two layers of lattice neighbors in the force calculation, and results in an interaction force that is isotropic up to the 8th order. The spurious velocity in the MRT-multirange model is consistently smaller than the MRT model under all viscosities, and its magnitude can often be reduced by more than half by using the multirange potential, as shown in Figure 5.5.

The spurious velocity near a 2D circular interface is shown in Figure 5.6. The three simulation are carried out under identical condition where $G=-5.0$ and $\nu = 0.05$. The dilute phase inside the circle has a density of 0.11, and the dense phase outside the circle has a density of 1.85. The maximum amplitude of the spurious velocities in BGK mode, MRT model, and MRT-multirange model are 0.028, 0.0053, and 0.0016, respectively. The vector plots Figure 5.6(a)-(c) clear demonstrates that the combination of MRT and multirange potential model can effectively reduce the spurious velocity.

5.3.4. Bubbles with high Re

The buoyant rise of a gas bubble in liquid is simulated in a 256*256 2D domain. The diameter of the bubble is 55 lattice units. The kinematic viscosity is 0.01 in both phases,
which results in a relaxation time $\tau = 0.53$. The bubble dynamics can be characterized by the non-dimensional numbers, including $Eo = 1.16$, $Mo = 6.18 \times 10^{-9}$, and $Re = 148.5$. Figure 5.7(a) shows the history of the bubble rise velocity, which increases rapidly in the first 5000 steps and then gradually rises to 0.027 in 20000 steps. The snapshots of the bubble shape and streamlines are shown in Figure 5.7(b). The bubble shape has little change after 10000 steps. However, a pair of vortices continues growing in the bubble wake. The vortices are the characteristic flow pattern in the high Reynolds number flows around a deformed bubble.

5.4. Conclusions

This chapter introduces the interaction potential based two-phase LBM with multi-relaxation time. Detailed algorithm of the MRT technique is presented, in which the collision step in transformed and operated in the moment space, while the propagation step remains to operate in the velocity space as in the single relaxation time algorithm. Numerical results are analyzed for both the equilibrium conditions and the flow conditions. It is demonstrated that the MRT algorithm does not change the equilibrium densities or the surface tension as long correct form of the force term is used. The extra freely adjustable relaxation parameters can be used to fine tune the stability of the algorithm. The MRT algorithm is shown to be able to reduce the minimum stable viscosity by an order of magnitude under equilibrium conditions. Moreover, together with the multi-range interaction force, the MRT can significantly reduce the magnitude of the undesirable spurious velocity near curved interfaces. The MRT algorithm is also
stable under flow conditions, which is demonstrated in the case of a bubble rising in a 2D domain with a kinematic viscosity of 0.01 and Reynolds number of 148.5.
Table 5.1 Simulated equilibrium densities and pressure at different viscosities. Simulations are carried out at G=−5.4.

<table>
<thead>
<tr>
<th>nu</th>
<th>tau</th>
<th>rho_l</th>
<th>rho_g</th>
<th>p</th>
<th>rho_l</th>
<th>rho_g</th>
<th>p</th>
<th>rho_l</th>
<th>rho_g</th>
<th>p</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>1.7</td>
<td>2.302</td>
<td>0.223</td>
<td>0.0383</td>
<td>2.179</td>
<td>0.0668</td>
<td>0.0185</td>
<td>2.178</td>
<td>0.0661</td>
<td>0.0184</td>
</tr>
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<td>2.252</td>
<td>0.1304</td>
<td>0.0300</td>
<td>2.179</td>
<td>0.0668</td>
<td>0.0185</td>
<td>2.178</td>
<td>0.0661</td>
<td>0.0184</td>
</tr>
<tr>
<td>0.1</td>
<td>0.8</td>
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<td>0.0834</td>
<td>0.0220</td>
<td>2.179</td>
<td>0.0668</td>
<td>0.0185</td>
<td>2.178</td>
<td>0.0661</td>
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</tr>
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<td>0.0186</td>
<td>2.179</td>
<td>0.0667</td>
<td>0.0185</td>
</tr>
</tbody>
</table>

Figure 5.1 Effect of relaxation time $\tau$ on the gas phase density in original Shan-Chen pseudo potential model (SC), Shan-Chen model with Guo’s forcing scheme (SC-Guo), and current MRT scheme.
Figure 5.2 Phase diagram obtained from the SC-Guo (BGK) scheme and current MRT scheme.

Figure 5.3 Laplace law tests for the SC-Guo model with BGK collision and the MRT model. Both models use the same interaction strength $G=-5.0$. The linear fit is made using the results obtained from the MRT model, and gives the surface tension coefficient of 0.041.
Figure 5.4 Effects of $s_2$ and $s_5$ on the magnitude of the spurious velocity in MRT model. 2D simulations are performed with $G=-5.0$, $s_3=1.5$, and $\nu = 0.02$ (i.e. $s_7=1.7857$). The BGK model, which corresponds to the choice $s_2 = s_3 = s_5 = s_7 = 1.7857$, is unstable under this condition. The simulation results using various values of $s_2$ and $s_5$ give a nearly identical surface tension value of 0.0378, with the largest deviation to be within 2%.

Figure 5.5 Magnitude of the spurious velocity as a function of viscosity. The SC-Guo model with BGK collision is unstable with viscosity less than 0.025. The MRT model uses the same force evaluation as the BGK model, which employs the 4th order discretization. The multi-range MRT model uses the 8th order isotropic discretization in the force calculation, which involves the second layer of neighboring lattice sites.
Figure 5.6 Spurious velocities at the gas-liquid interface in 2D. The same fluid properties are used in three simulations: G=-5.0, ν = 0.05. The gas and liquid densities are 0.11 and 1.85, respectively. The interface shown in the figures are plotted with density contours of 0.5 and 1.0. The spurious velocity is plotted under same magnification in the three figures.

(A) BGK model. \( |\mu_{s}|_{\text{max}} = 0.028 \); 

(B) MRT model. \( |\mu_{s}|_{\text{max}} = 0.0053 \); 

(C) MRT model with 8\(^{th}\) order isotropic force. \( |\mu_{s}|_{\text{max}} = 0.0016 \);
Figure 5.7 Simulation of 2D bubble rise, $E_0=1.16$, $M_0=6.18 \times 10^{-9}$, $Re=148.5$

(a) Variation of bubble rise velocity with time
(b) Snapshots of streamlines

107
CHAPTER 6

LATTICE BOLTZMANN SIMULATION OF THE BUOYANT RISE OF BUBBLES

Abstract

Understanding of the bubble dynamics is essential to the design and operation of many gas-liquid two phase reactors. In this chapter, the LBM with adaptive mesh and multi-relaxation time (LBM-AMR-MRT) schemes developed in previous chapters are employed to study the buoyant rise of a gas bubble in a viscous liquid. Simulations are conducted under various conditions for bubbles with large deformation or high Reynolds number. Comparison between the simulation results and experimental data in the literature proves the advantage of the current LBM-AMR-MRT approach over the traditional LBM techniques.

6.1. Introduction

Despite their ubiquitous existence in natural and industrial fluid systems, the behavior of bubbles is far from been fully understood. For a single bubble rising in a still liquid, the reason why it may follow a zigzag or spiral path instead of moving straight upward has
long puzzled scientists since the phenomenon was first pointed out, possibly by Leonardo da Vinci (Lohse, 2003; Prosperetti, 2004). For a large number of bubbles in a gas-liquid chemical reactor, the interactions between bubbles further complicate their behavior by affecting their velocity and the spatial distribution. The bubbles dynamics further influences the mass transfer between the gas and liquid phase as well as the rate of chemical reactions, and affects the overall performance of the reactor (Fan, 1989). Therefore, the dynamics of bubbles not only poses intriguing scientific questions, but is also of great importance to various engineering applications.

A bubble rising in a viscous liquid medium is a typical two-phase flow problem that has been studied extensively using both experimental and numerical approaches. In such flows, both the rise velocity and the bubble shape are determined by the properties of the gas and liquid phases as well as the magnitude of the gravitational force. These complicated nonlinear relations are often correlated in terms of three dimensionless groups, including the Reynolds number \((Re)\), the Eötvös number \((Eo)\), and the Morton number \((Mo)\):

\[
Re = \frac{\rho dU}{\mu} \quad (6.1)
\]

\[
Eo = \frac{\rho gd^2}{\sigma} \quad (6.2)
\]

\[
Mo = \frac{g\mu^4}{\rho \sigma^3} \quad (6.3)
\]
In the above equations, \( \rho \) and \( \mu \) are the density and viscosity of the liquid, \( d \) is the equivalent diameter of the bubble, \( U \) is the rising speed of the bubble, \( g \) is the acceleration of gravity, and \( \sigma \) is the surface tension coefficient of the gas-liquid interface. The bubble regime diagrams made by Grace (1973), and later modified by Bhaga and Weber (1981), are well-known graphical representations of such correlations.

In recent years, various direct numerical simulation techniques have been applied to study the bubble rise behavior. Van Sint Annaland et al. (2005, 2006) simulated different bubble regimes using the both VOF and Front Tracking methods. By VOF method, they simulated condition where \( E_o \) ranged from O(1) to O(10\(^2\)), and \( Re \) from O(1) to O(10). Using Front Tracking method, they could simulate much a wider range of the parameters, with \( E_o \) ranged from O(1) to O(10\(^2\)), and \( Re \) from O(1) to O(10\(^3\)), covering the spherical regime, ellipsoidal regime, and intermediate \( Re \) portion of the spherical cap regime. Yu and Fan (2008) performed similar simulations with the level set method, and focused on the conditions with high \( Re \) (~10\(^3\)) and large deformation (\( E_o \sim 10^2 \)). Simulations concerning the interactions between multiple bubbles in a cluster have been conducted by Bunner and Tryggvason (2002). There are several studies that apply LBM to investigate bubble dynamics, but only a few have reported convincing results by validating the simulation with experiment data, especially under different conditions. Sankaranarayanan et al (2002) used implicit formulation of the interaction potential based LBM to study the drag and virtual mass forces on bubbles. They obtained closures relations of those forces for regular array of spherical and slightly distorted bubbles with \( E_o \) between O(10\(^{-2}\)) and
$O(10^2)$, and $Re$ about 100~400. Other versions of LBM have also been employed to study the dynamics of bubbles, mainly in the spherical and ellipsoidal regimes (Kurtoglu and Lin, 2006; Frank, et al., 2006). In the simulations performed in the current study, the new LBM-AMR approach is employed to investigate the buoyant rise of bubbles under various conditions.

6.2. Model Description

The simulations of bubbles rising due to the buoyant force are carried out in 2D and 3D space with the advanced LBM approach described in previous chapters. For 2D simulations, both single component and multi-component interaction potential models are employed, while all 3D simulations are performed with the multi-component model.

The simulations are conducted in a rectangular domain. A typical grid set-up used in this study is shown in Figure 6.2, with a close-up view of the grid refinement near the bubble. For 2D simulations, usually 5~7 refinement levels are employed. And for 3D simulations, typically 4~5 refinement levels are used due to the limitation on the computational resources. Periodic conditions are applied for all boundaries of the computation domain. The bubbles are assumed to have spherical initial shapes, and the estimated fluid densities in the gas and liquid phase are assigned to the regions in and out of the initial bubble. The simulations then run without the presence of gravity for a certain periodic of time until the two phases reach equilibrium and the bubble volume remains constant. This
initialization process usually takes a few thousand steps, depending on the accuracy of the initial guess of the densities. The initialization step is essential to ensure mass conservation in the subsequent dynamics simulation of bubble rise. Since in the interaction potential based LBM the phase segregation is maintained by spontaneous particle interactions, stable phase distribution is only possible when the two phases are in equilibrium. When the bubble travels through the computation domain, it moves into contact with different part of the liquid phase, and its volume tends to change unless the gas phase inside bubble is in equilibrium with the liquid phase everywhere in the entire domain. After initialization, gravity is turned on using the standard technique for bubble simulations (Bunner and Tryggvason, 2001; Sankaranarayanan et al., 2002), which is able to maintain the total momentum conservation of the entire simulation domain. The applied body force $a(x, t)$ in the fluid is expressed by

$$a(x, t) = g \left(1 - \frac{\bar{\rho}}{\rho(x, t)}\right)$$

where $g$ is the gravitational acceleration, $\bar{\rho}$ is the average density of the entire domain, and $\rho(x, t)$ is the local fluid density.

Figure 6.3 shows the snapshots during the rise of a bubble in a 3D simulation. A slice of the domain demonstrates the four levels of grids employed in the simulation. As the bubble travels upwards, the grids are automatically adapted to ensure the finest resolution near the bubble surface.
6.3. Cap and skirted bubbles

Large bubbles rising in a viscous liquid often exist in cap or skirted shapes. If the liquid viscosity is high, and the bubble Reynolds number is small, the bubble shape is an oblate ellipsoidal cap in side view, and has a dented region in the bottom. In a less viscous liquid, the bubble Reynolds number becomes larger, and its shape changes to the spherical cap with a flat bottom. For very large bubble, a thin annual film of gas trailing behind the rim of the bubble may be observed, which can give the bubble a skirted shape.

Figure 6.4 presents the simulated shapes of oblate ellipsoidal cap bubbles. These bubbles are characterized by large aspect ratio as well as the indentation at the bottom. Figure 6.4 suggests that the dimensionless width of the deformed bubble (the actual bubble width divided by its equivalent diameter) increases monotonically with $Re$, which is in agreement with the experimental observation reported by Bhaga and Weber (1981). Generally, the dented region also grows with the Reynolds number and the Eötvös number. Figure 6.5 shows typical flow patterns by plotting the streamlines drawn with the relative velocity, which is the absolute velocity subtract the bubble velocity. When the bubble deformation is small and no significant dent is present at the bubble base, the liquid passes the bubble smoothly without the formation of vortices. As the deformation becomes more significant with larger dented area, two pairs of counter-rotating vortices start to form in the dented area. For such large bubbles, information of the flow inside the dented region is difficult to obtain experimentally and earlier researchers speculated that a pair of secondary vortices with reverse motion would be necessary in the internal
circulation of the bubble to satisfy the velocity and stress continuity (Clift, et al, 1978). However, instead of being inside the bubble, the secondary vortex appears to be in the dented region outside the bubble as demonstrated by most recent numerical studies using front tracking (Hua, et al, 2008), level-set (Yu and Fan, 2008), and LBM (Kurtoglu and Lin, 2006). The results obtained in this work are consistent with those in above numerical studies. Similar ellipsoidal cap shape is also observed in 3D simulations with Eo=31.4 and Mo=0.21, as shown in Figure 6.6. The bottom view clearly shows the indentation at the bubble base.

With further increase in Reynolds number, the indentation becomes more significant and the rear of the bubble gets more stretched. In this process, the thickness of bubble tail keeps decreasing, and the bubble shape becomes closer to the skirted regime. AMR techniques can provide the sufficient grid resolution that is required to resolve the thin skirt region, as shown in Figure 6.7(a). The streamlines are shown in Figure 6.7(b), which have the similar vortex pattern as in Figure 6.5(c) in the ellipsoidal cap regime, but with large size and further stretched in the flow direction.

Spherical cap shaped bubbles are simulated for the conditions Eo=23.1, Mo=0.33 and Eo=38.4, Mo=0.55, as depicted in Figure 6.8. Compared to ellipsoidal cap bubbles, the spherical cap bubbles have a higher Reynolds number, and a more flat base with little indentation and therefore only one pair of large vortices are seen in the wake region.
6.4. Ellipsoidal bubbles

Small or intermediate size bubbles rising in a low viscosity liquid due to gravity usually take ellipsoidal shapes. The Morton number is on the order of $10^{-5}$ or smaller, due to the low liquid viscosity. The Eötvös number is between O(1) and O(10), so that the bubble shape has a small finite deviation from a sphere. The Reynolds number is often above $10^2$ for such bubbles, so they may exhibit complex vortex structures in their wakes. The typical cases of 1~4 millimeter air bubbles in water fall into this category. For most LBM simulations, the low viscosity and high Reynolds number pose a severe problem in the numerical stability of the algorithms. Fortunately, the numerical instability can be overcome in the current LBM approach with the help of the MRT scheme.

Using the 2D single component model, a series of bubbles with the same Morton number ($Mo=2.3 \times 10^{-5}$) are simulated, which correspond to varying only the bubble size while keeping all fluid properties constant as in real experiments. With the Eötvös number varying from $10^{-1}$ to 10, the bubble gradually transform from spherical to ellipsoidal shape, as shown in Figure 6.9 (b)-(d). Many correlations exist for predicting the rise velocity of the bubble. Here the terminal velocities obtained from the simulation are compared against Fan and Tsuchiya’s (1990) correlation, which combines the linear prediction for low Reynolds number with the Mendelson equation for intermediate Reynolds numbers:

$$u_b = \left( \frac{\sigma g}{\rho} \right)^{1/4} \left[ \left( \frac{Eo}{K_b Mo^{1/4}} \right)^{-n} + \left( \frac{2C}{Eo^{1/2}} + \frac{Eo^{1/2}}{2} \right)^{-n/2} \right]^{-1/n} \quad (6.5)$$
In the equation, $K_b$, $C$, and $n$ are parameters determined by the liquid property and surface condition, and are chosen to be 15, 1.2, and 1.0, respectively. Both the predictions from Equation (6.5) and the numerical results of the velocities are shown in Figure 6.9(a), and a good agreement is found between the two.

Zenit and Magnaudet (2008) conducted a series of experiment of millimeter bubbles rising in several type of silicone oil with different viscosities, and obtained their terminal velocities. Using the 3D multi-component model, simulations are carried out under the same conditions as those in Zenit and Magnaudet’s experiments. Comparisons between numerical and experimental results for the Reynolds number are shown in Figure 6.10.

Two types of silicon oils are included in the comparison: the DMST-05 ($\rho = 918 \text{ kg/m}^3$, $\mu = 45.9 \text{ mPa} \cdot \text{s}$, $\sigma = 19.7 \text{ mN/m}$) and DMST-02 ($\rho = 870 \text{ kg/m}^3$, $\sigma = 18.7 \text{ mN/m}$, $\mu = 17.5 \text{ mPa} \cdot \text{s}$). The Morton number calculated from their properties are $6.2 \times 10^{-7}$ and $1.6 \times 10^{-8}$, respectively. The bubble diameters are in the range of 0.5 to 3 millimeters, so the Eötvös number lies between 0.1 and 5.5. For both liquid, the Reynolds number increases with bubble size, or equivalently, the Eötvös number. For DMST-05, the Reynolds number grows from 30 to over 100 when the Eötvös number increases from 0.8 to 3.5. Meanwhile, the Reynolds number in DMST-02 is much higher than that in DMST-05 due to its lower viscosity, and it also demonstrate a higher growth rate with the Eötvös number. In general, the LBM simulation results have a good agreement with the experiment in both liquids. In comparison, the agreement is better for DMST-05 which
has a higher viscosity. For DMST-02, the simulation tends to slightly under-predict the Reynolds number for larger bubbles.

The extent of the deformation of ellipsoidal bubbles is often characterized by their aspect ratio, which is the ratio between bubble width $b$ and bubble height $h$. In recent experiments of bubbles in silicon oil DMST-05 (Zenit 2009), measurements of bubble aspect ratio are obtained for bubbles with diameters of 1.5~3.5 mm. The experimental results for aspect ratio are plotted in Figure 6.11. Lattice Boltzmann simulations are performed for similar conditions in order to examine the prediction of the bubble shape in the ellipsoidal regime. The properties of DMST-05 yields a Morton number of $6.2 \times 10^{-7}$, and the Morton number is $4.4 \times 10^{-7}$ in the simulations. Two simulations are performed with Éötvös numbers of 2.3 and 4.0, which roughly correspond to 2.5 and 3.0 mm bubbles in DMST-05. The simulation results for the aspect ratio in these two conditions are 1.43 and 2.01, which are slightly smaller than the experimental data, as shown in Figure 6.11.

Various experimental correlations exist for the prediction of aspect ratio in different liquids. For example, the Vakhrushev-Efremov (1970) correlation gives the relation between aspect ratio and liquid and bubble properties in the following form:

$$b / h = \left[0.81 + 0.2 \tanh\left[1.8(0.4 - \log_{10} Ta)\right]\right]^{-3}$$  \hspace{1cm} (6.6)

where $Ta$ is the Tadaki number.
In the above expression, \( d_e \) is the equivalent bubble diameter, and \( U_b \) is the terminal velocity of the rising bubble. The Vakhrushev-Efremov correlation has proven to predict the bubble shape with reasonable accuracy for various liquids. However, the calculation of the Tadaki number needs the value of terminal bubble velocity, which cannot be easily determined from the physical properties of the fluids. In order to compare it with the simulation results, the terminal velocities measured from Zenit’s experiment were used in Equation (6.6) and (6.7) to obtain the aspect ratio. The correlation prediction for the aspect ratio are plotted as a function of the Eötvös number rather than the Tadaki number for better comparison, as seen in Figure 6.11. The correlation predictions matches the experimental data well, although they are slightly higher than experimental results at Eötvös number smaller than 3.8, and lower than experimental results at Eötvös number larger than 3.8. On the other hand, the simulation results for the aspect ratio are lower than both the experiment and the correlation, indicating that the current simulation tends to result in a more spherical bubble shape than that in the physical system.

The bubbles corresponding to the simulation in Figure 6.11 are shown in Figure 6.12. Both the bubble shape and the streamlines of the relative velocity are drawn for the two cases. For the bubble with \( Eo=2.3 \) and an aspect ratio of 1.43, its upper half and lower half are symmetry about the horizontal plane. In contrast, the bubble with \( Eo=4.0 \) and an aspect ratio of 2.01 has a more flat upper surface than the lower surface, and its lower
surface actually deviates from the ellipsoidal shape. With a Reynolds number of 80.7 and 106.3, both bubbles have a pair of counter-rotating vortices in their wakes. The bubble with Eo=4.0 has larger vortices compared to the smaller bubble, due to its large deformation and higher Reynolds number.

Two additional conditions are simulated for ellipsoidal bubbles in 3D, as shown in Figure 6.13(a) and (b). The simulation are performed for bubbles with $Eo=2.45$, $Mo=2.98 \times 10^{-5}$ and $Eo=9.81$, $Mo=1.19 \times 10^{-4}$. Compared to the conditions in the simulation presented in Figure 6.12, the current simulation conditions for the bubble in Figure 6.13 correspond to similar bubble sizes, but in more viscous liquids, as indicted by the larger Morton number. The Reynolds numbers obtained form the simulations are 30.0 and 36.0 for the two cases, respectively. These values of the Reynolds number are much lower than those in the Figure 6.12, since the higher liquid viscosity in this case poses a large resistance for the bubble. However, the changes in viscosity seem to have only small effects on the bubble shape. For the bubble with $Eo=2.45$, the aspect ratio is 1.43, which is identical to the bubble with $Eo=2.3$ and $Mo=4.4 \times 10^{-7}$ in Figure 6.12. The bubble with $Eo=9.81$ has an aspect ratio of 2.50, also consistent with the increasing trend of the aspect ratio with the Eötvös number. The velocity vectors in Figure 6.13(a) show that for the bubble with $Eo=2.45$ the liquid flows past the bubble smoothly without forming vortices in the bubble wake. This flow pattern is different from the flow field shown in Figure 6.12(a), in which the bubble has the same aspect ratio but higher Reynolds number. Similarly, the bubble with $Eo=9.81$ in Figure 6.13(b) has smaller vortices as compared to the bubble in Figure
6.12(b), even though it has a larger aspect ratio. These simulations show that while both the Reynolds number and the bubble deformation affect the generation of vortices, the Reynolds number has a more pronounced effect under the current simulation conditions for ellipsoidal bubbles.

It has been long observed that ellipsoidal bubbles in a low viscosity liquid may rise in either a rectilinear or an oscillatory manner (Lohse, 2003; Prosperetti, 2004). In recent years there has been considerable research effort to understand the origin of the instability that causes the transition from rectilinear rise to oscillatory rise. For air-water system, numerical models reveal that a ellipsoidal bubble with Reynolds number of 600 and aspect ratio of 1.25 will experience transitions from straight path to zigzag and spiral path (Mougin and Magnaudet, 2002). The lift force on the bubble during the transitions is also measured experimentally by ultrasound velocimetry (Shew et al, 2006). It has been recently found through experiments that the oscillation is controlled by the aspect ratio of the bubble (Zenit and Magnaudet, 2008). The streamwise vorticity measured in the bubble wake suggests that when the aspect ratio of the bubble exceeds a certain limit, two vortex tubes are developed in the bubble wake, and a horizontal force is induced and causes the sideways motion of the bubble (Zenit and Magnaudet, 2009).

Two cases with 2D ellipsoidal bubbles are presented in Figure 6.14. The bubble with \( Eo=2.1 \) and \( Re=18.3 \) rises in a rectilinear manner, and keeps the steady ellipsoidal shape. In the other case with a slightly higher \( Eo \) and \( Re \), the bubble follows a straight path.
initially when it gradually develops into the ellipsoidal disk shape, but then both the bubble shape and the path starts to oscillate. The simulated condition ($Mo=8.5 \times 10^{-5}$, $Eo=10.3$) corresponds to a liquid more viscous than water. Tomiyama et al. (2002) studied air bubbles in glycerol-water solutions, and found the oscillatory behavior for a bubble with a diameter of 5.5mm, which corresponds to $Mo=3.0 \times 10^{-6}$, and $Eo=5.8$. In the numerical simulation by Theodoropoulos et al. (2004), bubbles were found to oscillate when $Mo=4.1 \times 10^{-4}$, and $Eo=5.33$. The condition in current case falls between the two studies mentioned above (Tomiyama, et al., 2002; Theodoropoulos et al., 2004).

The snapshots of the streamlines in the two cases with straight and zigzag paths are compared in Figure 6.14(c) and (d). The streamlines for the rectilinearly rising bubble is symmetric about its vertical axis, which is parallel to the flow direction. On the contrary, the orientation of the oscillating bubble varies with time and the flow past the bubble is highly asymmetric, with vortex formation behind the bubble. In all the 3D simulations, however, no oscillation of the bubble path is observed. This fact may be attributed to the lower grid resolution used in 3D simulations. The transition to oscillatory path in clean water is also found to be affected by initial bubble shape. When starting form a spherical shape, the bubble moves considerably slower than the bubble of the same size but starting with a large disturbance of the shape. It also has a smaller aspect ratio in its subsequent rise and keeps a straight path, in contrast to the larger deformation and oscillating path for the bubble with larger initial disturbance (Wu and Gharib, 2002). Since all simulations performed in this study start with a spherical shape, the initial condition might explain the under-predicted aspect ratio and absence of path oscillation in the 3D simulations.
Simulation of air bubble in water is difficult for many direct numerical simulation techniques due to its low viscosity and high surface tension. However, with the enhanced numerical stability and improved accuracy, the current LBM can simulate small and intermediate air bubbles in water. The results for the terminal bubble velocity are compared with the experimental results shown in Figure 6.15. The bubbles in water are sensitive to the condition of the gas-liquid interface. When a small amount of surface active substance adsorbed on the interface, the bubble surface may change from a free-slip condition to a no-slip condition, and therefore changes the drag force on the bubble. Consequently, the contaminated bubbles rise slower than the clean bubbles, as shown in the lower and upper curves respectively for the ellipsoidal regime in Figure 6.15.

Simulations are carried out for 1~4 mm bubbles using MRT scheme with both uniform and adaptive grids. The Reynolds numbers for such bubbles are in the regime between 300 and 900. While the trend of the bubble velocities agrees reasonable well with the experiment, the bubbles seem to fall between the clean and contaminated conditions for the surface. When adaptive mesh is employed, it yields a slightly higher rise velocity, which is closer to that for a clean bubble. Theoretically, the gas-liquid interface in the current LBM corresponds to the free-slip condition. The simulation results indicate that this condition may not be accurately satisfied, probably due to the small but finite spurious velocity at the interface, or insufficient resolution in the boundary layer of the bubble.
The drag coefficients for the spherical and the ellipsoidal bubbles simulated in this work are plotted in Figure 6.16. The results are arranged in four groups depending on the Morton number, including the 2D simulations for $Mo=2.2\times10^{-5}$, and 3D simulations for $Mo=6.2\times10^{-7}$, $1.7\times10^{-8}$, and $2.6\times10^{-11}$. In Bhaga and Weber’s (1981) experiments, the relation between drag coefficient and the Reynolds number were shown to be presented by a single curve for small Reynolds numbers ($Re<10$) regardless of the Morton number:

$$C_D = [(2.67)^{0.9} + (16/Re)^{0.9}]^{1/0.9}$$  \hspace{1cm} (6.8)

For the intermediate Reynolds number ($10<Re<100$), however, the $C_D-Re$ relationship may become a function of the Morton number. The comprehensive review of literature data by Loth (2008) shows that the drag coefficient of uncontaminated bubbles at $Re>10$ first follows that of the clean spherical bubble, which can be calculated using

$$C_D = \frac{16}{Re}$$  \hspace{1cm} (6.9)

Then the drag coefficient gradually increases with in increasing $Re$, and eventually approaches the correlation of Bhaga and Weber at high Reynolds number. The simulation results in Figure 6.16 are consistent with the experimental measurements in the above literature. The drag coefficients fall between the upper and lower bound set by Bhaga and Weber correlation and clean spherical bubble limit respectively. For a given Morton number, the drag coefficient changes from decreasing to increasing trend as the Reynolds number increases. And for a smaller Morton number, the transition occurs at a higher Reynolds number. However, when compared quantitatively to the experimental data (for example, Figure 14 in Loth (2008)), the current simulated drag coefficients exhibit large
deviation from the clean bubble limit even at intermediate Reynolds numbers. In connection to the simulated rise velocity in Figure 6.10 and 6.15, it may again lead to the conclusion that the current simulation tends to under predict the bubble velocity, or over predict the drag coefficient.

6.5. Conclusions

Simulations of the buoyant rise of a gas bubble in a viscous liquid are performed in 2D and 3D for various conditions. The simulation results are compared to experimental results and correlations in the literature. Good agreement for bubble shape and rise velocity is found between the current simulation and the experimental results. Compared to the applicable conditions of the traditional interaction potential LBM model shown in Figure 6.1, typical conditions simulated in the current work as summarized in Figure 6.17 clearly demonstrate that the current LBM-AMR-MRT model significantly expands the accessible regimes of the simulation. Particularly, the cap bubbles with large deformation and ellipsoidal bubbles with high Reynolds number can both be simulated using the current numerical technique. For ellipsoidal cap and skirted bubbles, the mesh refinement ensures the accurate representation of the bubble interface. For bubbles with high Reynolds number, the MRT algorithm ensures the numerical stability of the simulation. Quantitative comparison of aspect ratio, velocity, and drag coefficient with experimental data shows good agreement in general. However, for ellipsoidal bubbles, the simulation tends to under predict the aspect ratio and the velocity of the bubble. Oscillatory motion
is observed for 2D ellipsoidal bubbles, but is absent in 3D simulation. The ellipsoidal bubbles with high Reynolds number are difficult to study since their dynamics is sensitive to a number of factors such as bubble surface condition and initial bubble shape, and considerable scattering the data are also found in experiments. Particularly, the effects of the accuracy of the gas-liquid interface condition on the transient shape and motion of the bubble requires further study in the future.
Figure 6.1 Bubble regime diagram (Bhaga and Weber, 1981).

s: spherical; oe: oblate ellipsoidal; oed: oblate ellipsoidal (disk-like); oec: oblate ellipsoidal cap; scc: spherical-cap with closed steady wake; sco: spherical cap with open unsteady wake; sks: smooth steady skirt; skw: wavy unsteady skirt. The circle represents the accessible regime of conventional LBM based on the interaction potential model.

Figure 6.2 Grid arrangements for 2D simulation of an ellipsoidal cap bubble with $Eo=49.8$ and $Mo=137.4$.
(a) entire computation domain
(b) close-up of bubble region
Figure 6.3 Time sequence of a 3D bubble rise with $Eo=9.81$ and $Mo=1.19\times10^{-4}$.
Figure 6.4 Simulated shapes of oblate ellipsoidal cap bubbles.
(a) $E_0=15.3$, $M_0=13.6$
(b) $E_0=43.4$, $M_0=27.1$
(c) $E_0=49.8$, $M_0=137.4$
(d) $E_0=62.3$, $M_0=135.7$
(e) $E_0=99.6$, $M_0=274.9$

Figure 6.5 Streamlines of relative velocity
(a) $E_0=15.3$, $M_0=13.6$
(b) $E_0=43.4$, $M_0=27.1$
(c) $E_0=99.6$, $M_0=274.9$
Figure 6.6 3D ellipsoidal cap bubble. $E_0=31.4$, $M_0=0.21$.
(a) grid configuration
(b) bottom view showing the dented region

Figure 6.7 Skirted bubble. $E_0=86.8$, $M_0=54.3$
(a) grid configuration
(b) relative streamlines
Figure 6.8 Spherical cap bubble in 2D
(a) $Eo=23.1, Mo=0.33$
(b) $Eo=38.4, Mo=0.55$
Figure 6.9 2D ellipsoidal bubbles with $Mo=2.3\times10^{-5}$
(a) Comparison of simulated bubble rise velocity with Fan-Tsuchiya correlation
(b) Bubble shape with $Eo=0.67$.
(c) Bubble shape with $Eo=1.33$.
(d) Bubble shape with $Eo=7.68$
Figure 6.10 Reynolds number of bubbles rising in silicon oil DMST-05 (Mo=6.2*10^{-7}) and DMST-01 (Mo=1.6*10^{-8}).

Figure 6.11 Aspect ratio of ellipsoidal bubble in silicon oil DMST-05.
Figure 6.12 Simulated shape and streamlines of ellipsoidal bubbles with $Mo=4.4\times10^{-7}$
(a) $Eo=2.3$, $Re=80.7$
(b) $Eo=4.0$, $Re=106.3$

Figure 6.13 Simulated shape and flow field of ellipsoidal bubbles.
(a) $Eo=2.45$, $Re=30.0$, $Mo=2.98\times10^{-5}$
(b) $Eo=9.81$, $Re=36.0$, $Mo=1.19\times10^{-4}$
Figure 6.14 Path and streamlines of 2D ellipsoidal bubbles
(a) Rectilinear path, $Eo=2.1$, $Mo=1.7\times10^{-5}$, $Re=18.3$
(b) Oscillatory path, $Eo=10.3$, $Mo=8.5\times10^{-5}$, $Re=23.2$
(c) Streamlines of a bubble with $Eo=2.1$, $Mo=1.7\times10^{-5}$, $Re=18.3$
(d) Streamlines of a bubble with $Eo=10.3$, $Mo=8.5\times10^{-5}$, $Re=23.2$
Figure 6.15 Simulation results for millimeter air bubbles in water. The experimentally obtained velocity map for air bubble in water at 20°C from Clift, et al. (1978) is used for comparison.

Figure 6.16 Drag coefficients for spherical and ellipsoidal bubbles.
Figure 6.17 Summary of typical simulation conditions in the current work on the regime map
CHAPTER 7

COLLISION OF A DROPLET WITH A POROUS SURFACE

Abstract

Direct simulation of the collision between a liquid droplet and a porous surface is a challenging task due to the separation of scales, complex geometry, and complicated contact conditions between three phases. The LBM-AMR-MRT technique provides a promising approach to solve such a problem. In this study, the collision process of a droplet with a porous surface is analyzed using the LBM-AMR-MRT simulation. The porous surface is constructed from a large number of small particles. Firstly, simulation is run for single phase flows, and the flowrate in the pore space between the particles is validated against empirical correlations. Then simulations are carried out for droplet collision on impermeable and porous surfaces under various conditions, and the droplet dynamics are analyzed based on the simulation results.

7.1. Introduction

The impact of a liquid droplet on a porous surface is relevant to many important processes both in nature and in industry. In environmental applications, the behavior of a droplet
on soil affects the release rate of the liquid into the soil and its evaporation into the atmosphere. For inkjet printing technology, the spreading of the ink droplet on the porous paper surface determines the printing quality. In many cases, the droplet dynamics is coupled with other processes such as heat and mass transport, phase change, or even chemical reactions. In the example of a method proposed to produce hydrogen from nonvolatile fuels, cold liquid droplet first collides with a high temperature porous catalytic surface. Then evaporation takes place and the gaseous reactants diffuse into the pores of the catalytic surface and react to produce hydrogen, which is subsequently transported again out of the porous surface (Salge, et al, 2006).

The dynamic behavior of the droplet during its collision with the porous surface is dictated by the competition among a number of forces, including the inertial force associated with the kinetic energy of the droplet, the viscous force due to the liquid viscosity, the surface tension force, and the morphology and wetting condition of the porous surface. Typical behavior of a droplet on a porous surface includes full and partial adsorption, rebounding, disintegration, and splashing. The dynamics of the droplet is the result of the competition among the various forces mentioned above, and is often correlated to the dimensionless group including the Reynolds number ($Re$), the Weber number ($We$) and the Darcy number ($Da$):

\[
\frac{R}{e} = \frac{ud}{\nu} \quad We = \frac{\rho u^2 d}{\sigma} \quad Da = \frac{K}{d^2}
\]  

(7.1)
where $d$ is the droplet diameter, $\rho$, and $\nu$ are the liquid density and kinematic viscosity, $u$ is the impact velocity, and $K$ is the permeability of the porous surface.

There have been a number of experimental studies concerning the droplet dynamics on a porous surface. The conditions for droplet rebound from a porous superhydrophobic polymer surface is studied by Rioboo, et al. (2008) using a high-speed camera. The transitions between Cassie-Baxter and Wenzel regimes are also discussed for different droplet sizes. When in contact with a high-temperature surface, the evaporation of the droplet may generate a vapor layer that levitates the droplet above the surface, which is well-known as the Leidenfrost phenomenon. However, studies using high-speed camera show that the droplet behavior on a hot ceramic porous may be significantly different from that on an impermeable surface. When the porosity exceeds a certain limit, the droplet cannot be levitated regardless of the surface temperature (Avedisian and Koplik, 1987). Since the liquid droplet may partially or fully penetrate into the porous medium during the collision, information of droplet shape inside the porous medium may become difficult to obtain. In those situations, techniques such as the magnetic resonance imaging (MRI) have been used to visualize the droplet embedded inside the porous surface (Reis Jr., et al., 2003). However, it is difficult for the MRI technique to capture the transient impact dynamics that occurs on the time scale of milliseconds. Therefore, it is only used to analyze the final shape of the droplet or the slow evaporation process, but cannot provide sufficient resolution to investigate the collision while it is occurring.
While numerical models can be employed to study the collision mechanism inside the porous surface as well as provide the sufficient resolution for the small time scales, they still face the challenges because of the separation of scales. While the droplet is usually around millimeter size, the pore size of the substrate is often only micrometers. Directly resolving the flow on the two spatial scales at the same time is a complex problem itself, and it is further complicated by the multiple interfaces between gas, liquid, and solid phases. If resolved in 3D space, the problem involves tracking of droplet surface and moving contact lines, which are both challenging to numerical simulation algorithms.

As a result, to the best of the authors’ knowledge, no attempt has been made to address this two-phase flow on both the droplet and the pore scale at the same time. Most previous numerical studies involving droplet and porous substrate employ a macroscopic model for the porous media, in which the substrate is described by a few parameters such as pore size and porosity. Due to the simplified assumptions made in these studies, they can only treat a certain type of droplet behavior, mostly deposition and partial absorption. For example, Reis, et al. (2004, 2008) used a 2-D model to study the impact of liquid droplets on a porous surface, which is partly absorbed into the porous media. The computation results were in good agreement with the MRI images, and the effects of various factors on the flow characteristics were investigated. Alam et al. (2007) studied the impact and spreading-absorption behavior of small droplets (50 µm in diameter) on topographically irregular porous materials using VOF simulation. Both kinetic energy driven impacts and capillarity driven impacts were investigated and the surface roughness
was found to be a crucial factor during spreading. Alleborn et al. (2004) modeled the spreading and sorption of droplets on a porous substrate. The model was derived using the lubrication theory, and the saturated part of the porous substrate was assumed to be governed by the Darcy’s law. The droplet profile above the substrate and the wetting front inside the substrate were analyzed, and the evolution of the apparent contact angle was discussed. Yu et al. (2008) simulated an evaporative droplet colliding with a high-temperature porous surface. Mass transport of the phase inside porous media was considered and the simulation results for the rebound of the droplet agreed well with the experiment.

In this study, a new numerical model for the collision between a droplet and a porous surface is developed based on the lattice Boltzmann method. With its advantages in handling both the gas-liquid flow and complex fluid-solid boundaries, the LBM is an ideal candidate for droplet-surface collision problems. The interaction potential model provides the LBM with a unified approach to model the gas-liquid interface as well as the wetting of the droplet on the solid surface, and the moving contact line in complex geometries can be treated in a much more elegant manner than other interface tracking or capturing methods, such as front tracking, VOF, or level-set. In addition, the adaptive mesh refinement technique ensures sufficient resolution inside small pores and affordable overall computation cost. The multi-relaxation time scheme is also used to further enhance the numerical stability of the simulation in the presence of different scales. With
the combination of these efforts, the direct simulation that addresses simultaneously the droplet scale and the pore scale becomes feasible.

In the following sections, the numerical model will be briefly described first. The construction of the porous surface used in the simulation and the computational characterization of flow inside the porous surface will be illustrated in sections 7.4 and 7.5. The surface wetting condition will be discussed in section 7.6, focused on the equilibrium contact angle of the droplet on the surface. Then the droplet impingement on non-porous surfaces and porous surfaces will be studied in sections 7.7 and 7.8, respectively. Finally, section 7.9 will provide some conclusions and visions of the future work.

7.2. Model Description

The model system is schematically illustrated in Figure 7.1, which consist of a droplet and a porous surface. The porous surface is directly discretized into solid particles and void space that can be occupied by either gas or liquid phase. The computations are performed in a 3D cubic domain with the LBM-AMR-MRT approach for two fluid components described in previous chapters. Before the simulation, a separate program is run to generate the porous surface from thousands of spherical particles, as described in section 7.3. Information of the particle in the porous surface is used to mark the corresponding locations in the discretized computation simulation. The equilibrium densities of the gas and liquid phase are used to initialize the density distribution. The
droplet has initially a downward impact velocity, while the surrounding gas phase is assumed to be static. Then the simulation starts, and the droplet shape, droplet velocity, and flowfield both inside and outside the porous surface are obtained from the simulation for analysis.

7.3. Generation of porous substrate

Accurate representation of the geometric properties of the porous media is essential to the prediction of their transport properties. A number of techniques have been developed to reconstruct the porous media used with specified geometric information, such as grain or pore shape, porosity, tortuosity, and connectivity. The microstructure of the porous material can be obtained by X-ray microtomography, and 3D structure of the material can be directly constructed from a stack of tomographic images for difference slices of the sample (Martys and Chen, 1996). Using a thin section micro-CT image of the material, 3D microstructure that preserve the typical pore space patterns of the thin section can also be generated by multiple-point statistics method (Okabe and Blunt, 2004). These tomographic imaging techniques are usually employed in the analysis of the microstructures of sandstones (Okabe and Blunt, 2004) and filter cakes (Selomuya, et al, 2006). But more often the random porous medium is reproduced from statistical-based average properties rather than detailed tomographic information. For example, the quartet structure generation set (QSGS) method allows the pore space to grow from an initial distribution to the desired porosity by following a directional growth probability (Wang, et al, 2007). Such method has been applied to reconstruct the random open-cell porous
foams in the analysis of its effective thermal conductivity (Wang and Pan, 2008).

Another typical approach to generate random porous medium is the packing of particle grains that construct the porous medium by steepest descent deposition method, Monte-Carlo deposition method, or discrete element method (DEM) (Bertrand, et al, 2004). In this study, the Monte-Carlo deposition method is adopted to construct the porous substrate by allowing a large number of spherical particles to consolidate under gravity.

The packing algorithm is similar to that developed by Vidal et al. (2003), in which the particles move with a random walk in each iteration and their motion is accepted or rejected based on the value of the Energy of the system. With coordinates of the N particles denoted as \( \mathbf{R} = \{ \mathbf{x}_i \}_{i=1}^{N} \), the energy of the system is defined as

\[
E(\mathbf{R}) = E_{\text{interaction}}(\mathbf{R}) + E_{\text{gravity}}(\mathbf{R})
\]

(7.2)

The second term of the above equation represents the potential energy of the particle system in the gravitational field. For spherical particles, it can be calculated form:

\[
E_{\text{gravity}}(\mathbf{R}) = \frac{4}{3} \pi g \sum_i \rho_i r_i^3 z_i
\]

(7.3)

Where \( g \) is the gravitational acceleration, \( \rho_i, r_i, z_i \) are the density, radius, and elevation of the \( i \)th particle. The interaction energy \( E_{\text{interaction}}(\mathbf{R}) \) is used to prevent the overlap of particles during their motion. It is defined to be the sum of pair-wise potentials of hard spheres:

\[
E_{\text{interaction}}(\mathbf{R}) = \frac{1}{2} \sum_i \sum_j E_{ij}
\]

(7.4)
The particles are initially loosely located in a 3D domain. Then at the beginning of each iteration step, a trial move $R_{j+1}$ is made to update the locations of the particles. The change in the total energy of the system is calculated by comparing the new energy value to that in the previous step.

$$
\Delta E = E(R_{t+1}) - E(R_t)
$$

(7.6)

If the change in energy is negative, the new particle configuration is always accepted. Otherwise, it is accepted with a probability defined by $\Delta E$. A random number $\xi$ is generated and compared to the Boltzmann distribution to determine if the new configuration is to be accepted. Therefore, the configuration for the new iteration step can be expressed as

$$
R_{j+1} = \begin{cases} 
R_{t+1} & \text{if } \Delta E < 0 \text{ or } \xi < e^{-\Delta E/kT} \\
R_t & \text{otherwise}
\end{cases}
$$

(7.7)

During the iteration, the porosity of the porous substrate is monitored, and the process runs until the desire porosity is achieved. This iteration process ensures that the particles gradually consolidate under the effect of gravity. Figure 7.2 illustrates the change of particle configuration in different steps of the Monte-Carlo deposition process. A group of 3000 particles are initially put into the domain with a porosity of 0.80. As the system evolves, the porosity gradually reduces to 0.53 after 1000 iterations, and finally reaches 0.49 after 7000 iterations.
It should be noted that the Monte-Carlo deposition algorithm described above does not represent the actual packing process of particles, since many important factors such as friction and collision are not taken into account. Nevertheless, it is sufficient for the current purpose of this study, which is to generate a random porous medium with a desired porosity. Also, the algorithm usually gives a porosity larger than the real system. Taking spherical particles with identical size for example, the random close packing limit is about 0.36. However, the lowest porosity the algorithm is able to reach is about 0.46 even after a long time of iteration. This phenomenon has been attributed to the lack of contact forces in the Monte-Carlo deposition algorithm (Bertrand, et al, 2004).

7.4. Flow in porous media

In order to validate the current LBM for flows inside porous medium, 3D single phase flow simulations are performed to compare the numerical results with the classical Darcy’s theory. A cluster of 120 randomly packed spherical particles is placed into a cubic domain. The particles have an identical diameter of 8 lattice units, and the overall porosity of the domain is 0.52. Periodic conditions are imposed in the y and z directions, while a pressure difference is specified in the x direction.

The simulated velocity-pressure drop relation is compared against the theoretical results predicted by the classic Darcy’s equation for low Reynolds number flow in porous media:

\[ \mathbf{u} = -\frac{K}{\mu} \nabla p \]  

(7.8)
The permeability of the medium, $K$, can often be approximated using the Carman-Kozeny correlation which has been widely applied for porous media with $\varepsilon < 50\%$:

$$K = \frac{1}{c_0 \tau^2} \frac{1}{S^2} \frac{\varepsilon^3}{(1 - \varepsilon)^2}$$  \hspace{1cm} (7.9)

in which $c_0$ is a pore shape factor, $\tau$ is the tortuosity, $S_0$ is the specific area of the particles, and $\varepsilon$ is the porosity. For mono-sized spherical particles, $c_0 \approx 2$, $\tau = \pi/2$, and $S_0 = 6/d_p$, where $d_p$ is the particle diameter (Bertrand, et al, 2004).

The LB simulation for single phase flow is first carried out for a porous media made of ordered array of mono-sized spherical particles. As shown in Figure 7.3 (a), the particles are placed in a 3×3×3 simple cubic array. The relationship between the pressure gradient and the mean velocity, which is defined as the volumetric flow rate divided by cross-section area, is plotted in Figure 7.3(b) for two different viscosities. Linear relationship between pressure drop and velocity can be clearly found, as predicted by the Darcy’s equation. On the other hand, the mean velocity is found to decrease linearly with the viscosity under the same pressure drop, as in Figure 7.3(c). However, rather than having a slope of -1 as predicted by the Darcy’s equation, the line in Figure 7.3(c) has a slope of $-0.74$. This effect is probably caused by the treatment of the particle boundary conditions in the current LBM. The bounce back condition is known to produce a rough solid surface with a limited spatial resolution of the particle, and therefore the effective radius (“hydrodynamic radius”) of the particle in the simulation will deviate from the specified value. In fact, the hydrodynamic radius has been found to decrease when
viscosity increases (Ladd, 1994). In this situation, the reduced particle size could resulted in a higher porosity, and therefore mitigate the reduction in velocity due to increased viscosity.

The flow inside a random porous medium is shown in Figure 7.4(a). The porous medium is constructed with 150 spherical particles with the same diameter of 8 lattice units, and has a porosity of 0.52. Using the relationship between velocity and pressure drop obtained from the simulation, as shown in Figure 7.4(b), the permeability of the material was found to be 0.21. It is in good agreement with the permeability value calculated from the Carman-Kozeny correlation, which is 0.23 in the current case.

7.5. **Wetting condition of the surface**

The wetting condition of the surface plays an important role during the collision between the droplet and the surface. The surface wettability is usually represented by the contact angle, which is the angle between the gas-liquid interface and liquid solid interface. The thermodynamically based LBM is an ideal method for the modeling of three phase contact problems with complex wetting conditions and moving contact lines, which are extremely difficult to handle using other interface models such as the VOF or level-set method. Instead of directly manipulating the interface geometry near the contact line, the interaction potential based LBM specifies the wetting condition by changing the interaction potential of the surface (Martys and Chen, 1996). Droplets with different equilibrium contact angles representing from wetting to no-wetting conditions are shown
in Figure 7.5(a), and the effect of the solid phase potential on the equilibrium contact angle is shown in Figure 7.5(b).

7.6. Collision on an impermeable surface

The collision of a small droplet on a super hydrophobic surface is simulated by setting the solid surface interaction potential equal to the gas phase potential, so that the contact angle is 180°. A cubic computational domain with 128 lattice units in each direction is used in the simulation. Initially the droplet has a spherical shape with a diameter of 30 lattice units, and is placed in contact with the surface. The Weber number is calculated based on the initial velocity of the falling droplet. Two conditions are simulated, with Weber numbers of 3 and 12, respectively. The droplet shapes during the collision are shown in Figure 7.6 for the two cases. After initial contact with the surface, the droplet starts to spread on the surface and the height of its center of mass continues to decrease. As the liquid moves radially outwards, the inertial energy of the droplet gradually transforms into the surface energy stored on the deformed droplet surface, until the maximum spreading diameter is reached. Then the surface energy starts to release and transforms back into the kinetic energy, while the droplet starts to recoil and attempts to restore its original spherical shape. Due to the nature of the super hydrophobicity, there is little resistance for the droplet motion on the surface so that the loss of energy due to friction is negligible. As the results, most of the kinetic energy is recovered at the end of the recoil stage, and the droplet has sufficient momentum to bounce off the surface.
Comparing the two cases, the droplet with the larger Weber number clearly goes through a larger deformation, which is in accordance with the fact that more kinetic energy needs to be stored by large deformation of the droplet surface.

The extent of the droplet deformation is often characterized by the spreading factor $d^*$ and dimensionless droplet height $h^*$, which are the diameter of the contact area and the height of the droplet nondimensionalized using the initial droplet diameter, respectively. The variation of $d^*$ and $h^*$ with time are plotted in Figure 7.7(a) and (b), respectively. The droplet with $We$ of 12 has a maximum spreading fact of 0.6, while the droplet with $We$ of 3 has a maximum spreading ratio of 0.4. The minimum height of the center of mass is about 0.4 for the droplet with $We$ of 12, and is about 0.6 for the droplet with $We$ of 3. Both quantities show that the droplet with larger $We$ spreads to a larger extent than the droplet with smaller $We$, which is consistent with the images shown in Figure 7.6.

Comparing the spreading time and recoiling time for the two cases shows that the droplet with a higher $We$ reaches its maximum deformation earlier than that with a smaller $We$. When $We$ is 12, the spreading time consumes about 40% of the entire contact time, while for the droplet with $We$ of 3, the spreading time spans almost half of the entire contact time. The $d^*$ and $h^*$ curves also indicate that the deformation process of the droplet with $We$ of 3 is more symmetric for the spreading and recoiling stages.

The contact time of the droplet on the surface can be obtained from Figure 7.7(a) by finding the time when the diameter of the contact area decreases to zero, and it is found to
be 800 and 880 for \( \text{We}=3 \) and 12, respectively. On the other hand, the contact time can be calculated from Rayleigh’s approximation (Wachters and Westerling, 1966)

\[
\frac{t^*}{\text{d}} = \frac{\pi d}{4} \sqrt{\frac{\rho d}{\sigma}}
\]  

(7.10)

Given the parameters used in the current simulation, the contact time calculated from the Rayleigh’s equation is 801. The contact times obtained from the simulations are in good agreement with Rayleigh’s approximation, especially for the droplet with a lower impact velocity.

Snapshots in Figure 7.8 show the process of a droplet with \( \text{We}=6.14 \) colliding with an impermeable surface. The equilibrium contact angle of the droplet on the surface is 60°. The corresponding spreading factor and nondimensional droplet height are given in Figure 7.9(a) at various instants. The droplet first spreads on the surface until about \( t=1500 \), when it starts to recoil. There is a small shape oscillation after the recoil, and the droplet finally reaches the stable shape at about \( t=5000 \). The variation of the dynamic contact angle and the speed of the moving front are shown in Figure 7.9(b). During most part of the collision, the dynamics contact angle is only slightly above its equilibrium value of 60°, except for the initial contact stage and the abrupt change at \( t=3200 \). The cause of the sudden change in contact angle may be related to the change in the velocity of the moving contact line, which changes from receding (recoiling) to advancing (spreading) at \( t=3200 \). The simulation indicates that for the receding contact line, the dynamic contact angle is close to the equilibrium value. However, when the contact line
changes from static or receding state to advancing state, the dynamic angle exhibits a value much larger than the equilibrium contact angle, and this value decreases with decreasing advancing speed.

7.7. Collision on a porous surface

The simulation of the collision of a droplet with a porous substrate is carried out in a 256×256×256 domain. In the first case, the porous substrate is made of particles with diameters of 8 lattice units, and the porosity of the substrate is 0.51. The fluid-solid interactions potential is specified such that the equilibrium contact angle on the solid surface is 60°. The droplet has a diameter of 60 lattice units, and the Reynolds number and Weber number of the droplet are 300 and 6.14, respectively. The Darcy number of the system is 6.5×10⁻⁵. Three snapshots at different instants during the collision are demonstrated in Figure 7.10, showing the partial adsorption of the droplet into the porous surface. Since the ratio of the droplet diameter to particle diameter is only about 8, the porous surface appears to be a heterogeneous material to the impacting droplet. The non-uniformity of the surface results in the irregular shape of the contact region, which is demonstrated in the side view and top view of the droplet. The normally accepted assumption of the axis-symmetric droplet shape is unable to predict the irregular droplet shape under current conditions. Figure 7.11 shows a slice of the computation domain which cur through the center of the droplet. The adaptive mesh applied near the droplet and inside the porous surface is illustrated using the boundary of the mesh blocks, which
each contain 8*8*8 cubic grids. The bottom of the droplet has penetrated into the void space of the porous surface as the result of the high pressure generated due to the impact. The velocity field in the vicinity of the droplet is given in Figure 7.12. The downward flow inside the droplet indicates that the droplet is spreading on the surface and penetrating into the pores. Vortices are observed in the gas phase near the droplet surface, showing a typical flow pattern often recognized in droplet-surface collision problems. There is also considerable gas flow inside the porous surface, which may assist the transport of gaseous species in case of evaporation or chemical reaction.

The diameter of the contact area, droplet height, and penetration depth of the droplet are defined in Figure 7.13(a), and variations of their dimensionless values with time are plotted in Figure 7.13(b). As the droplet spreads on the porous surface, both the spreading factor and the penetration depth increases, while the droplet height decreases. Comparisons of the droplet behavior can be made between the two cases shown in Figure 7.8 and 7.10, since the two collisions have the same droplet size, Weber number, and equilibrium contact angle,. The droplet on the porous surfaces reaches a spreading factor of 1.5 at t=2000, which is much smaller than that of 1.8 on the impermeable surface shown in Figure 7.9(a). The corresponding dimensionless droplet height is about 0.3 on the porous surface, while it is 0.25 on the impermeable surface. The comparisons suggest that the droplet spreads to a less extent on the porous surface than on the impermeable surface. The downward flow that penetrates into the void space apparently contributes to the smaller spreading factor on the porous surface. In addition, the dynamic contact angle
shown in Figure 7.12 for the droplet on the porous surface also seems to be much larger than the value of near 60° on the impermeable surface. This larger dynamic contact angle caused by the surface roughness may also be used to explain the slower spreading on the porous surface. This fact is also in accordance with the experimental observations that the microscopic roughness often makes the surface more hydrophobic (Jung and Bhushan, 2008).

When made up of superhydrophobic particles, the porous surface maintains the superhydrophobic property. Droplets in collision with the superhydrophobic porous surfaces are able to completely rebound from the surface when the pore size is much smaller than the droplet size. Figure 7.14 shows the collision of a droplet with $We=6.41$ impinging on two superhydrophobic porous surfaces. The droplet diameter is 60 lattice units, while the particles in the upper and lower row are 10 and 12 in diameter, respectively. The droplets in both cases rebound from the surface. The initial symmetric droplet shape is lost after rebounding due to the randomness of the particle locations of the surface. Using Rayleigh’s approximation in Equation 7.10, the contact times in the two cases are both estimated to be 2267.7, which is in good agreement with the contact time observed in the simulations. This suggests that although Equation 7.10 is originally developed for impermeable surfaces, its application might be extended to porous surfaces with small pore size and porosity.
7.8. Conclusions

Direct simulations are performed to study the collision between a liquid droplet and a porous surface. Due to the different scales of the pore and the droplet, the complex geometry in the porous medium, and complicated interactions between the three phases, currently the LBM-AMR-MRT seems to the only viable approach to simulate such a problem. For single phase flow inside porous medium, the simulated flowrate and permeability are in good agreement with the empirical correlations in the literature. For droplets impinging on a wettable impermeable surface, the dynamic contact angle is close to the equilibrium contact angle, except during the initial contact and when the moving contact line changes from receding to advancing. For droplet colliding on a porous surface, the spreading factor is smaller than that on an impermeable surface under the same droplet size, Weber number, and equilibrium contact angle. The apparent contact angle on the porous surface is also larger than that on the impermeable surface. The Rayleigh’s approximation for the contact time is found to be valid for both impermeable superhydrophobic surface and porous superhydrophobic surface with small pore size and porosity.
Figure 7.1 Schematic illustration of the model system with a droplet and a porous surface. The solid/void space in the porous surface is represented in the discretized form, so that flow inside the pores can be simulated directly together with the flow on the droplet scale.

Figure 7.2 Generation of the porous surface with 3000 particle using Monte-Carlo deposition.
(a) Initial configuration, $\varepsilon = 0.80$
(b) After 1000 steps, $\varepsilon = 0.53$
(c) After 7000 steps, $\varepsilon = 0.49$
Figure 7.3 Single phase flow in a porosity medium made up of ordered particle array
(a) Particle configuration and velocity field
(b) Variation of mean velocity in the porous medium with pressure drop
(c) Variation of mean velocity in the porous medium with viscosity
Figure 7.4 Single phase flow in a porosity medium made up of randomly packed particles
(a) Particle configuration and velocity field
(b) Variation of mean velocity in the porous medium with pressure drop
Figure 7.5 Equilibrium contact angles of a droplet on a surface
(a) Droplet shapes on a solid surface with different contact angles
(b) Variation of the contact angle with the solid surface potential
Figure 7.6 Snapshots of the collision of a droplet with a non-porous superhydrophobic surface
Figure 7.7 Spreading factor and dimensionless height of the droplet
(a) Comparison of the spreading factor during collision for two droplets with different $We$
(b) Comparison of the non-dimensional height during collision for two droplets with different $We$

Figure 7.8 Snapshots of a droplet colliding with a surface with $We=6.14$ and equilibrium contact angle of $60^\circ$
Figure 7.9 Spreading dynamics of the droplet on the surface
(a) Variation of spreading factor and nondimensional droplet height with time
(b) Variation of spreading speed and dynamic contact angle with time
Figure 7.10 Collision of a droplet on a porous substrate. The first row shows the snapshots in 3-D view, and the middle and bottom row show the corresponding side view and top view, respectively.

Figure 7.11 A slice of the mesh and phase distribution at t=1920. Each block represents a patch of 8*8 grids
Figure 7.12 Velocity field in a cross section at t=1920.

Figure 7.13 Droplet deformation on the porous substrate.
(a) Definitions of the droplet spreading diameter, droplet height, and penetration depth
(b) Variation of non-dimensional spreading factor, droplet height, and penetration depth with time $t$
Figure 7.14 Droplet collisions on superhydrophobic porous surface. Upper row: porous surface permeability is 0.74, and particles diameter is 10. Lower row: porous surface permeability is 0.53, and particle diameter is 12. The droplet Weber number is 6.41 in both cases.
Abstract

Two-phase flows in microchannels have many advantages in heat and mass transfer compared to single-phase flows. In particular, segmented flows such as bubbly and slug flows are often used in microfluidic devices. In this chapter, experiments and lattice Boltzmann simulations are carried out to study the gas-liquid flow in microchannels under various conditions. Two types of mixer geometries are used, including the cross shape and the converging shape channels. The bubble shape, size, and formation mechanism are investigated for different flow rates and different mixer geometries. The simulation results and the experimental results are compared based on dimensionless numbers, and good agreement is found in general. The flow regimes, which dictate the general flow behavior as well as the bubble shape, are found to be dependent upon the Capillary number of the flow. The simulation data confirm that the bubble breakup was induced by the pressure difference in the two phases for small Capillary numbers. In addition, the geometry of the mixing section is also shown to have an impact on the size of the gas and liquid slugs.
8.1. Introduction

Multiphase flows in microfluidic devices have received much attention because of the foreseeable advantages that unique microscale properties have to offer. The performance of such multiphase microfluidic devices often have many favorable characteristics, such as enhanced heat and mass transfer efficiency, reduced axial dispersion, and smaller sample volume. In order to realize these benefits, a good understanding of the complex multiphase flow behavior in microfluidic devices must be developed. In particular, this study is focused on the micro gas-liquid flow systems. Such flows have been used extensively for different applications and offer enhanced performance over conventional systems. For example, in the synthesis of silica nanoparticles in a microfluidic chemical reactor, a narrow size distribution of the nanoparticles was achieved by using inert gas to divide the liquid phase into small segments and to reduce axial dispersion (Khan et al., 2004). Some other applications of the gas-liquid reactions in microchannels include fluorinations (Chambers, et al., 2001), hydrogenation (Kobayashi et al, 2004), and biochemical reactions such as DNA analysis (Burns et al., 1998). These reactions use molar flow rates of the reactant gas on the same order of the liquid reagent flow rate, and typically operate in the slug flow and annular flow regimes (Gunther and Jensen, 2006). Additionally, microchannel heat exchangers such as heat sinks have been developed, which operate using non-adiabatic flows with liquid-vapor phase change (Qu and Mudawar, 2002).
The two-phase flow characteristics in microchannels are determined by the flow conditions, the channel geometry, and properties of both fluids. Generally, it is found that the gas-liquid flow in microchannels could be categorized into three different basic regimes, namely, the bubbly flow, intermittent/slug flow, and the annular flow (Waelchli and Rohr, 2006). The flow regime map has been developed by several authors (Cubaud and Ho, 2004, Haverkamp et al. 2006). These maps are often drawn with respect to the superficial velocities of the gas and liquid phases. Waelchli and Rohr (2006) compared some of the regime maps developed by several research groups. These regime maps show similar trend in general: bubbly flow appears at high liquid velocity and low gas velocity, while annular flow are resulted from at high gas velocity. At intermediate gas and liquid velocities, long gas bubbles are formed and divide the continuous liquid phase into segments so that slug flows occur. Despite the above general trend, there are some discrepancies between those flow maps in detailed demarcation of the regimes, which are probably caused by the different conditions under which the data were obtained. Most studies that aimed to explore the transitions between different regimes are focused on the air-water systems (Zhao and Bi, 2001, Cubaud and Ho, 2004), while some other liquids and gases have also been used, such as isopropanol and nitrogen (Haverkamp et al. 2006). The size of the microchannel ranges from 100 microns to about 1 mm in different studies. The cross sections of the channels used in these studies include triangular, circular, or square shapes (Zhao and Bi, 2001, Chung, et al, 2004). All these factors may contribute to the variations between different flow regime maps. Therefore, a more general regime
map still needs to be developed in order to have thorough understanding of the gas-liquid
flow behavior in microchannels.

To generalize the flow behavior under different conditions, the study of microchannel
flows often uses non-dimensional scaling laws that reveal the relative importance of
different factors. The most important forces in multiphase flows in microchannels are the
inertial force, viscous force, and interfacial force. One important dimensionless number is
the Reynolds number (Re), which describes the ratio of the inertial force to the viscous
force.

\[ Re = \frac{\rho_l u L}{\mu_l} \]  (1)

where \( \rho_l \) is the liquid density, \( u \) is the characteristic velocity, \( \mu_l \) is the dynamic viscosity
of the liquid, and \( L \) is the characteristic length. On the other hand, the ratio between the
viscous force and the surface tension is often characterized by the Capillary number (Ca):

\[ Ca = \frac{\mu_l u}{\sigma} \]  (2)

where \( \sigma \) is the surface tension between gas and liquid. For many typical multiphase
flows in microfluidic devices, both \( Ca \) and \( Re \) are small, due to the small length scale and
low velocity.

The formation pattern of bubbles or slugs in the microchannels is highly sensitive to the
flow conditions, the channel geometry, as well as the wetting condition of the channel
wall. Garstecki, et al. (2005) used the flow focusing device with a small an orifice to
generate monodispersed bubbles. They found that in their device the bubble formation was due to the pressure gradient and the breakup could be controlled by the flowrate of the continuous liquid phase. Garstecki, et al (2006) later found that the breakup mechanism in microfluidic T-junctions was also due to the pressure drop generated by the high flow resistance to the continuous phase induced by the emerging bubble/droplet. However, the breakup in a similar T-junction device but with a much smaller gas inlet was reported to be controlled by shear rapture (Xu, et al. 2006). Cubaud and Ho (2004) studied the bubbles generated in a cross-shaped mixing section in square microchannels. They found that the breakup mechanism in their device could be understood as the competition of pressure drops in the gas and the liquid phase. The bubble length in their experiment could be predicted by the ratio of the gas/liquid flowrate (Cubaud, et al. 2005). The effect of the mixing geometry was investigated by Haeverkamp and co-workers (2006). They designed two mixing geometries, namely, the “T-type” and the “smooth” mixers, and studied the flow of nitrogen-water as well as nitrogen-isopropanol system in both mixers. They reported that the breakup by pressure gradient was only observed in the T-type mixer, while the jet instability was the only mechanism for bubble formation in the smooth mixer.

Compared to the experimental studies, there are relatively fewer research works that use numerical approaches to investigate multiphase flows in microfluidic devices. Although interface tracking and interface capturing methods have been used extensively in unbounded domains to study the dynamics of bubbles and droplets, the complex
geometries in microfluidic devices and the complicated wetting conditions often make these methods difficult to apply. Weber and Shandas (2007) used VOF approach provided by the commercial CFD-ACE package to simulate the bubble formation in the flow focusing devices. By examining the simulated pressure profile, they were able to validate the bubble formation mechanism proposed in the previous experimental work. Qian and Lawal (2006) studied the gas-liquid slug flow regime in T-junction microchannels using VOF based commercial CFD package FLUENT. The slug lengths at various operating conditions were in good agreement with experimental data. Besides the conventional CFD methods based on Navier-Stokes equations, recently novel simulation techniques such as the Lattice Boltzmann Method (LBM) have also been applied in microfluidic multiphase flows. Dupin et al. (2006) used LBM to study the flow-focusing device. They were able to simulate the droplet formation in the flow-focusing device at low $Re$ and $Ca$, and their results matched well with the experiments by Anna et al (2003). However, since they used sharp interface in their simulation and no phase separation mechanism was included, the breakup/coalescence had to be taken care of explicitly. The wetting condition at the wall also required special treatment.

In this chapter, the LBM simulation of gas-liquid flow in microchannels will be presented. The simulation results will be related to the experimental work, which uses either silicon oil or aqueous sugar solutions as the liquid phase, and air as the gas phase. The flow regime and bubble formation mechanisms are investigated under different conditions. The effects of mixing geometries are also analyzed. This study demonstrates the
prediction capability of LBM in multiphase microfluidic applications. The results from this study will provide useful information for understanding the nature of gas-liquid flow in microchannels and can help the design of multiphase microfluidic devices.

8.2. Model Description

The LBM simulation is carried out for two-phase flows in microfluidic devices using the multi-component model developed by Shan and Chen (1993). Although a single component with non-ideal equation of state can also result in separation of liquid and vapor phases, it faces the problem of excessive condensation and evaporation, which is not typically expected under the conditions in this study. By including the second component, the repulsive interaction between the two components will keep them in two different phases (Sankaranarayanan, et. al., 2002). In this work, all simulations were performed using the two-component model described in Chapter 2.

The computation domain is a 2-D projection of the experimental device, including the inlet and mixing sections. 20 grid points are used across the width of both the central channel and the inlet channels. In most simulations in this study, 600 grid points are used in the length of the channel. However, in some cases, in order to reduce simulation time, a short channel with 300 grid points is used. The velocities of each component are specified at the inlet boundaries, while the pressure is held constant at the outlet boundary. Bounce back conditions are used on the fluid-solid boundaries in order to obtain no-slip condition for the velocity. Initially, the equilibrium gas and liquid phases with zero
velocity are specified in the gas and liquid inlet, respectively. The main channel is filled with liquid at rest. When simulation starts, gas and liquid flow into the domain according to the specified velocities at the inlets. The variables used in the simulation were all in the dimensionless form, and the results are compared with experiments based on dimensionless numbers such as $Ca$, and flow rate ratio $u_l / u_g$.

### 8.3. Experiment setup

The experiment setup for the microfluidic experiment was shown schematically in Figure 8.1(a). The microchannels are fabricated in polymethyl methacrylate (PMMA) using an Aerotech ultra precision micromilling system with 125 and 250 micron bits for the channels and 1 millimeter bit for the inlet and outlet. All channels are 125 microns deep and are sealed by thermobonding a transparent thin film of PMMA. Inlet and outlet ports are glued over the inlet and outlet holes with 1/8” barbed tubing ports. The Liquid inlet is immediately split into 2 channels that travel around the air inlet and converge at the mixing zone, which has either a cross shape or a converging shape, as shown in Figure 1 (b) and (c). A dual syringe pump is used to push the liquid and air streams into the microchannels. When setting a new flowrate, the system is allowed to run for 5 minutes to reach steady state before images were taken. Images are captured using an inverted microscope with a 4x objective and a high speed CMOS camera capable of 1000 frames per second at full resolution. Two types of liquid are used as the continuous phase:
aqueous solution of sucrose and glucose with a viscosity of 30~60 centipoises, and mineral oil with a viscosity of 75 centipoises. Air is used as the dispersed phase.

8.4. Effect of Ca on flow regime

Because of their wide applications in microfluidic devices, this study is mainly focused on the segmented gas-liquid flows, i.e., flows in bubbly and slug regimes. It has been recognized that Capillary number ($Ca$), which describes the ratio between the viscous force and the surface tension force, has a strong influence on the flow patterns, especially the mechanism of the formation of the bubbles/slugs. Generally, in flow focusing devices, when $Ca$ is small (<0.01), the formation of bubbles is dominated by the pressure drop across the bubble (Gunther and Jensen, 2006). On the contrary, when $Ca$ is large, the viscous force is strong enough to overcome the surface tension and the bubbles are usually formed by shear instability. In order to investigate the effect of $Ca$, simulations are performed with different values of the surface tension, flow speed, and liquid viscosity. Experiments are also carried out using two different liquids: silicon oil and sugar solution.

Figure 8.2 shows the formation of bubbles at $Ca$=0.2. The surface tension in these cases is not strong enough to overcome the shear force, and the gas phase is squeezed into a thin stream in the mixing section. Spherical bubbles are formed at the tip of the gas stream, with a radius much smaller than the channel width. In Figure 8.2(a), the ratio of the gas flow rate to the liquid flow rate is 1:8, and the bubble size and formation
frequency are non-uniform. In Figure 8.2(b), the ratio of the gas flow rate to the liquid flow rate is increased to 1:4, which results in a regular pattern of the bubbles with a uniform radius and a fixed frequency, except the first bubble which is much larger compared to the others.

When $Ca$ is reduced to about 0.03, bubbles with bullet shapes are formed in the mixing section. These bubbles are similar to the typical “Taylor bubbles” in the gas-liquid flow in tubes and channels (Taha and Cui, 2006). A thin liquid film layer is always present between the bubble and the channel wall, preventing the direct contact of the two. Figure 8.3 shows the image of the bubbles obtained from experiment using silicon oil and air in 125$\mu$m wide channels. The effects of different $Ca$ and flow rate ratio are tested by changing the gas and the liquid flow rate. It is observed that larger gas to liquid flow rate ratio leads to longer gas bubbles. Under the same flow rate ratio, a smaller $Ca$ number yields a longer bubble. The bubbles shown in Figure 8.3(a) are almost spherical, while the bubbles in (b) and (c) have elongated shapes. In the numerical simulation, by increasing the surface tension and reducing the flow rate, a lower $Ca$ can be reached, as shown in Figure 8.4. The $Ca$ number in the simulation was comparable to the experiment condition used in Figure 8.3, and the bubbles shapes in the simulation were close to those observed experimentally.

The bubble formation process for $Ca=0.04$ is shown in Figure 8.5. The experiment is conducted in a cross-shaped channel 250$\mu$m in width using sugar solution as the liquid
phase. The formation of the bubble starts with the co-flow of the gas and liquid in the mixing section. After the front of the gas stream enters the main channel, the tip of the gas phase keeps expanding, and the neck connecting the bubble tip and the gas stream keeps thinning. The thinning of the neck ultimately leads to the breakup of the bubble from the gas stream. In this case, the breakup point is located in the main channel downstream of the mixing section, and the width of the bubble is almost the same as the width of the channel. The bubble formation process was also simulated under the same $Ca$ number and flow rate ratio, as shown in Figure 8.6. The simulation was able to reproduce the shape of the bubble during the formation as well as the location of the breakup point.

With further decrease of $Ca$, the surface tension force starts to dominate over the viscous force. As a result, the gas-liquid interface is able to expand after the mixing section until it is constrained by the channel walls, almost blocking the entire liquid flow, as shown in the experimental picture in Figure 8.7(a). This in turn leads to increased pressure in the liquid phase, and this increased pressure enables the liquid to pinch off the gas stream and form a gas slug. Such bubble formation process caused by pressure drop across the interface is believed to the main mechanism for bubble formation at low $Ca$ numbers (Garstecki, et al. 2006). Simulation results under the same flow condition are shown in Figure 8.7(b). It is observed in both experiment and in simulation that the gas phase in the main channel is in the slug shape, which has a much larger contact area with the channel wall compared to the bullet shape bubbles. The breakup point is located at the end of the
mixing section, rather than in the downstream channel as in the previous case in Figure 8.5 and Figure 8.6.

In order to verify that the bubble formation is induced by pressure drop, the pressure profiles at the gas inlet and the liquid inlet are extracted from the simulation data. The sample point in the gas phase is chosen at the center of the gas inlet. The sample point for the liquid phase is chosen on the centerline of the liquid channel, 5 grid spaces upstream the mixing region in order to ensure that it is always in the liquid phase. Figure 8.8(a) shows the snapshots of the simulated bubble formation under the condition $Ca=0.006$, and $Q_g:Q_l=1:2$. The variation of the pressure at the gas and liquid inlets with time is shown in Figure 8.8(b), in which the corresponding instants to the snapshots in Figure 8.8(a) are also marked.

It is clear that during the waiting period (before the gas stream goes past the mixing section), the pressure in gas inlet is always higher than that in the liquid, due to the Laplace pressure across the concave interface (point A). As the interface moves forward, the pressure difference between the two phases decreases due to the decrease of the interface curvature. Once the gas stream passes the mixing region and blocks the liquid flow, the pressure in the liquid starts to build up. The interface also changes from concave to convex, and therefore the liquid pressure becomes higher than the gas pressure (point B). The liquid pressure reaches its maximum when the width of the gas stream is at minimum (point C). When the bubble breaks away from the gas stream, the
liquid pressure drops while the gas pressure goes up. The gas inlet pressure again
becomes higher than the liquid inlet pressure (point D). The previous bubble formation
cycle is also included in the same figure, which shows a consistent pattern of pressure
fluctuation. The pressure difference in the two phases can be interpreted using the
Laplace pressure, indicating that the bubble formation process can be viewed as a series
of equilibrium states. The variation of pressure with time confirms the hypothesis that the
pressure difference is the main mechanism for bubble formation at low $Ca$ number.

For the simulations in the slug regime, it should be noted the liquid film between the gas
bubble and the channel wall is almost invisible. This may partly be attributed to the
limited resolution of current simulation. On the other hand, as observed by Serizawa, et al.
(2002) and Cubaud et al. (2004), the liquid film could become very thin or even partially
dry out in small channels with a width about 50 micron. The film thickness depends on
the strength of the surface tension, the bubble length, the bubble velocity, as well as the
surface property of the channel wall. When dry patches are formed, the flow problem
becomes much more complicated, with complex moving contact lines and small
droplets/bubbles sticking on the wall. This poses tremendous challenges for numerical
simulation, and cannot be solved by increasing the spatial resolution alone.

van der Graaf, et al. (2006) used free-energy based LBM approach to study the formation
of droplets in a T-junction. The $Ca$ number range in that paper was similar to the one in
the present work. They observed similar regimes of droplet shapes, i.e., small droplets
were formed at large $Ca$ numbers while longer slugs were formed at small $Ca$ numbers. In particular, they found that the wetting condition on the boundaries could slightly affect the droplet size. There might be similar effects of wettability in the interaction potential based LBM used in the current study, which could contribute to the discrepancy between the experiments and the simulation results.

8.5. Effect of channel geometry

To investigate the effect of the geometry of the mixing section on the flow characteristics, both experiments and simulations are carried out for two types of mixers. One is the cross-shaped mixer, in which the liquid inlet channels are perpendicular to the main channel. The other type is the converging mixer, where the two liquid channels are at 45 degrees to the main channel. The width of the channels in both geometries is 125µm.

Figure 8.9 shows the comparison of the experimental results in both geometries under the same flow conditions. Two different flow conditions are tested for each geometry. The different flow conditions are achieved by fixing the gas flow rate while changing the liquid flow rate. In each case, the figures present the flow in the mixing section as well as the flow in the downstream channel where the bubbles reached stable shapes. For the same geometry, increasing the ratio of gas flow rate to liquid flow rate yields an increase in the bubble length. Flows in both geometries show the same trend for the change of bubble shape and size with increasing liquid flow rate. For the flows in different
geometries under the same flow condition, the shapes of the bubbles are similar. However, as shown in Figure 8.9, the size of the bubble and the spacing between the bubbles can be quite different.

The simulation results in Figure 8.9 also show that the mixer geometry affects the bubble length and the spacing between the bubbles. For the case where \( Ca=0.035 \), and \( Q\text{l}:Q\text{g}=4:1 \), the bubble size in both geometries are similar. However, the converging channel leads to longer liquid plugs between the bubbles. For the case where \( Ca=0.006 \), \( Q\text{l}:Q\text{g}=1:1 \), the length of the gas bubbles and the liquid plugs are both larger than that in the cross-shaped channel. The simulation results show some discrepancy with the experiments. The possible reasons might be that the simulation is unable to completely capture the wetting conditions between the fluid and the channel wall, and the flow in the narrow liquid film between the bubble and the wall.

Figure 8.10 shows the bubble formation in the two types of channels obtained from simulation results under the same operating conditions. In both cases, the \( Ca \) number is 0.07, and \( Q\text{g}:Q\text{l}=1:4 \). It can be seen from Figure 8.10(a) that the cross-shaped mixer gives a relatively consistent bubble size and shape. For the converging mixer shown in Figure 8.10(b), since the liquid coming into the mixing section has a higher velocity parallel to the main channel, the gas stream is stretched much longer towards downstream, resulting in a longer bubble. After the detachment of the long bubble, a smaller bubble with a more
spherical shape is generated. The long bubble and short bubble are formed in an alternating pattern.

8.6. Pressure drop and flow field

The multicomponent LBM can be used to simulate two phases with various density and viscosity ratios. In this work, the interaction potential model for binary mixture is employed, with the first component having the non-ideal potential of the form

\[ \psi_1(\rho) = 1 - \exp(-\rho) \]  

And the other component is assumed to be an ideal gas. The density and viscosity ratios between the two phases resulted from such potentials is about 30. Although not matching the real density and viscosity ratio of the gas-liquid system, they shed some light on the flow characteristics of two phases with different densities and viscosities.

The snapshots of simulation results are shown in Figure 8.11. The Ca number in this case is 0.017, and the flow rate ratio between the two phases is 1:1. The liquid phase has a dynamic viscosity 26 times higher than that of the gas phase. The pressure-drop mechanism of the bubble formation can be clearly seen from the evolution of the interface shape in the mixing region. The breakup process is found to be similar to those obtained from simulations using two identical components.
The pressure drop along the centerline of the channel was shown in Figure 8.12(a). The discontinuities in pressure are caused by the curved interface between and two phases and the pressure jump across the interface equals to the Laplace pressure. The Laplace pressure is higher at the front edge of the bubble than at the rear at the bubble, since the front interface is more curved and has a smaller radius of curvature. The pressure inside the bubble is almost flat, compared to the large pressure drop in the liquid phase. This can be attributed to over 20 times difference in the dynamic viscosity of the two phases in the simulation.

The streamlines drawn using the relative velocity to the bubble is shown in Figure 8.12(b). The relative velocity is obtained by subtracting the average bubble velocity from the velocity field. A pair of counter rotating vortices are found in the liquid region between two consecutive gas bubbles. This flow vortex pattern is consistent with the theories for typical Taylor bubbles and PIV measurements reported in the literature (Waelchli, and von Rohr, 2006). Similar vortex pairs are also found inside the bubble.

8.7. Conclusions

The Lattice Boltzmann simulation is carried out to study the gas-liquid flow in microchannels. The bubble shape, size, and formation mechanisms are investigated under different flow conditions. The simulation results are compared with experimental results using dimensionless numbers, and reasonable agreement is found between the two. It is
observed that at higher $Ca$ number ($Ca > 0.03$), the bubbles are generally formed by shear instability, characterized by the stretching of the gas stream. In this case, the bubbles have spherical or bullet shapes. At lower $Ca$ number ($Ca < 0.01$), the bubbles are usually pinched off by the pressure difference between the two phases, and are present in slug form. The geometry of the mixing section also affects the bubble size and the spacing between the bubbles. Simulations with different density and viscosity ratios are performed, and the results are consistent with the previous conclusions. Some of the discrepancy between the simulation and the experiment might be attributes to the inaccurate wetting condition and the 3-D effects, which require further investigation.
Figure 8.1 Experimental setup
(a) Schematic illustration of the experiment setup
(b) Channel with cross-shape intersection
(c) Channel with smooth (converging) intersection
Figure 8.2 Simulation results for $Ca=0.2$. The region in red represents the gas phase, and the region in blue represents the liquid phase.

(a) $Q_g:Q_l=1:8$

(b) $Q_g:Q_l=1:4$
Figure 8.3 Experimental results for air-silicon oil in 125 µm channel.
(a) $Ca=0.034$, $Q_g:Q_l = 1:1$
(b) $Ca=0.034$, $Q_g:Q_l = 2:1$
(c) $Ca=0.017$, $Q_g:Q_l = 2:1$

Figure 8.4 Simulation results for $Ca=0.03$. $Q_g:Q_l = 1:2$
Figure 8.5 Air bubble formation in sugar solution in 250µm channel. $Ca=0.04$. $Q_s:Q_l = 1:2$

Figure 8.6 Simulation results for $Ca=0.04$, $Q_s:Q_l = 1:2$
Figure 8.7 Experimental and simulation results for slug regime
(a) Experiment for Air-silicon oil in 125 µm channel, $Ca=0.003$, $Q_g:Q_l=1:1$
(b) Simulation result for $Ca=0.003$, $Q_g:Q_l=1:1$. 
Figure 8.8 Simulation results for $Ca=0.006$, $Q_g:Q_l=1:2$.
(a) Snapshots of the bubble formation process
(b) Pressure variation at the gas and liquid inlet during bubble formation, time points A to D correspond to the four snapshots in (a)
Figure 8.9 Comparison of simulation results in “cross” and “converging” channels.

(a) $Ca=0.035$, $Q_g:Q_l=1:4$
(b) $Ca=0.006$, $Q_g:Q_l=1:1$
Figure 8.10 Comparison of bubble formation process in different geometries with $Ca=0.07\;Q_g:Q_l=1:4$
(a) “cross” channel
(b) “converging” channel
Figure 8.11 Simulation results for Ca=0.017, Q_g:Q_l=1:1, μ_g:μ_l=1:26.
Figure 8.12 Pressure and velocity field
(a) Pressure distribution along the centerline of the channel
(b) Vortices in the gas and liquid slugs, drawn by the streamlines of the relative velocity
CHAPTER 9

CONCLUSIONS AND RECOMMENDATIONS

9.1. Conclusions

In this study, a novel numerical technique is developed to improve the performance of the lattice Boltzmann method in simulating multiphase flow problems. The followings are the major accomplishments regarding the newly developed LBM:

1. High density ratio between the liquid phase and the gas phase

Previous interaction potential based LBM for multiphase multi-component simulation is limited to stable density ratios less than 50. Although a high density ratio model has been developed for the single-component LBM, no high density ratio multi-component model has been reported. In this study, the high density ratio multi-component model is developed by modifying the form of the interaction potentials. The interaction potential for the self interactions in the non-ideal component is calculated based on the Carnahan-Starling equation of state, while the cross-interaction between the non-ideal and ideal component is treated separately to ensure equilibrium between the two components. As the results, stable density ratios of 1000 can be achieved in the simulation.
2. Adaptive mesh refinement technique

The adaptive mesh refinement capability is developed for the interaction potential based LBM. The block-structured mesh is generated and managed using an open source code PARAMESH. Special algorithm is designed to exchange information between fine and coarse grids, and care has been taken to maintain consistent physical properties for different grid sizes. When a moving gas-liquid interface is involved, it is always located in the finest grids, and the mesh resolution is automatically adjusted according to the motion of the interface. The adaptive mesh is shown to provide accurate predictions of the interface and to significantly reduce the computational cost.

3. Improved stability for simulations of low viscosity fluids

The stability of the multiphase LBM is appreciably improved by incorporating the multi-relaxation time algorithm into the interaction potential model. The collision term of the lattice Boltzmann equation is transformed into the moment space, and a matrix representation is adopted to calculate the post-collision distributions. The propagation step is performed in the velocity space as usual. This approach introduces a number of adjustable parameters that can be used to fine-tune the stability of the algorithm. Test cases prove that the lower limit of the stable kinematic viscosity can be reduced by an order of magnitude. In the simulations of bubbles, the new multi-relaxation time scheme is still stable when the Reynolds number reaches about 1000, while the original LBM model is often limited to Reynolds numbers below 100.
Using the lattice Boltzmann method, a number of multiphase flow problems are investigated in this study. The buoyant rise of a gas bubble in a viscous liquid is simulated under various conditions. Particular attention is paid to two types of bubbles: ellipsoidal cap bubbles and skirted bubbles with larger deformation, and ellipsoidal bubbles with high Reynolds number. The predicted bubble shapes and rise velocities are compared to the experimental results in the literature and good agreement is found between the two. Compared to the original LBM that is only able to simulation bubbles with small deformation and low velocity, the newly developed model can simulate bubbles under much broader conditions. The simulation is also carried out for the droplet collision with a porous surface. The unique feature of this simulation is that both the droplet scale flow and pore scale flow are directly simulated at the same time. This can only be done with the newly developed LBM model with adaptive mesh. The simulation predictions for flow inside porous media and the wetting of liquid droplet on a solid surface are analyzed and validated against widely used correlations. The droplet dynamics on porous surfaces are investigated and compared to that on impermeable surfaces. It is found that the droplet spreads slower on the porous surface than on the impermeable surface. The contact time of a droplet on a non-wetting porous surface can be estimated using the same equation as that for the impermeable surface if the pore size is small. Finally, the bubble formation in microchannels is simulated under different gas and liquid flow rates. The simulation shows that when the Capillary number is small, the flow is in the bubbly regime, in which small bubbles are generated by the shear force.
between the gas and liquid. When the flow rate is larger, large slugs are formed due to the pressure difference between the gas and liquid phase.

9.2. Recommendations for future studies

Although the parameter range of the new LBM model is significantly larger than that of the original model, it still has difficulties to reach some of the desired conditions. In general, the parameter range of the LBM is mainly limited by the magnitude of the velocity, the density ratio, the viscosity, and the surface tension. In order to perform simulations under various conditions, it is desired that the algorithm remains stable when all above parameters are adjusted independently. Although the value of the surface tension in the current LBM model can be varied to some extent, it can not be specified freely. The reason is that in the current LBM model both the phase equilibrium and the surface tension come from the interaction potential, and therefore are not completely independent. The surface tension values in the current model are often too large for practical applications. Consequently, it is difficult to simulate large deformation of the bubbles due to the large surface tension in the simulation. Moreover, when the surface tension is force to be small, the simulation often loses isotropy and square interface emerges. The reason for such non-isotropic interfaces can be understood from the pressure tensor analysis (Shan, 2008). Currently the bubbles with small surface tension (large Eötvös number) can only be simulated with very fine grid resolutions, which is not computationally efficient. Clearly, a model with larger range of surface tension values is desired. It is noted that the free-energy based LBM can adjust surface tension in a much
The technique needs to be investigated for the possibility to adopt an alternative surface tension model for the interaction potential LBM.

The multiphase flow problems are often coupled with heat and mass transfer processes. However, the coupling between heat/mass transport and multiphase LBM is scarcely reported. Although heat/mass transfer can be computed using the lattice equation for scalar transport, it has only been coupled with single phase LBM. The difficulty to integrate heat/mass transfer with the multiphase LBM lies in the interface between the two phases, where the coupling of the density distribution and the heat/mass flux often causes instabilities and inaccurate results. The problem is even more severe when phase change takes place at the interface, for example, during droplet evaporation or vapor bubble growth. A coupled model for LBM and mass/heat transport will be useful for such applications.

The bubble simulations in this study emphasize the steady state characteristics of the bubbles. However, the transient properties of the bubbles are also important, especially in bubble swarms. In the current simulation, no oscillation is found for 3D ellipsoidal bubbles, and the reason is not yet identified. The simulation also tends to underestimate the aspect ratio and rise speed of the ellipsoidal bubble. Experimentally, the ellipsoidal bubbles with high Reynolds numbers are observed to have unstable paths and shapes. The different patterns of the bubble is largely due to the different surface conditions: when contaminates are adsorbed on the interfaces they change the surface condition form free
shear to no-slip, and make the surface more rigid. In addition, the oscillation is also affected by other factors such as the initial bubble shape. Future simulations of such bubbles need to take these factors into account in order to accurately model the bubble behavior.

For droplet collision on a porous surface, more parametric analysis need to be performed to investigate the effects of the pore size, porosity, and liquid properties on the droplet spreading and penetration. Particularly, simulation needs to be carried out to compare its predictions with the experimental data available in the literature, such as the MRI images of the droplet shape inside the porous surface. A very interesting application of such simulation is the collision between a fuel droplet and a high-temperature catalyst particle, which involves heat and mass transfer, phase change, and chemical reactions. The simulation, however, requires the coupling of the LBM with heat and mass transfer models and reaction kinetics models. It can also be used to investigate the rebounding condition of an evaporative droplet on the porous surface for different pore sizes, porosities, and thermal conductivity of the porous surface.

The ultimate goal of the direct numerical simulation on the bubble and droplet scale is to provide closures to reactor scale models. Such closures are often based on the collective behavior of bubble swarms or groups of droplets. Therefore, simulation of multiple bubble or droplet is needed. The difficulty lies in the treatment of the topology changes involving breakup or coalescence of the bubbles or droplets. This is largely an unresolved
issue in any type of direct numerical simulation techniques. For the current LBM model, the feasibility of controlling such topology changes of the interface by manipulating interaction potentials needs to be studied.
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205


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