Lattice Boltzmann Simulation To Study Single And Multi Bubble Dynamics

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LATTICE BOLTZMANN SIMULATION TO STUDY SINGLE
AND MULTI BUBBLE DYNAMICS

by

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B.Tech. Indian Institute of Technology Delhi, 2004

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ABSTRACT

In recent years, the lattice Boltzmann method (LBM) has emerged as a powerful tool that has replaced conventional macroscopic techniques like Computational Fluid Dynamics (CFD) in many applications. The LBM starts from meso- and microscopic Boltzmann’s kinetic equation to determine macroscopic fluid dynamics. The origins of LBM can be drawn back to lattice gas cellular automata (LGCA); however, it lacks Galilean invariance and creates statistical noise in the system. LBM on the other hand does away from these drawbacks of LGCA, and is easy to implement in complex geometries and can be used to study microscopic flow behavior in complex fluids/fluid mixtures. In this work, the LBM is used as a tool to study isothermal bubble dynamics of single and multiple bubbles in heavier fluids. Some benchmark problems have been solved to prove the effectiveness of LBM over conventional solvers and results have been compared to analytical/existing solutions. Flow behavior at different flow parameters have been recorded and presented. Bubble shape regimes have been classified based on the important two-phase flow parameters, namely the Eotvos number, Morton number, Reynolds number and the Weber number. Single bubble simulations have been conducted in fairly large domains to capture terminal velocities, which have been compared to existing theoretical solutions, obtained using the potential flow theory. The terminal velocities so obtained have also been used for the estimation of drag and drag coefficient for a range of Eotvos and Reynolds numbers, and the drag coefficient so computed has been compared with those predicted by existing correlations and analytical expressions. Bubble dynamics and collision and coalescence for multiple bubbles rising under the influence of gravity in fully periodic domains have been simulated using LBM, and the flow behavior around such bubbles prior to and after coalescence have been studied and
the results presented. The study of multiple bubble dynamics reveals the influence of the wake on the shape and collision of downstream bubbles, and yields valuable insights into the physics of intermediate stages when multiple bubbles collide and form an elongated/stretch bubble. The flow and bubble coalescence behavior predicted in this study compares very well with experimentally captured bubble dynamics and with data present in literature. Possible extensions of the present study have been highlighted for future research.
Dedicated to my parents Uma and Banshi Dhar.
ACKNOWLEDGEMENTS

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Lastly, I am grateful to my parents Uma and Banshi Dhar, whom I hold in high regard. They have led me by example, have given me the strength to follow my dreams and have been instrumental in motivating me to do my best. To them I dedicate this thesis. Nothing would have been possible without the encouragement shown by my brother Puneet and my girlfriend Nanditha, two people who have made me smile in times of distress.
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# LIST OF ABBREVIATIONS

- **a**: acceleration
- **a**: index for velocity-space discretization
- **c**: lattice unit length
- **c_s**: speed of sound
- **C_D**: drag coefficient
- **d**: diameter of the bubble
- **D**: diameter of the spherical cap
- **e_i**: lattice speed of particles moving in direction *i*
- **Eo**: Eotvos number
- **f**: particle distribution function
- **g**: acceleration due to gravity
- **g_ij**: interaction strength between components *i* and *j*
- **G**: Green’s function
- **m**: molecular mass
- **Mo**: Morton number
- **N**: number of links at each lattice point
- **p**: pressure
- **p**: momentum
- **r**: radius of the bubble
- **Re**: Reynolds number
- **s**: curvature of the stagnation point
$S$ number of phases
$t$ time
$\mathbf{u}$ velocity vector
$U$ velocity in the rise direction
$V$ interaction potential
$We$ Weber number
$\rho$ density
$\sigma$ surface tension
$\nu$ kinematic viscosity
$\tau$ relaxation time
$\Omega$ collision operator
$\delta_{\alpha\beta}$ Kronecker delta
$\Psi$ effective mass function
$e$ effective
$i$ index
$b$ bubble
$L$ liquid
$sph$ sphere
$\sigma$ phase index
* non-dimensional quantities
$eq$ equilibrium
$\sigma$ phase index
CHAPTER ONE: INTRODUCTION

Boiling and two-phase flow situations are of major importance to many industries and domestic applications. The flow topology in micro-sized channels is an area where the need is most for proper investigation and subsequent understanding. Such micro- and mini-channels are very commonly used these days in residential air-conditioners, and thin compact evaporators that are being used in automotive and aerospace industries. Channels of different shapes find uses in variety of applications. For instance, square and rectangular geometries in the millimeter range are being used in the electronic cooling industry. The high heat flux density used in miniaturized electronic circuits requires efficient cooling techniques. Proton Exchange Membrane (PEM) fuel cells, that employ two-phase flow in millimeter and micron sized channels, are being developed as nonpolluting energy sources which combine hydrogen and oxygen to produce electrical current and only water as a by-product. These cells use very high gas velocity in the flow channels that does not allow for flooding of the channel in case too much water is present.

Kandlikar (2002) has classified thin channels based on their hydraulic diameters. According to his classification, microchannels (10 µm to 200 µm) are employed in inkjet printers and many Micro-Elecro-Mechanical Systems (MEMS), minichannels (200 µm to 3 mm) in compact plate-fan evaporators, and conventional channels (>3 mm) in steam tube boilers, evaporator tubes, etc. This classification is bound to undergo changes as our knowledge in this field advances.
In microchannels, nucleating bubbles grow in size and quickly span the gap, and therefore the slug and churn-turbulent regimes are dominant in microchannels. This increases the pressure gradient and the heat transfer coefficient of these thin channels compared to the large channels. The existing correlations work for large channels, and do not predict thin channel data. These correlations have taken only the gravity and vapor shear forces into account; however, in thin geometries the surface tension effects become significant. It is still not clear whether there is a critical channel size at which the surface tension effect begins to dominate.

One of the issues with microchannels is the geometric shape. It is known that flow in rectangular channels is more complex and less well understood than in circular geometries. The behavior of bubbles and slugs in a confined space between two walls has been observed to be different from that in a circular geometry. Thus, the number of flow and geometric variables, for instance the shape and flow passage, system pressure, mass flux and fluid properties, increases and it becomes even more important to focus on the fundamental understanding of two-phase flow behavior and rely less on empirical correlations.

Since the past decade, researchers have begun using an alternative computational technique, called the lattice Boltzmann method (LBM), to simulate fluid flow as opposed to Computational Fluid Dynamics (CFD). The lattice Boltzmann method of simulating fluids has been proven to be an efficient algorithm, as it can handle flows in complex geometries, porous media, and in multiphase systems with relative ease.
The earliest remnants of LBM go back to 1986 when Frisch, Hasslacher and Pomeau (1986) developed a simple cellular automaton that obeyed conservation laws at the microscopic level and was able to reproduce real fluid flows. This method was known as the lattice gas cellular automaton (LGCA) and was soon found to suffer from the lack of Galilean invariance, anomalous velocity dependence of the fluid pressure, statistical noise, high viscosity, exponential complexity and spurious invariants (Succi (2001)). Later work by McNamara and Zanetti & Higuera and Jiménez helped circumvent two obstacles of LGCA, namely statistical noise and exponential complexity of the collision rule. This version of lattice Boltzmann evolved under the Bhatnagar-Gross-Krook (BGK) collision operator, and is the ultimate version of LBE in terms of simplicity, elegance and efficiency.

The Boltzmann’s kinetic equation is a well established mathematical model of a fluid at the microscopic level which describes the evolution of the single particle distribution function. Unlike conventional schemes that are based on discretization of continuum based macroscopic equations, the lattice Boltzmann method models the microscopic and mesoscopic kinetic equations. The fundamental idea of LBM is to construct simplified kinetic models that incorporate the essential physics of microscopic or mesoscopic processes so that the macroscopic averaged properties obey the desired macroscopic equations.

In multiphase flows, the standard technique is to use either the fluid-mixture or the two-fluid model. Each fluid is modeled by a modified Navier-Stokes (NS) equation, with extra source terms accounting for interfacial effects and forces. But the interface is dynamic, which is difficult
to handle numerically with conventional methods. Table 1 below lists some of the methods used in modeling multiphase flows with the spatial resolution that can be achieved as given by Tomiyama (1998).

Table 1: Numerical Methods for Computational Bubble Dynamics after Tomiyama (1998)

<table>
<thead>
<tr>
<th>Spatial Resolution</th>
<th>Method</th>
<th>Fundamental Equations</th>
<th>Applicability to practical problems</th>
</tr>
</thead>
<tbody>
<tr>
<td>low ((\Delta x &gt;&gt; d))</td>
<td>Averaging methods (homogenous, drift-flux, two fluid models)</td>
<td>Averaged field equation + constitutive equation</td>
<td>high</td>
</tr>
<tr>
<td>intermediate</td>
<td>Bubble tracking method (one-way, two-way methods)</td>
<td>Equation of bubble motion + constitutive equations</td>
<td>Intermediate</td>
</tr>
<tr>
<td>high ((\Delta x &lt; d))</td>
<td>Interface tracking method (front-tracking, volume tracking, level set).</td>
<td>Navier-Stokes equation + Surface tension</td>
<td>Low</td>
</tr>
<tr>
<td>high ((\Delta x &lt;&lt; d))</td>
<td>Microscopic method (Lattice Gas, lattice Boltzmann method).</td>
<td>Translation and Collision and Pseudo molecules</td>
<td>Low</td>
</tr>
</tbody>
</table>

\(\Delta x\): cell size, \(d\): Bubble diameter.

According to Tomiyama (1998), applicability of LBM to practical problems is considered to be low. This has changed over the past decade with the advent of new models that can handle
complex multiphase behavior like phase separation and modeling of liquid droplets and bubbles in the presence of another medium. One of the many interesting advantages of LBM over other conventional multiphase methods like level-set and volume-of-fluid methods is that in LBM the interface is no longer a mathematical boundary or needs to be tracked unlike these former techniques. Rather, it is a post-processed quantity that can be detected by monitoring the variation in fluid properties.
CHAPTER TWO: LITERATURE REVIEW

In this chapter, a discussion of the literature that is considered the foundation and motivation for bubble dynamics has been presented. Various experimental and numerical techniques that involved multiphase flows have been discussed, and the reasons for our departure from these techniques to LBM have been illustrated. Some of the traditional methods discussed are the VOF, marker-and-cell method, and the level-set method.

It has been noticed that almost all proposed schemes to handle boundaries in LBM are more or less based on some speculation of flow properties on the wall (Chen et al (1996)). As a closing discussion, in section 2.3, various ways of dealing with velocity and pressure boundary conditions using the Bhatnagar-Gross-Krook (BGK) variant of the lattice Boltzmann equation have been described.

2.1 Experiments and correlations

One of the classical works on classifying bubble shapes and velocities on the basis of three most important parameters in two-phase flows was done by Bhaga & Weber (1981). These three parameters were the Eotvos number, Reynolds number and the Morton number, and are defined as

\[ Eo = \frac{g \Delta \rho d_e^2}{\sigma} \]  \hspace{1cm} (2.1)

\[ Re = \frac{U_x d_e}{\nu} \]  \hspace{1cm} (2.2)

\[ Mo = \frac{g \rho_i^2 \Delta \rho u^4}{\sigma^3} \]  \hspace{1cm} (2.3)
The commonly used Weber number can be written in terms of these three parameters as

$$We = \frac{Re^2 Mo^{1/2}}{Eo^{1/2}}$$

(2.4)

In their work on flow field measurements around rising bubbles, experimental data was presented with correlations for bubble rise velocity and shape of the rising bubbles. They used hydrogen tracer technique to visualize the flow around single isolated bubbles, and studied the behavior of the wake that is shed by the upward rising bubbles. They concluded that for Morton numbers greater than $4 \times 10^{-3}$, the drag coefficient and dimensionless bubble shape were functions only of the Reynolds number. The commonly used drag coefficient was defined by them as

$$C_D = \frac{4gd_e}{3U_b^2}$$

(2.5)

where ‘g’ is the acceleration due to gravity, ‘$d_e$’ is the volume equivalent diameter of a bubble of volume ‘V’ and ‘$U_b$’ is the terminal bubble rise velocity. Most of the data presented by Bhaga & Weber (1981) was in the high Morton number regime. For this high Morton number class of liquids, the non-dimensional drag was found to obey

$$C_D = \left[ (2.67)^{0.9} + \left( \frac{16}{Re} \right)^{0.9} \right]^{1/0.9}$$

(2.6)

They classified three most distinct bubble shapes, namely, spherical, oblate ellipsoidal and spherical cap with flat rear end.

Grace (1973) has collected almost all experimental measurements of his time and generated a map of bubble shapes at different Eotvos, Reynolds and Morton numbers. In his single plot, data
for 21 different liquids were used to develop correlations for fluids as diverse as mercury
\( Mo = 3.6 \times 10^{-14} \) to a very viscous liquid like glass melt \( Mo = 1 \times 10^7 \).

Two phase bubbly flow in a vertical circular tube has been studied by several investigators in air-
water (Serizawa (1975); Liu (1990); Liu (1993)) and in sub-cooled boiling flows (Shiralkar
(1972); Delhaye (1972); Hasan (1991)). There have been relatively few detailed bubble size
obtained data in modeling refrigerant fluid which simulates upward boiling systems at high
pressures. They used a rectangular geometry to capture the three-dimensional effects of this
rising vapor phase. They also proposed correlations for both departure size and bubble size.
According to them, the bubble shapes could be classified in different groups based on only
Eotvos number.

Recently, Joseph (2003) in his work on predicting the rise velocities of spherical cap bubbles has
derived the theoretical terminal velocities of such bubbles, which is written in terms of the
curvature of the bubble at the stagnation point and the ‘apparent’ diameter of the spherical cap.
He also suggested a drag coefficient that was independent of any Morton number effects unlike
the one given by Bhaga and Weber (1981).

2.2 Numerical simulations

Although efforts to compute the motion of multiphase flows are as old as computational fluid
dynamics, the difficulty in solving the full Navier-Stokes equations in the presence of a
deforming phase boundary has proven to be considerable (Tryggvason et al (2001)). There are
many methods that have been written about and discussed in literature. These methods can be classified into four broad categories. These are

1. Front capturing methods.
2. Boundary fitted method.
3. Lagrangian methods.
4. Front Tracking methods.
5. Lattice Boltzmann modeling.

### 2.2.1 Front capturing method

One of the oldest and most popular techniques to study multiphase flows though simulations is the marker-and-cell (MAC) method. In this method, a marker function is used to identify each fluid. The movement of the interface is captured in the post-processing of the solution of a single continuum mixture with properties being discontinuous at the interface. An illustration of the MAC method is shown in figure 1.

![Figure 1: A schematic of the MAC method solved for a two-phase flow situation (from Yuan (2005).)]
The volume-of-fluid (VOF) method is another way of solving multiphase problems using conventional techniques. In this method, instead of tracking a large number of markers like the MAC method, the void fraction of each cell is used to track the movement of the interface. This makes the method computationally less expensive as compared to MAC. However the gain in computations is at the cost of inaccuracies in resolving and tracking the right position of the fluid-vapor interface.

Another way of solving multiphase problems is through the level-set method, introduced by Osher and Sethian (1988). It relies on an implicit formulation of the interface, that is represented through a time-dependent initial-value partial differential equation (Sethian & Smereka (2003)). The method was particularly designed for problems in multiple space dimensions in which the topology of the interface changes during the course of the simulation. But for a 3-D problem, this method would cost time of $O(N^4)$, where ‘$N$’ is the number of grid points in any direction, to advance the front throughout the domain, thus rendering the method highly computationally expensive.

### 2.2.2 Boundary fitted method

In the boundary fitted method, each fluid has its own set of governing equations that are solved over the domain. The interface is resolved such that at all times it coincides with a grid line, as shown in figure 2. The displacement of the interface is determined by a force balance between the multiple fluid phases that are separated at this grid line.
2.2.3 Lagrangian methods

In this class of solving multiphase flow problems, the grid is allowed to follow the fluid. Work using this method has been to simulate droplet breakup, axisymmetric computations of the collision of a single drop with a wall, and unsteady simulation of two-dimensional motion of several particles.

2.2.4 Front tracking methods

This class of methods tracks the location of the two-phase interface directly without the use of any marker cells. Each phase in this method is treated separately and has its own set of governing equations. One of the variants of this class is the ‘hybrid method’ developed by Tryggvason et al (2001) which is shown in figure 3. In this hybrid method, which is a cross-over of conventional front tracking and front-capturing method, a stationary regular grid is used for the fluid flow, but
the interface is tracked by a separate grid of lower dimension. However, unlike front-tracking methods where each phase is treated separately, this method treats all phases together and solves a single set of governing equations for the whole flow field. Tryggvason et al (2001) have used this method to study aspects of bubbly flows.

![Diagram showing fixed grid and front between Fluid 1 and Fluid 2](image)

Figure 3: Computations of flow containing more than one phase using ‘hybrid’ method developed by Tryggvason et al (2001).

### 2.2.5 Numerical simulations of multiphase flow using LBM

Hou et al (1997) in one of the earliest works on multiphase LBM studied the Rothman-Keller (RK) and the Shan-Chen (SC) models. Their simulations were done for a static bubble with the ideal equation of state and in a static medium. They showed that the SC model is a major improvement over the RK model. This static bubble test has since then been used as a
benchmark for conducting multiphase simulations using LBM. Recent work has been focused towards development of new methods that could simulate high density ratios for the liquid-vapor mixture. Inamuro et al (2004) used the projection method together with Swift’s free energy model to deal with immiscible fluids with large density ratios. In their work, they demonstrated the applicability of the algorithm developed for the case of droplet collisions surrounded by a lighter fluid. In another work, Inamuro et al (2004) conducted simulations for bubbly flows with large density ratios using the projection method. Takada et al (2001), in their work on bubble motion under gravity, developed a 3-D version of the binary fluid model that introduces a free energy function into the lattice Boltzmann equation (LBE). Their results showed that LBM is suitable for numerical analysis of bubble motion under gravity. Their simulations were conducted using a two-dimensional hexagonal lattice arrangement. They have also shown bubble migration towards the center of the channel for wall-driven shear flows. In more extended simulations, they demonstrate binary bubble coalescence and the stages involved in the process. Yang et al (2001) used the SC model for their lattice Boltzmann (LB) based simulations and have qualitatively proved that results from LBM are very similar to experimental observations for saturated pool boiling. Sankaranarayanan et al (2002) proposed closures for drag and virtual mass terms that appear in two-fluid models through simulations performed using an implicit LBM. They also used Shan-Chen’s method to model the liquid-vapor interaction. More recently, Kurtoglo and Lin (2006) used the phase-field method to assess its applicability to single bubble dynamics.
2.3 Boundary conditions in LBM

A lot of work has been done on creating newer and reliable boundary conditions in the LB BGK model. The simplest form of wall boundary condition that has been quoted innumerably in literature is the pure wall bounceback proposed by Wolfram (1986) and Lavallée at al (1991). In this form, the particle distribution function (PDF) streamed to the wall is scattered/reflected along the direction it came from. Because of its simplicity and ease of handling even in complex geometries and flow situations, wall bounceback is still the most preferred of all no-slip boundary conditions that can be found in literature.

But it was soon found by many groups (Cornubert et al (1991), Ziegler (1993) and Guinzbourg and Adler (1994)) that wall bounceback boundary condition is of first order numerical accuracy, although the lattice Boltzmann equation (LBE) is second order accurate in space. Skordos (1993) suggested that to eliminate this fallacy, velocity gradients should be included in the equilibrium distribution function at the wall nodes. It was also found that in certain situations, using wall bounceback resulted in a fictitious slip velocity near the wall nodes. Inamuro et al (1995) proposed a new form of LBE in which a slip velocity was included to nullify the effect of the ‘false’ slip created at the boundary because of the use of bounceback. In their study, unknown distribution functions at the wall, whose velocity points to the fluid region, were assumed to be an equilibrium distribution function with a counter slip velocity. This velocity was determined in a way such that the fluid velocity at the wall is equal to the wall velocity. But their method had shortcomings in dealing with corners. In a separate work, Noble et al (1995) proposed the use of hydrodynamic boundary conditions on no-slip walls by enforcing a pressure gradient. During each time step in the LBM procedure, the particle distribution at each node is modified by
collision, forcing and streaming. The goal of the hydrodynamic approach was to prescribe this process in such a way that the desired velocity conditions are satisfied at the end of the time step. Maier et al (1996) in their work modified the bounceback condition to nullify net momentum tangent to the wall and preserve momentum normal to the wall. In their work, they proposed that for the case in 3-D lattices where the number of unknown particle distribution functions at the boundaries exceeds the number of equations to be solved, supplementary rules for the external links need to be enforced, which employ extrapolation for density conditions and mass addition and redistribution for velocity conditions. Their methods were tested for standard benchmark problems like Poiseuille flow, Couette flow and duct and pipe flow. Zou and He (1997) extended the wall bounceback boundary condition for the non-equilibrium part of the particle distribution function. They used the known boundary velocity/pressure values to determine the unknown distribution functions pointing into the fluid by using bounceback for the non-equilibrium part of the PDF. Their method was found to be second order accurate for Poiseuille flow. Ziegler (1993) in his work found that shifting the wall (boundary) half-mesh unit into the fluid, in other words applying the bounceback between the nodes, yields second order accuracy at the walls. This scheme is popularly known as the half-way bounceback method. It has been further extended by authors, but has been found to be too difficult to be implemented for arbitrary geometries.

Chen et al (1996) adopted a staggered mesh discretization from the traditional finite difference methods and proposed using a second-order extrapolation scheme of distributions in the flow to obtain the unknown PDFs. Chen et al (1996) proposed a simple extrapolation scheme in place of wall bounceback method (figure 4). They argued that the bounceback scheme works well only
when $\tau = 1$. For other values of the relaxation parameter, the bounceback scheme does not yield results that match analytical solutions. It was also emphasized that since the relaxation parameter is a measure of the fluid viscosity, and since high velocities cannot be simulated in LB-BGK because of the low Mach number restriction, simulating high Reynolds number flows can be a problem with conventional treatment of the wall.

Figure 4: Basic cell for the '9 speed' lattice Boltzmann model. The center of the cell is occupied by the rest particle (after Chen et al (1996)).

Their extrapolation employed one additional set of nodes beyond the boundary nodes which lie inside the wall. The PDFs at this row of nodes was calculated using the PDF values at the wall and the layer of one lattice nodes of fluid adjacent to the boundary nodes. Thus if $f_i^{-1}, f_i^0$ and $f_i^1$
are the PDF on the outside layer, the wall layer and the first layer inside the fluid respectively, then

\[ f_{i}^{-1} = 2f_{i}^{0} - f_{i}^{1} \]  \hspace{1cm} (2.7)

After this, streaming of the distribution functions is carried out. The collision step is the normal collision carried out for all fluid nodes, except the wall nodes where velocity or pressure boundary conditions are enforced using the equilibrium distribution functions. The important thing to note about this method is that it does not require any assumptions about the incoming distribution functions as was the case with other schemes like that proposed by Zou and He (1997). This scheme was tested by the authors for Poiseuille flow, flow in a lid-driven cavity and flow over a column of cylinders among other standard problems with success.

Mei et al (1999) developed a second accurate treatment of boundary conditions for curved boundaries. Until then, a standard way to deal with curved boundaries was to treat the surface as a series of stairs, which resulted in less accurate solution. Their scheme was found to give better accuracy than standard bounceback. Also, flows at a lower value of the relaxation parameter could be computed without the system becoming unstable. In a later work, Mei et al (2000) extended the idea to deal with arbitrary curved 3-D solid geometry and found the method to give second order accuracy and possess stability characteristics.
CHAPTER THREE: METHODOLOGY

In the following sections, the lattice Boltzmann equation (LBE) has been derived from Boltzmann’s kinetic equation. The collision operator has been derived using the Chapman-Enskog expansion of the collision operator. This gives a linear differential equation for the particle distribution function. The Chapman-Enskog expansion also yields a simple form of the collision operator, which can be replaced by a single-time relaxation term.

There are three important features of LBM that distinguish it from other numerical methods. These are:

1) The convection operator in velocity (phase) space is linear, which has been brought from kinetic theory and is in stark contrast with the non-linear convection terms in other approaches like the Navier-Stokes equations.

2) The incompressible form of the Navier-Stokes equations can be obtained in the nearly incompressible limit of LBM.

3) In the Maxwell-Boltzmann equilibrium distribution, the phase space is a complete functional space, due to which the averaging involves the whole of the velocity (phase) space. In LBM, only a few moving directions are used and thus the transformation that relates the microscopic properties is simplified.

To show that indeed the LBE bridges the gap from microscopic physics to the real world fluid phenomenon, the Navier-Stokes equations have been derived starting from the BGK form of the
collision operator together with the zeroth and first order moments of the particle distribution functions, and the special form of the equilibrium distribution function. The numerical implementation of the LBGK has been described in section 3.3. Finally the multiphase model used in the current study for simulating two-phases has been described in section 3.4.

3.1 Lattice BGK from Boltzmann’s equation

The evolution equation for the particle distribution function is very similar to the kinetic equation in lattice gas automata, given by

\[ f_i(x + e_i \Delta t, t + \Delta t) = f_i(x, t) + \Omega_i \left[ f_i(x, t) \right] \]

where \( i = 0, 1, \ldots, M \)

(3.1a)

\[ \rho = \sum_i f_i ; \quad \rho u = \sum_i f_i e_i \]

(3.1b)

\( \Omega_i \) has to satisfy

\[ \sum_i \Omega_i = 0 \quad \& \quad \sum_i \Omega_i e_i = 0 \]

(3.2)

at each lattice location.

If equation (3.1) is expanded in a Taylor series about \( \epsilon \) which is a small parameter proportional to the Knudsen number, i.e.

\[ |\Delta x| \Delta t \approx O(\epsilon) \]

(3.3)

Then on expansion, we get

\[ f_i(x + e_i \Delta t, t + \Delta t) = f_i(x, t) + \epsilon \frac{\partial f_i}{\partial t} + \epsilon e_i \cdot \nabla f_i + \frac{\epsilon^2}{2} \frac{\partial^2 f_i}{\partial t^2} + \frac{\epsilon^2}{2} (e_i \cdot \nabla f_i)^2 + \frac{\epsilon^2}{2} (e_i \cdot \nabla^2 f_i) + O(\epsilon^3) \]

\[ = f_i(x, t) + \Omega_i \]

(3.4a)
\[
\Rightarrow \frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i + \varepsilon \left[ \frac{1}{2} \frac{\partial^2 f_i}{\partial t^2} + \frac{1}{2} \left( \mathbf{e}_i, \mathbf{e}_i \cdot \nabla \nabla f_i \right) + \frac{1}{2} \left( \mathbf{e}_i, \mathbf{V} \right) \frac{\partial f_i}{\partial t} \right] + O(\varepsilon^2) = \frac{\Omega_i}{\varepsilon} \quad (3.4b)
\]

Using the Chapman-Enskog expansion, where we use
\[
\frac{\partial}{\partial t} = \varepsilon \frac{\partial}{\partial t_1} + \varepsilon^2 \frac{\partial}{\partial t_2} ; \quad \frac{\partial}{\partial \mathbf{x}} = \varepsilon \frac{\partial}{\partial \mathbf{x}_1} \quad (3.5)
\]

where \( t_1 \) is the convection time scale and \( t_2 \) is the diffusion time scale such that \( t_1 \gg t_2 \). Further, the particle distribution functions can be expanded as
\[
f_i = f_i^{eq} + \varepsilon f_i^{neq} \quad \& \quad \sum_i f_i^{eq} = 0 \text{ , } \sum_i f_i^{eq} \mathbf{e}_i = \mathbf{0} \quad (3.6a)
\]

\[
f_i^{neq} = f_i^{(1)} + \varepsilon f_i^{(2)} + O(\varepsilon^2) \quad (3.6b)
\]

and
\[
\sum_i f_i^{1,2} = 0 ; \quad \sum_i f_i^{1,2} \mathbf{e}_i = \mathbf{0} \quad (3.6c)
\]

Thus the collision operator up to third order is given by
\[
\Omega_i(f) = \Omega_i(f^{eq}) + \varepsilon \frac{\partial \Omega_i}{\partial f_j} f_j^{eq} f_j^{(1)} + \varepsilon^2 \left( \frac{\partial^2 \Omega_i}{\partial f_j^2} f_j^{eq} f_j^{(2)} + \frac{\partial \Omega_i}{\partial f_j} \frac{\partial \Omega_i}{\partial f_k} f_j^{eq} f_j^{(1)} f_k^{(1)} \right) + O(\varepsilon^3) \quad (3.7)
\]

For small \( \varepsilon \), \( \lim_{\varepsilon \to 0} \Omega_i(f^{eq}) = 0 \). Thus the above equation would reduce to
\[
\frac{\Omega_i(f)}{\varepsilon} = \frac{\partial \Omega_i(f^{eq})}{\partial f_j} f_j^{(1)} + \varepsilon \frac{\partial \Omega_i(f^{eq})}{\partial f_j} f_j^{(2)} + O(\varepsilon^2) \quad (3.8a)
\]

\[
= \frac{\partial \Omega_i(f^{eq})}{\partial f_j} [f_j^{(1)} + \varepsilon f_j^{(2)}] = \frac{\partial \Omega_i(f^{eq})}{\partial f_j} [f_j^{neq}]
\]

\[
= \frac{1}{\varepsilon} \frac{\partial \Omega_i(f^{eq})}{\partial f_j} (f_j - f_j^{eq}) \quad (3.8b)
\]

\[
= \frac{M_{ii}}{\varepsilon} (f_j - f_j^{eq})
\]
where ‘$M_{ij}$’ is the collision matrix (Higuera and Jiminez (1989)). Further assuming that the local particle distribution function relaxes to an equilibrium state at a single rate ‘$\tau$’, so that

$$M_{ij} = -\frac{1}{\tau}\delta_{ij}$$  \hspace{1cm} (3.9)

we arrive at the lattice BGK collision term,

$$\frac{\Omega_i}{\epsilon} = -\frac{f_{i}^{eq}}{\tau} = -\frac{\left(f_i - f_i^{eq}\right)}{\epsilon\tau}$$  \hspace{1cm} (3.10)

This form of the collision operator with the single time relaxation approximation is also known as the lattice BGK (Bhatnagar-Gross-Krook) operator. This form of the collision operator reduces (3.1) to a differential equation of the form

$$\frac{\partial f_i}{\partial t} + \mathbf{e}_i \cdot \nabla f_i = -\frac{\left(f_i - f_i^{eq}\right)}{\tau}$$  \hspace{1cm} (3.11)

Equation 3.11 can be discretized in time and discrete-velocity space. This gives

$$\frac{f_i(x + \mathbf{e}_i \delta t, t + \delta t) - f_i(x, \delta t, t)}{\delta t} + \frac{f_i(x + \mathbf{e}_i \delta t, t) - f_i(x, t)}{\delta x} = -\frac{\left(f_i - f_i^{eq}\right)}{\tau}$$  \hspace{1cm} (3.12)

Assuming $\delta x = \delta t = 1$, equation 3.12 simplifies to the most commonly used ‘explicit’ lattice Boltmann equation (LBE), given as

$$f_i(x + \mathbf{e}_i \delta t, t) - f_i(x, t) = -\frac{\left(f_i - f_i^{eq}\right)}{\tau}$$  \hspace{1cm} (3.13)

This is the lattice BGK (LBGK) equation. The density per node and the macroscopic momentum flux are defined in terms of the particle distribution functions by

$$\rho = \sum_i f_i \quad ; \quad \rho \mathbf{u} = \sum_i f_i \mathbf{e}_i$$  \hspace{1cm} (3.14)
The equilibrium distribution functions depend only on local density and velocity and they can be expressed in the following form:

\[
\begin{align*}
  f_i^{eq} &= \frac{\rho - d_0}{b} + \frac{\rho D}{c^2 b} \mathbf{e}_i \cdot \mathbf{u} + \frac{\rho D (D + 2)}{2 c^4 b} (\mathbf{e}_i \cdot \mathbf{u}) \mathbf{u} - \frac{\rho D}{2 c^2 b} (\mathbf{u} \cdot \mathbf{u}), \\
  f_0^{eq} &= d_0 - \frac{\rho}{c^2} (\mathbf{u} \cdot \mathbf{u})
\end{align*}
\]  

(3.15)

where \( f_i^{eq} \) is the equilibrium distribution of particles moving in direction ‘i’, \( f_0^{eq} \) is the equilibrium distribution of rest particles, \( D \) is the dimension rank (2 for two-dimensions), \( b \) is the number of lattice directions (six for hexagonal lattice), \( c \) is the lattice unit length (unity for two-dimensions), and \( d_0 \) is the average rest particle number (Noble et al (1995)). Also, the leading truncation error of such a velocity-space discretization is then taken into account exactly by modifying the viscosity in the NS equation derived from equation 3.11 to

\[
\nu = \left( \tau - \frac{1}{2} \right) c_s^2 \delta t
\]  

(3.16)

The positivity of the viscosity requires that \( \tau > 1/2 \).

3.2 Navier-Stokes from LBE

The particular form of the collision operator with the single time relaxation approximation, also known as the lattice BGK (Bhatnagar-Gross-Krook) operator leads to a differential equation of the form given by equation 3.11 for the Boltzmann’s kinetic equation. In the low frequency, long wavelength limit, the Chapman-Enskog expansion can be used under the assumption that \( \delta x \approx \delta t \approx \epsilon \), where \( \epsilon \) is a small parameter as compared to the macroscopic scales and is proportional to the Knudsen number. Thus, the particle distribution functions can be expanded in a Taylor series about \( \epsilon \),
\[ f_i = f_i^{eq} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + O(\varepsilon^3) \]  

Similarly, the time and space derivatives can be expanded as

\[ \frac{\partial}{\partial t} = \varepsilon \frac{\partial}{\partial t_1} + \varepsilon^2 \frac{\partial}{\partial t_2}, \quad \frac{\partial}{\partial x} = \varepsilon \frac{\partial}{\partial x_1} \]  

To recover the Navier-Stokes equations from the BGK form of the LBE, we need to substitute equation 3.17 and 3.18 into 3.11. This would give

\[ \left( \frac{\partial f_i^{eq}}{\partial t_1} + \mathbf{v}_i \cdot \nabla f_i^{eq} + \frac{1}{\tau} f_i^{(1)} \right) \varepsilon^0 + \left( \frac{\partial f_i^{eq}}{\partial t_2} + \left( 1 - \frac{1}{2\tau} \right) \frac{\partial f_i^{(1)}}{\partial t_1} + \mathbf{v}_i \cdot \nabla f_i^{(1)} \right) + \frac{1}{\tau} f_i^{(2)} \varepsilon^1 + O(\varepsilon^2) = 0 \]  

where higher order terms have been grouped together. Filtering out \( O(\varepsilon^0) \) and \( O(\varepsilon^1) \) terms leads to

\[ \frac{\partial f_i^{eq}}{\partial t_1} + \mathbf{v}_i \cdot \nabla f_i^{eq} = -\frac{1}{\tau} f_i^{(1)} \]  

and

\[ \frac{\partial f_i^{eq}}{\partial t_2} + \left( 1 - \frac{1}{2\tau} \right) \frac{\partial f_i^{(1)}}{\partial t_1} + \mathbf{v}_i \cdot \nabla f_i^{(1)} = -\frac{1}{\tau} f_i^{(2)} \]  

Using the condition that the zeroth and first order moments of the equilibrium particle distribution function give the macroscopic density and momentum flux respectively (equation 3.14), and the form of the equilibrium distribution function as given in equation 3.15 simplifies equation 3.20 to the governing equations that have the form given by,

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot \rho \mathbf{u} = 0 \]  

\[ \frac{\partial (\rho \mathbf{u})}{\partial t} + \nabla \left[ \sum_i \mathbf{e}_i \mathbf{e}_i f_i^{eq} + \left( 1 - \frac{1}{2\tau} \right) \sum_i \mathbf{e}_i \mathbf{e}_i f_i^{(1)} \right] = 0 \]  

Chen and Doolen (1998) show that the two summations in equation 3.22b can be reduced to
\[ \sum_i (\mathbf{e}_i)_\alpha (\mathbf{e}_i)_\beta f_i^{(\alpha)} = p\delta_{\alpha\beta} + \rho u_\alpha u_\beta \]
\[ \left(1 - \frac{1}{2\tau}\right)\sum_i (\mathbf{e}_i)_\alpha (\mathbf{e}_i)_\beta f_i^{(\alpha)} = \nu \left( \nabla_\alpha (\rho u_\beta) + \nabla_\beta (\rho u_\alpha) \right) \]

(3.23)

where \( p = c_s^2 \rho \) & \( \nu = c_s^2 (\tau - 1/2) \). The resulting momentum equation is
\[ \rho \left( \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nu \nabla^2 (\rho \mathbf{u}) + \nu \nabla \cdot (\rho \mathbf{u}) \]

(3.24)

Thus the lattice Boltzmann’s equation is able to bridge the gap between the microscopic fluid interactions and the macroscopic world as it yields Navier-Stokes equation in the low Mach number limit using the Chapman-Enskog expansion, and is second order accurate in space.

### 3.3 Numerical implementation

In this work, the D2Q9 form of the discrete velocity space has been used that gives a square lattice for the space discretization. For such a model, the nine velocities are shown below in figure 1. The velocity vectors are given as
\[ e_a = \begin{cases} (0,0), & a = 0; \\ (\pm 1,0)c, (0,\pm 1)c, & a = 1,2,3,4; \\ (\pm 1,\pm 1)c, & a = 5,6,7,8. \end{cases} \]

(3.25)

where ‘c’ is the lattice speed and is given by \( c = \delta x/\delta t \). The other forms of the velocity discretization are D2Q7 (hexagonal lattice), D3Q15 (15 velocity 3-D model) and D3Q19 (19 velocity 3-D model).
Broadly, the lattice Boltzmann scheme consists of two computational steps,

**collision step:**
\[
\tilde{f}_i(x,t) - f_i(x,t) = -\frac{1}{\tau} \left[ f_i(x,t) - f_i^{eq}(x,t) \right]
\]

**streaming step:**
\[
f_i(x, t + \delta t) = \tilde{f}_i(x, t)
\]

where \( \tilde{f}_i \) and \( f_i \) denote the pre- and post-collision state of the distribution function, respectively.

This form of an implementation itself justifies the very reason why the LBE has been regarded as a preferred tool over the Navier-Stokes equations and solvers. The LBE is a simple time-marching algorithm for the PDFs, whereas the NS involves linear non-linear advection terms that make the process iterative. Because of its explicit form, the LBE is easy to implement, and natural to parallelize as the collision step is completely local and the streaming step takes very little computational effort at every time step. However unlike the macroscopic solvers for which a no-slip boundary condition for the velocity \( \mathbf{u} \) on the wall is easily satisfied, there is no similar
form available for boundary condition on the PDFs. Various ways and treatments have been proposed in literature to date, and have been summarized in section 2.1.

3.4 Multiphase models in LBM

Numerous methods have been used by researchers over the past decade to conduct multiphase simulations using LBM. These include the model proposed by Rothman and Keller or better known as the R-K model (1988), where the two fluids are denoted by different colors. In this model, phase separation is produced by the repulsive interaction based on the color gradient. The R-K model was originally meant for lattice gas simulations. Grunau et al (1993) introduced some free parameters in this model.

The lattice Boltzmann implementation was first introduced by Shan & Chen (1993). In Shan-Chen’s (S-C) model, multiphase phases were simulated by introducing non-local interactions between particles at each lattice site, thereby making it hard to parallelize. Swift et al (1996) proposed the “free-energy” approach. In this model, unlike the S-C model, the local momentum conservation was satisfied. However, Swift’s model suffered from the lack of Galilean invariance.

In this work, the S-C model has been used extensively to study isothermal flow behavior of immiscible components and multiple phases. The model is described below.
3.4.1 S-C model for multiple phases and components

Shan & Chen (1993) in their work proposed a lattice Boltzmann based model that could simulate multiple phases and components. They incorporated non-local interactions amongst particles to simulate multiple component fluids. The interaction potential between components \( \sigma \) and \( \bar{\sigma} \) was defined as

\[
V(\mathbf{x}, \mathbf{x}') = G_{\sigma\bar{\sigma}}(\mathbf{x}, \mathbf{x}') \psi^\sigma(\mathbf{x}) \psi^{\bar{\sigma}}(\mathbf{x}')
\]  

(3.27)

where \( G_{\sigma\bar{\sigma}}(\mathbf{x}, \mathbf{x}') \) is the Green’s function. The quantity \( \psi^\sigma \) is the “effective mass”. If only nearest neighbor interactions were considered, then

\[
G_{\sigma\bar{\sigma}}(\mathbf{x}, \mathbf{x}') = \begin{cases} 
0 & ; |\mathbf{x} - \mathbf{x}'| > c \\
G_{\sigma\bar{\sigma}} & ; |\mathbf{x} - \mathbf{x}'| = c 
\end{cases}
\]

(3.28)

The magnitude of \( G_{\sigma\bar{\sigma}} \) controls the strength of the interaction between components \( \sigma \) and \( \bar{\sigma} \), while its sign determines whether the interaction is attractive or repulsive.

This form of the potential gives the rate of net momentum change at each lattice site to be

\[
\frac{d\mathbf{p}^\sigma}{dt}(\mathbf{x}) = -\psi^\sigma(\mathbf{x}) \sum_{\sigma=1}^{N} G_{\sigma\bar{\sigma}} \sum_{a=0}^{h} \psi^{\bar{\sigma}}(\mathbf{x} + \mathbf{e}_a) \mathbf{e}_a
\]

(3.29)

Therefore, this change in momentum is applied at each lattice site in the equilibrium distribution function before the collision, as shown by Buick and Greated (2000):

\[
\rho^\sigma \mathbf{u}^\sigma = \rho^\sigma \mathbf{u} + \tau^\sigma \frac{d\mathbf{p}^\sigma}{dt}(\mathbf{x})
\]

(3.30a)

where

\[
\rho^\sigma = m^\sigma f^\sigma(\mathbf{x})
\]

(3.31b)
is the mass density of the $\sigma^{th}$ component and

$$u = \frac{\sum_{\sigma} m_{\sigma} \sum_{a} f_{a} \sigma e_{a} / r_{\sigma}}{\sum_{\sigma} m_{\sigma} \sum_{a} f_{a} \sigma / r_{\sigma}}$$  \hspace{1cm} (3.31c)$$

and

$$f_{\sigma}(x) = \sum_{a} f_{a} \sigma$$  \hspace{1cm} (3.31d)$$

In this study, the interaction model given by Shan and Chen (1994) has been used extensively to study isothermal bubble dynamics in periodic domains with gravity as the only external force for the two-phase system. The vapor has been denoted by index ‘1’ and the continuous liquid phase would be denoted by ‘2’. The next chapter presents the results of single and multiple bubble simulations of lighter vapor phase rising in a heavier liquid.
CHAPTER FOUR: RESULTS

This chapter details the numerical simulation part of the current study. It contains typical benchmark problems that have been solved using LBM both in single- and two-phase flows. Some of these benchmark problems are: pressure driven flow in a channel (Poiseuille flow), flow in a lid-driven cavity and the static bubble test. Computer codes were developed for all the problems and solved with appropriate form of boundary conditions. For the static bubble test, the simulation was done under the absence of gravity to isolate a single-bubble as an initial condition for further tests on rising bubble(s).

4.1 Validation

Some of the test problems that were conducted to test the understanding of the lattice Boltzmann method are described in the next few sections.

4.1.1 Poiseuille flow

Pressure driven flow in a rectangular channel is a problem that has an exact analytical solution. For such a flow situation, the velocity profile at any location ‘x’ and along the vertical ‘y’ direction is given as

$$u = \frac{h^2 G y}{2\nu} \left(1 - \frac{y}{h}\right)$$

(4.1)

where $G$ is the pressure gradient per unit density along the ‘x’ axis and ‘h’ is the height of the channel in lattice units.
A channel length of 41 lattice units was simulated for this case with a relaxation time of 1. The pressure gradient per unit density was fixed at 0.001. Half-way bounceback boundary condition is used at the walls, which implies that any particle distribution functions that are streamed to the nodes inside the wall are reversed back to get a zero velocity on the particular node of the wall. The so obtained velocity profile is found to match very well with the analytical solution, as is shown in figure 6.

Figure 6: Velocity profiles at the outlet for a channel with length 41 units and pressure gradient of 0.001 obtained using LBM with the bounceback boundary condition. Comparison has been shown with the analytical solution for $\tau=1$. 
In another simulation, the extrapolation scheme used by Chen & Martinez (1996) is used to model the wall boundary conditions. The details of this implementation have already been discussed in section 2.3. The simulation was again done with the same number of lattice nodes as the half-way bounceback case, and the results have been compared to the analytical solution in figure 7. It was found that the extrapolation scheme yields better match for the velocity profile close to the walls because of the second-order accurate treatment of the wall particle distribution function, unlike the case in figure 6.

Figure 7: Velocity profiles at the outlet for a channel with length 41 units and pressure gradient of 0.001 obtained using LBM with the extrapolation scheme with proposed by Chen et al (1996). Comparison has been shown with the analytical solution for $\tau=1$. 

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The Poiseuille flow problem was also solved for different values of the relaxation parameter ‘\( \tau \)’. These values were \( \tau = 0.8, 0.9, 1.0, 2.5 \) and 5. The results of the velocity profile as compared to the analytical solution are shown in figure 8 for an equal pressure gradient of 0.001. The extrapolation scheme was used to model the no-slip boundary condition at the wall. The

Figure 8: Velocity profiles at the outlet for a channel with length 41 units and height 10 units and pressure gradient of 0.001 obtained using lattice Boltzmann method with the extrapolation scheme proposed by Chen et al (1996) for different values of the relaxation parameters. The symbols show the analytical values of the velocity: (a) □ \( \tau = 0.8 \), (b) Δ \( \tau = 0.9 \), (c) \( \nabla \tau = 1 \), (d) ◊ \( \tau = 2.5 \), and (e) ○ \( \tau = 5 \).
simulation shows very good match of the numerical calculations with that of the analytical solution. It was also observed that the least error occurred for the case when the relaxation parameter was chosen to be 1.

### 4.1.2 Lid-driven cavity

To further check the applicability of the method, steady state simulations were done for a lid-driven cavity flow with the upper wall moving at a fixed velocity of $U_w$. The extrapolation scheme proposed by Chen and Martinez (1996) is used for all the walls (see section 3.2 for more details about this method) This gives a better accuracy for the flow field at smaller relaxation parameters as compared to the pure bounceback that yields accurate results only at relaxation time of close to 1. A square grid of $167 \times 167$ nodes was used for the simulation that gives grid independent results. The driving lid is placed on top of the cavity and moves at a velocity of $U_w=0.052$ lattice units. The relaxation time was chosen to be 0.7 in order to simulate flow with Reynolds number of 250. The streamlines inside the cavity at steady state are shown in figure 9.

The flow behavior obtained is in good agreement with previous studies. Figure 9 shows the streamlines of the flow obtained at Re=250. The two recirculation zones (secondary vortices) at the bottom corners of the domain are captured very well with the present grid resolution. To study the deviation of the vertical centerline velocity with the Reynolds number, a new case with Re=100 was run, and the results compared with that of Re=250. The vertical centerline velocity for the cavity flow compared for the two Reynolds numbers is shown below in figure 10.
Figure 9: Streamlines for a 2-D lid-driven cavity simulation obtained using LBM at a Reynolds number of 250.
Figure 10: Center-line velocity for two different Re values of 100 and 250 for the lid-driven cavity.

These results of single-phase LBM simulations show that the technique is strong enough to be considered a candidate for study of incompressible flow situations and can yield valuable insights without solving the sometimes highly non-linear Navier-Stokes equations. For a case like the lid-driven cavity flow, upwinding schemes would have to be used when solved using CFD techniques like the finite-difference (FD) or the finite-volume (FV) method, and the solution might become unstable for the combination of grid-resolution and the time step chosen. With LBM, all these stability criterion are condensed into one single Courant number, which is given by $\frac{c\delta t}{\delta x}$. This number is always equal to unity in the explicit version of LBM, and hence
stability considerations regarding the resolution of the grid and the value of the time step are never encountered.

4.2 Multiphase Simulations using LBM

The most important parameters in the study of two-phase flows are the Eotvos number, \( Eo = \frac{g \Delta \rho d_e^2}{\sigma} \), Morton number, \( Mo = \frac{g \rho L^2 \Delta \rho \nu^4}{\sigma^3} \), Reynolds number, \( Re = \frac{U_b d_e}{\nu} \) and the Weber number, \( We = \frac{\rho L^2 U_b^2 d_e}{\sigma} \). Fan and Tsuchiya (1990) have described the importance and distinction between the Weber and the Reynolds number in a classical manner. The Weber number is a ratio of the dynamic pressure \( \sim \rho L U_b^2 \) to the surface tension pressure \( \sim \sigma / d_e \), whereas the Reynolds number is a ratio of the inertial force \( \sim \rho L U_b d_e \) to the viscous force \( \sim \mu U_b d_e \) from the surrounding liquid. The Weber number becomes even more important for \( We \ll 1 \), because for flows of this kind the bubbles maintain a spherical shape all throughout the flow domain. These parameters have been used in this study to record and observe bubble shapes and flow regimes.

Multiphase simulations in LBM were started with conducting static bubble tests to generate a good initial condition with one or more than one bubble in a fully periodic domain. The nearest neighbor SC model as explained by Yuan & Schaefer (2006) has been used in which the next-nearest neighbor is also used in the force discretization. Accordingly, equation 3.17 is modified to account for the nearest and second nearest neighbors as
This leads to a non-ideal equation of state that is given by

\[ p = c_s^2 \rho + \frac{3}{2} g \Psi^2(\rho) \]  \hfill (4.3)

where \( c_s = 1/\sqrt{3} \) is the speed of sound. It should be noted here that if there is no interaction amongst the same kind of fluid, then the equation of state would reduce to the ideal gas equation of state given by \( p = c_s^2 \rho \). The ‘effective mass’ function, \( \Psi \), used for the liquid is the same as proposed by Shan & Chen (1993), given by

\[ \Psi(\rho) = \rho_0 \left[ 1 - \exp\left( -\rho / \rho_0 \right) \right] \]  \hfill (4.4)

This leads to a value of the critical interaction strength to be \( g_{\text{crit}} = -\frac{4}{9 \rho_0} \). Any value of the interaction strength below \( g_{\text{crit}} \) would result in phase separation of the liquid phase. In most simulation results described below, \( \rho_0 = 1 \) unless otherwise specified. For the vapor phase, \( \psi \) value is set to be equal to \( \rho_0 \).

Studies have reported that using the SC model for multiphase simulations can sometimes lead to non-zero velocity vectors near the liquid-vapor interface. This phenomenon is a result of the non-local momentum conservation for the fluid mixture at each lattice location, and the velocity vectors are known as ‘spurious currents’. Shan (2006) suggested that this could be due to lower order discretization of the force field, and that taking the contribution of many more neighbors can lead to lowering of these spurious currents. It was suggested that the force be discretized...
among the nearest, next-nearest and next-next-nearest neighbors by the following discretization
that allows for a smaller and smaller interaction strength as the distance from the central node
gets higher. So,

\[ \mathbf{F} = -G \left( |\mathbf{e}_a| \right) \Psi(\mathbf{x}) \sum_b \Psi(\mathbf{x} + \mathbf{e}_b) \mathbf{e}_a \]  

(4.5)

This leads to an interaction strength at each location to be of the form

\[ G(\mathbf{x}) = G_w \left( |\mathbf{x}|^2 \right) \]  

(4.6)

He suggested a list of weighting factors for 2-D situations and these have been listed below in

\[ E^{(n)}_{k_{12} \ldots -n} = \sum_a \mathbf{w} \left( |\mathbf{e}_a|^2 \right) (\mathbf{e}_a)_{i_1} (\mathbf{e}_a)_{i_2} \ldots (\mathbf{e}_a)_{i_n} \]  

(4.7)

and the force has been discretized as

\[ \sum_a \mathbf{w} \left( |\mathbf{e}_a|^2 \right) \Psi(\mathbf{x} + \mathbf{e}_a) \mathbf{e}_a = (\nabla \Psi) \cdot \mathbf{E}^{(2)} + \frac{1}{3!} (\nabla^3 \Psi) \cdot \mathbf{E}^{(4)} + \frac{1}{5!} (\nabla^5 \Psi) \cdot \mathbf{E}^{(6)} + \ldots \]  

(4.8)

In this study, sixth order weighting factors as suggested by Shan (2006) have been used to create
higher isotropy and reduce the magnitude of the spurious currents. Using this form of the force
discretization leads to an equation of state for the liquid to be of the form

\[ \rho = c_{\rho}^2 \rho + \frac{15}{8} g \Psi^2 (\rho) \]  

(4.9)
Table 2: Weights that yield unit $E^{(2)}$ and $E^{(n)}$ tensors in two dimensions. The tensor given in the first column is the highest isotropic tensor with the corresponding weights (taken from Shan (2006)).

<table>
<thead>
<tr>
<th>Tensor</th>
<th>w(1)</th>
<th>w(2)</th>
<th>w(3)</th>
<th>w(4)</th>
<th>w(5)</th>
<th>w(6)</th>
<th>w(8)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E^{(4)}$</td>
<td>1/3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$E^{(6)}$</td>
<td></td>
<td>1/10</td>
<td></td>
<td></td>
<td></td>
<td>1/120</td>
<td></td>
</tr>
<tr>
<td>$E^{(8)}$</td>
<td></td>
<td>4/45</td>
<td></td>
<td>1/60</td>
<td>2/315</td>
<td></td>
<td>1/5040</td>
</tr>
</tbody>
</table>

4.2.1 Static bubble test

Figure 11 shows the density contours of a static bubble test done in a periodic domain of $100 \times 100$ with an initial diameter of the bubble to be 50 lattice units. The parameters for the interaction strengths have been chosen to be $g_{12} = 0.1$ and $g_{22} = -0.35$ and the relaxation time was chosen to be equal to 1. With time, an interface is observed to develop on the surface of the vapor bubble. The lighter fluid obeys an ideal equation of state, because $g_{11} = 0$. The density ratio of the lighter vapor to the heavier liquid is 2.4. The velocity vectors visible on the surface of the bubble are spurious currents that have been discussed in the previous section. They are a consequence of the non-conservation of fluid momentum on each lattice site because of the form of the SC model. But the total fluid momentum is conserved and hence the bubble center does not migrate in the domain in the absence of any external force. The bubble is equilibrated for 10,000 timesteps, which is a sufficiently long time at which the velocity in the domain does not change by more than $1 \times 10^{-6}$. 

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Figure 11: Density contours and velocity vectors for a static bubble test done with $g_{12} = 0.1$ and $g_{22} = -0.35$. The bubble diameter is 50 lattice units initially and the bubble is left to evolve for 10,000 lattice time steps under no external force.
The density profile through the centerline of the static bubble has been shown in figure 12. Vapor phase is denoted by 1 and the liquid phase is denoted by 2. It can be seen that near the interface the density does not drop sharply as would be expected in a real system. Instead, the density transition occurs over an interface width of 3 lattice units. This value of the interface thickness is the same as reported by Hou et al (1997). Due to this reason, multiphase simulations of bubbles with diameter less than 6 lattice units is not possible using the current method as they cannot be resolved.
The static bubble test acts as a good validation exercise and a starting point for all multiphase flow simulations conducted in this work. The density field obtained as a result of this test is a stable initial condition for the simulation of bubble motion under gravity. At this time, the clock is turned back to \( t=0 \), and the external force is switched on, and the dynamics of the bubble are recorded. The results of these tests for different bubble sizes and different values of the external force are presented in the next section on single-bubble dynamics.

### 4.2.2 Single-bubble dynamics

The static bubble test yields a good initial guess for the density and pressure distribution in the domain for the multiphase simulation, even before gravity is introduced. After letting the bubble(s) equilibrate for a long time in the domain, a steady state is achieved. This state of the bubble(s) is then recorded, and from here on gravity is switched on to study the motion and dynamics of the single isolated bubble under buoyancy. All simulations have been done in fully periodic domains. The gravitational force is directed in the negative vertical direction. Sanakaranarayanan et al (2002) have suggested that this external force can be introduced into the force equation using the expression

\[
\mathbf{a}_{\text{ext}} = \mathbf{g} \left( 1 - \frac{\langle \rho \rangle}{\rho} \right)
\]  

where \( \rho \) is the mixture number density at the node of interest and \( \langle \rho \rangle \) is the average number density of the mixture in the entire domain. This choice ensures that the average value of the external force is zero in the periodic domain, and hence the mass-average velocity of the mixture is constant.
To capture bubble motion for a long enough time and to achieve steady state, the domain size is then increased to $100 \times 300$ lattice units and a new static bubble for this size of the domain is created. For all the liquid-vapor simulations described below, $\tau=1$. Figure 13 shows bubble snapshots at different instants of time as the bubble shape evolves under the influence of gravity.

Figure 13: Bubble shape evolution under gravity at an Eotvos number of 10.7. The time instants are at (a) initial condition, and (b) time=3000 timesteps. Red depicts the lighter vapor and blue denotes the heavier liquid surrounding the bubble.

The simulation was done at $Eo = 10.7$ and $Mo = 2.38 \times 10^{-3}$. At this Eotvos number, the bubble shape changes from a sphere to an ellipse. Liquid to vapor density ratio was 2.66. The interaction strengths were taken to be $g_{11} = 0, g_{22} = -0.3, g_{12} = 0.15$. The velocity vectors around the bubble are shown in figure 14. The presence of closed wakes behind the bubble is clear. The bubble
forms an oblate ellipsoidal shape as has been discussed by Bhaga & Weber (1981), who did experiments to study wake behavior behind moving bubbles with hydrogen bubble tracer technique.

Figure 14: Velocity vectors around the bubble as it forms an ellipsoidal shape for an Eo=10.7.

Figure 15 shows a comparison of the single bubble flow behavior and the bubble shape deformation/change as a function of Eotvos and Morton numbers. It is clear that as the Eotvos number increases, the bubble deformation and wake characteristics change very dramatically. The parameters for the single-bubble simulations are listed in table 3. It can be seen that as the
Eotvos number increases, the bubble shape changes from an ellipsoid (figure 15(a)) to a disk (figure 15(b)) and then for even higher Eotvos numbers, the bubble takes a skirt-like shape (figure 15(c)). These shapes and numbers match very well with the chart created by Bhaga & Weber (1981) and the numerical results of Tomiyama (1998). Figure 16 shows the well-known bubble shape regime map constructed by Grace (1971) using flow visualization. For various Re and Eo, the bubbles were characterized as spherical (s), oblate ellipsoid (oe), oblate ellipsoidal disk-like (oed), oblate ellipsoid cap (oec); spherical cap with closed wake (scc), and skirted (sks). Several cases were run using the current LBM for various Re, Eo and Mo as given in the APPENDIX and have been characterized as spherical, oblate ellipsoid and oblate ellipsoidal cap bubbles. Six representative cases are plotted along with Grace’s (1971) regime map in Figure 16. This figure shows that the current numerical simulation using LBM yields excellent quantitative and qualitative results for single bubble simulations.
Figure 15: Bubble deformation as computed using LBM for different sizes of the initial bubble. Density ratio is 2.68 for all the simulations. The Eotvos number for each case is (a) $Eo=37.2$, (b)$Eo=74.5$ and (c) $Eo=297.2$.

Table 3: Parameters for single bubble simulations as shown in figure 15.

<table>
<thead>
<tr>
<th></th>
<th>$\rho_l/\rho_g$</th>
<th>$d_e$</th>
<th>$Eo$</th>
<th>$Mo$</th>
<th>Shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>2.68</td>
<td>50</td>
<td>37.28</td>
<td>0.026</td>
<td>Oblate ellipsoidal</td>
</tr>
<tr>
<td>(b)</td>
<td>2.68</td>
<td>50</td>
<td>74.56</td>
<td>0.052</td>
<td>Oblate ellipsoidal disk-like</td>
</tr>
<tr>
<td>(c)</td>
<td>2.68</td>
<td>60</td>
<td>297.18</td>
<td>0.276</td>
<td>Skirted</td>
</tr>
</tbody>
</table>
Figure 16: Shape regime map for isolated bubbles in liquids taken from Bhaga & Weber (1981). The pictures in the inset show the results of the numerical simulations using LBM; s, spherical; oe, oblate ellipsoidal; oed, oblate ellipsoidal disk-like and wobbling; oec, oblate ellipsoid cap; scc, spherical cap with closed wake; sks, skirted with smooth steady wake.
Figure 17: Plot of $\log(Eo^{1/2})$ vs $\log(We)$. For initial bubble diameters much less than $d_{sph}$, the bubble deviates from perfect sphericity.

Calculations were also done for the Weber number and its relationship with the effective diameter of the bubble has been shown in figure 17. The effective diameter of the single bubbles has been non-dimensionalized using $d_{sph}$, which effectively yields $Eo^{1/2}$. This was done to study the bubble shape behavior as a function of the bubble diameter. As has been explained earlier, when $We<<1$, the surface tension pressure dominates over the dynamic pressure, and hence the bubble shape remains purely spherical. Figure 17 shows that for small effective bubble diameters, or small $Eo$, the Weber number is also small, and the shape is observed to be pure spherical. As
the diameter increases, the Weber number also increases and a higher distortion in the bubble shape is noticed, which explains that the surface tension pressure can no longer hold the bubble as a sphere and hence the dynamic pressure of the bubble dominates, creating a distorted and a highly distorted bubble.

Figure 18: Non-dimensional rise velocity as a function of time compared with the potential flow solution of Joseph (2003) for bubbles with very low Weber number (i.e. $\text{We}<<1$). The symbols show current LBM results, and the dotted lines show the theoretical predicted value.

Joseph (2003) has used potential flow theory to derive the terminal rise velocities of spherical cap bubbles. According to his work, such bubbles obey a dependence of the velocity on the fluid
viscosity and the diameter of the spherical cap, and also the curvature at the stagnation point of the bubble. The terminal velocity is given by

\[
\frac{U}{\sqrt{gD}} = \frac{-8\nu(1+8s)}{3\sqrt{gD^3}} + \frac{\sqrt{2}}{3}\left[1 - 2s - \frac{16s\sigma}{\rho gD^2} + \frac{32\nu^2}{gD^3}(1+8s)^2\right]^{1/2}
\]

(4.11)

where ‘s’ is the curvature at the stagnation point of the bubble, and is equal to zero for a perfectly spherical bubble. In the small Weber number limit, i.e. \(\text{We} \ll 1\), the expression can be simplified and written as

\[
U^* = \frac{U}{\sqrt{gD}} = \frac{-8\nu}{3\sqrt{gD^3}} + \frac{\sqrt{2}}{3}\left[1 + \frac{32\nu^2}{gD^3}\right]^{1/2}
\]

(4.12)

Joseph (2003) has called the non-dimensional form of the velocity as the Froude number. The non-dimensional velocity calculated through the code as the bubble attains a steady terminal velocity is shown in figure 17 for two cases of \(E_0=0.64\) and \(E_0=1.6\). The development of the rise velocities has been plotted as a function of the non-dimensional time, given as \(t^* = t/\sqrt{d_c/g}\).

The results show a perfect match of the computed velocity profile in the Stokes flow limit when compared to the derived Froude number of Joseph (2003).
4.2.3 Drag force and drag coefficient calculations

Most of the available correlations for drag have been developed for a single bubble in an infinite medium. Although the ideas can be extended to small tubes and channels for very small bubbles, for larger bubbles that are confined by the walls this may not always hold true. When the bubbles are confined, they start elongating with a spherical cap and a cylindrical tail in the case of a tube, and a planar cap in the case of a thin rectangular channel (Kumar (2004)). Beyond a certain size slug, the vapor is considered to be a continuous vapor field. In order to calculate the drag coefficient for a bubble in the dispersed field, the spherical equivalent size of the capped bubble is one that is widely considered. Where the bubble ceases to be dispersed and becomes a continuous field will of course depend on the dimensions of the channel, i.e., the hydraulic diameter. Even within the dispersed field, the bubbles go through distinct regimes and have different rise velocities. The rise velocity given as a function of the equivalent bubble diameter is an important component in the development of bubble drag models.

The bubble diameter at which the bubble ceases to be spherical is proportional to \( d_{\text{sph}} = (\sigma/\Delta \rho g)^{0.5} \).

This quantity simply comes from the force balance between the buoyancy and surface tension acting on the bubble. This can also be recast in terms of the parameter, Eotvos number, \( E_o \), defined as \( E_o = g\Delta \rho d^2/\sigma \). Tomiyama (1998) classified bubbles in several groups based on their \( E_o \).

For each field or group, he used a drag coefficient based on Eotvos and Morton number. Based on the proposed drag coefficient, he calculated the terminal rising velocities of single bubbles in stagnant liquids, and plotted \( Re \) vs. \( E_o \) for various Morton number to compare with available data. He classified the bubble shapes for \( Mo < 10^{-6} \) into spherical and ellipsoidal (oblate spheroid, \( E_o < 40 \)) and spherical-cap (\( E_o > 40 \)) with a flat rear surface. This is an effective approach in thin
tubes if the flow regime is predominantly bubbly and slug flow. It is not clear whether the drag relations given by Tomiyama (1998) for air-water systems are applicable for other fluids and at high pressures. Zun (1987) describes the intrinsic fluctuating bubble motion in terms of Eo, and reports that the magnitude of the fluctuation increases with Eotvos number. Using an interface tracking method, Tomiyama (1998) predicted single bubble motions to determine the effect of Eotvos number. Their predicted velocity field indicates that the bubble fluctuation is closely related to the periodic vortex shedding, and Eo is the most appropriate parameter to define the lateral movement of the bubbles.

In our study, drag coefficient calculations were conducted using buoyancy-driven single bubble simulations at low void fractions and the velocity of such isolated bubbles was computed till it reached a steady value. This terminal bubble velocity was then used to compute Re and We together with the effective bubble diameter, \( d_e \). The drag coefficient is defined as the ratio of the buoyancy force to the inertial force, and is given by

\[
C_D = \frac{4\Delta \rho g d_e}{3\rho \ell U_b^2} \quad \text{in 3-D and} \quad C_D = \frac{\pi \Delta \rho g d_e}{2\rho \ell U_b^2} \quad \text{in 2-D.}
\]

The calculations for the drag coefficient have been compared to the correlation of Bhaga & Weber (1981), in which the drag coefficient for fluids with high Morton numbers \( (Mo > 4 \times 10^{-3}) \) is said to obey the relationship

\[
C_D = \left[ (2.67)^{0.9} + \left( \frac{16}{\text{Re}} \right)^{0.9} \right]^{1/0.9} \quad \text{(4.13)}
\]

Results of the numerical computations have also been compared to the empirical correlation of Joseph (2003) in which \( C_D \) is given by

\[
C_D = 0.445 \left( 6 + \frac{32}{\text{Re}} \right) \quad \text{(4.14)}
\]
The results of the numerically computed drag coefficient have also been compared with the correlation of Tomiyama (1998), in which the drag coefficient is a function of the Reynolds and the Eotvos numbers.

\[ C_D = \max \left[ \min \left( \frac{24}{\text{Re}} \left( 1 + 0.15 \text{Re}^{0.687} \right), \frac{72}{\text{Re}} \left( 8 \frac{\text{Eo}}{3 \text{Eo} + 4} \right) \right) \right] \]  (4.15)

For comparisons with his correlation, the numerically computed Eotvos and Reynolds numbers are used together to determine which component is bigger and should be used to quantify the drag. The results of this exercise have been shown in figure 19. With the current explicit formulation of LBM, bubble Reynolds numbers are limited to 100. This was mainly done to capture a wide range of Morton numbers. Tomiyama’s (1998) \( C_D \) relation consists of independent functions of \( \text{Re} \) and \( \text{Eo} \). At low Reynolds number (\( \text{Re} < 10 \)), the drag coefficient is completely determined by the Reynolds number part of Tomiyama’s (1998) correlation. For \( \text{Re} > 25 \), neither part of the correlation is predominant in the determination of the drag coefficient for a single isolated bubble.
Figure 19: The drag coefficient (○-current simulation results) as computed for single bubbles at different Reynolds numbers compared with the correlation in Bhaga and Weber (1981), by Joseph (2003), and (*) computed using the correlation given by Tomiyama (1998). Pictures in the inset show bubble deformation at different Reynolds numbers.
4.3 Multi bubble simulations

Simulations were also done for multiple vapor bubbles in a periodic domain. In one of the earlier, beautiful collections of two-phase flow photographs in thin vertical rectangular channel, followed by excellent flow descriptions, Jones and Zuber (1975) observed that the slug regime seldom contains Taylor-type bubbles. Instead, the bubbles in the slug flow oscillated wildly from side to side and snakewise along the upward flow direction. They observed the Karman vortex street behavior by the entrained bubbles behind major voids using the high-speed motion pictures. Under the influence of the trailing vortex street, the nose of the elongated bubbles moved from side to side. They noted that slug-like flows occur for void fraction between ~0.2 and ~0.8. Later from geometric considerations, Mishima and Hibiki (1998) showed that the possibility of collisions and coalescence would increase if the maximum distance between two bubbles were less than the projected diameter of flat bubble. Figure 20 and 21 show two such cases in which LBM has been used to study bubble coalescence. Figure 20 shows the flow situation for two bubbles at an initial \( Eo=53.74 \) and \( Mo=0.297 \) separated by an initial separating distance of \( 2.5d \) and figure 21 is at \( Eo=29.6 \) and \( Mo=0.279 \) with an initial separation of \( 2.0d \), where ‘\( d \)’ is the initial diameter of the bubble. The preliminary cases were run with two bubbles, whose line connecting the centers is parallel to the gravitational vector. The objective was to study the influence of the wakes left by the upper bubble(s), which subsequently move downstream into the path of the lower bubble(s). It can be observed that for bubbles with an Eotvos number of 53.7, the upper bubble deforms much more than the lower rising bubble. This can be explained by the fact that the upper bubble flows ‘through’ the freely falling liquid, while the lower one is traveling ‘into’ the wake left behind the upper bubble. Thus, the wake left behind by the former
enables lesser drag for the latter. As a result, the relative velocity of the bubbles is non-zero, because of which the distance between the two bubbles keeps decreasing with time. Eventually the bubbles touch (see figure 20(a) & 21(a)), and soon after form a larger bubble with twice the volume as the initial bubble. The shape of this intermediate larger bubble (see figure 20(b) & 21(b)) is different for the two cases shown here, thereby indicating that bubble coalescence and behavior is a function of the Eotvos number and is not the same for all situations. In our case, we have studied the change in Eotvos number by changing the size of the initial bubble(s). Eventually at steady state, the bubble streamlines and the shapes for the two cases are found to be much different as was expected. Simulations were also done for cases with more than two bubbles, with axially and non-axial starting conditions. It was found that if the line connecting the centers of the bubbles is aligned to the gravity, then the motion of the bubbles is purely rectilinear. This can be explained as the initial bubble distribution has an axis of symmetry that runs through the center of the bubbles, as can be seen in figure 22. So the bubbles do not deviate in the lateral direction. The way these bubbles coalesce has been captured in figure 22(c)-(g). It can be observed that the uppermost bubble flowing upstream into the path of the falling liquid has the maximum shape deformation, because of the highest drag experienced by this vapor phase. Figure 22(g) shows an instance when some liquid is trapped inside the bubble after the small-big bubble collision. This is because the inertia of the bubbles is so high that at the time of impact, the liquid does not get enough time to squeeze out completely through the narrow gap left between the two bubbles, thus, getting trapped inside the vapor phase. Eventually, as can be seen in figure 22(h), the liquid ‘pops’ out from the bottom surface of the vapor. This phenomenon has also been observed by Takada et al (2001).
To study how the wakes behind the bubbles effect the motion of the downstream bubbles, a new simulation was run with three bubbles of the same size that do not have the line joining their centers parallel to the gravitational vector. The results of this test as shown in figure 23, 24 and 25. It was observed that as the bubbles move, the wake behind the upper bubbles creates an artificial lift force for the downstream bubbles, thereby causing the bubbles to move in a helical path. The effect of the lift force is such that the bubble shapes are no more oblate elliptical, rather change to oval-like. These oval bubbles seem

Figure 20: Bubble coalescence for a flow situation with two bubbles of equal size of diameter 40 lattice units separated by center to center distance of 2.5d initially. Bubbles touch at (a) $t^*=21.9$; (b) bubbles coalesce at $t^*=22.62$ to form a bell-shaped blob; (c) bubble attains a spherical cap shape at $t^*=27.6$. 
Figure 21: Bubble coalescence for a flow situation with two bubbles of equal size of diameter 30 lattice units separated by center to center distance of 2d initially. Bubbles touch at (a) $t^* = 11.0$; (b) bubbles coalesce at $t^* = 11.84$ to form a bell-shaped blob; (c) bubble attains an oblate ellipsoidal shape at $t^* = 20.4$.

to follow each other, into the wake left by the upstream vapor. Eventually these bubbles coalesce and the final shape of the eventual bubble is shown in figure 25 (a) and 25(b). The vortices for the two cases of rectilinear and helical bubble motion are also compared in figure 26. The shape of the vortex at either end of the major axis of the bubble is much different in both cases, and explains why the bubble in the latter case follows a helical path because of the oscillatory motion of the wake.
Figure 22: Dynamics of three bubbles separated by a continuous liquid phase at $Eo=2.88$ and $Mo=2.71 \times 10^{-3}$. Bubbles are aligned vertically; (a) $t^*=2.85$, (b) $t^*=6.12$, (c) $t^*=6.94$, (d) $t^*=7.35$, (e) $t^*=10.2$, (f) $t^*=11.02$, (g) $t^*=13.88$, and (h) $t^*=14.29$. 
Figure 23: Dynamics of three bubbles separated by a continuous liquid phase at $E_o=3.04$ and $M_o=3.16 \times 10^{-4}$. Bubbles are in staggered alignment with respect to the gravity vector; (a) $t^*=1.84$, (b) $t^*=4.9$, and (c) $t^*=7.96$. 
Figure 24: Dynamics of three bubbles separated by a continuous liquid phase at $Eo=3.04$ and $Mo=3.16 \times 10^{-4}$. Bubbles are in staggered alignment with respect to the gravity vector; (a) $t^*=8.57$, (b) $t^*=9.19$, and (c) $t^*=10.41$. 
Figure 25: Dynamics of three bubbles separated by a continuous liquid phase at $Eo=3.04$ and $Mo=3.16 \times 10^{-4}$. Bubbles are in staggered alignment with respect to the gravity vector.; (a) $t^*=11.64$, and (b) $t^*=15.92$. 

(a)  

(b)
Figure 26: Comparison of the streamlines around the bubble for the case of fig. 22 (shown in (a)) and 23, 24, 25 (shown in (b)). The flow field around (a) is symmetrical about the center axis unlike (b). This causes the bubble in (b) to oscillate as it moves upwards.
CHAPTER FIVE: CONCLUSIONS

The lattice Boltzmann method has been used to simulate single- and two-phase fluids. Benchmark studies were done to validate the code. These benchmarks included Poiseuille flow, lid-driven cavity, and the static bubble test. Shan-Chen’s (1993) interaction model has been used to simulate gravity driven two-phase flows. Bubble dynamics has been studied with single dispersed vapor bubble in a heavier liquid, and the results show that the bubble shapes fall into the shape-chart created by Bhaga & Weber (1981). Simulation of bubbles with different sizes shows that as the Eotvos number increases, the bubbles deform from a spherical to oblate-ellipsoid to disk-like and eventually at very high Eotvos numbers to skirt-like structures. For cases where the Weber number was very small as compared to unity, numeric terminal velocity calculations were compared to the potential flow solution of Joseph (2003), and the simulation results matched extremely well with that predicted by theory. Bubble drag calculations have also been done and the results have been found to compare well with existing empirical correlations of Bhaga and Weber (1981), Tomiyama (1998) and Joseph (2003). Current LBM results show that Tomiyama’s (1998) correlations that involve functions of Reynolds number and Eotvos number yield the best results for a wide range of parameters.

Multiple bubbles are also simulated in an infinite domain and bubble coalescence characteristics are studied for different initial size and distances of the bubbles. It is observed that as the Eotvos number increases, the uppermost bubble deforms the most because of the maximum drag that it experiences from the liquid flowing downstream. The bubble dynamics is dictated by vortex pattern of the leading bubble, which allows the bubbles to coalesce. Such
simulations have also been run for different configurations of the initial bubble distribution to show the effect of vortex shedding on the oscillatory motion of the bubbles. Staggered bubbles yield a qualitative overview of the process of bubble coalescence in channels in which lift forces come into play because of the presence of walls. Future work is directed towards the study of bubble nucleation and coalescence to form vapor slugs due to wall heating.
CHAPTER SIX: FUTURE WORK

A major challenge with the current model of LBM that has been used is that it cannot handle fluid mixtures with a very high density ratio (like water-air system which is typically of the order of 1000). The method needs significant work and needs to be developed where common day fluid phenomenon can be observed and studied without any criterion that decides the maximum density ratio that can be simulated successfully.

Another area where work needs to be directed upon is the simulation of bubble motion in the presence of walls in the lateral direction. The influence of walls on the motion of single- and multiple bubbles in a wall-bounded domain needs to be studied. Experimental observations show that a bubble with low Eotvos number does not move towards the wall significantly as compared to a bubble with larger Eotvos number (or a larger diameter), in which case the bubble quickly migrates towards the center of the duct. Simulating a two-phase system which can capture such bubble motion would lead to a better understanding of the physics of flows in narrow rectangular ducts. Lift forces need to be quantified in such simulations and the dependence of the lift coefficient on the Eotvos number needs to be investigated deeply. Subsequent work would be to study the effect of wall heating and phase separation on a wall-site, i.e. the creation of a bubble at one of the locations on the wall and subsequent bubble departure/peeling away from the wall once it reaches a critical bubble size. This in itself is a very challenging problem.
APPENDIX: PARAMETERS AND SHAPES FOR SINGLE-BUBBLE SIMULATIONS
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*for all cases, $\rho_{f}/\rho_{g}=2.66$*
LIST OF REFERENCES


