

Multiple-Relaxation-Time Lattice Boltzmann Method for Multiphase Flows with High Density and Viscosity Ratios - 10135

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ABSTRACT

In this paper, the lattice Boltzmann method is reviewed for specific applications to numerical simulation of multiphase flow problems. A thorough literature review regarding the multi-phase lattice Boltzmann method was conducted with special focus on flows with large density and viscosity ratios between the two phases. A multiphase model with the capability of handling large-density-ratios is crucial for the modeling efforts at Florida International University since Department of Energy related operations such as the pulsed-air mixing involve air bubbles formed in tanks where the liquid to gas density ratio is approximately 1000. It was observed that there have been four major interface tracking methods developed in the lattice Boltzmann framework, namely; the color method, the free-energy method, Shan-Chen's potential method and the index-function method. There have also been other methods proposed such as the hybrid level-set lattice Boltzmann method and the front-tracking lattice Boltzmann method, however, they have not been applied as extensively as the others. Lattice Boltzmann simulations are reported to be unstable when the density ratio between fluids are larger than 10. Of twenty-six papers reviewed on multiphase lattice Boltzmann method with the single-relaxation-time collision model, five have extended the capability of the multiphase methods into fluids with large-density-ratios up to 1000. However, the single-relaxation-time lattice Boltzmann method using the Bhatnagar-Gross-Krook collision model was found to have stability issues when the viscosity of the fluid is reduced or the Reynolds number is increased. Lattice Boltzmann method using the multiple-relaxation-time collision operator was proposed by researchers in order to simulate flows where viscosities are low or the Reynolds number is large. Twenty-five publications were reviewed on multiple-relaxation-time methods, seventeen of which were specific to multiphase flows. Six of the multiple-relaxation-time papers were focused on multiphase flows with large liquid to gas density ratios, which was identified as another source of numerical instabilities observed in multiphase simulations with the lattice Boltzmann method. The multiple-relaxation-time lattice Boltzmann method coupled with the modified index-function approach was observed to be capable of stable simulations of high-density-ratio, low viscosity multiphase flows.

INTRODUCTION

As a result of atomic weapons production, millions of gallons of radioactive waste was generated and stored in underground tanks at various U.S. Department of Energy sites. Department of Energy is currently in the process of transferring the waste from single shell tanks to double shell tanks. Various waste retrieval and processing methods are employed during the transfer of the waste. One such method, pulsed-air mixing, involves injection of discrete pulses of compressed air or inert gas at the bottom of the tank to produce large bubbles that rise due to buoyancy and mix the waste in the tank as a result of this rising motion. Pulsed-air mixers are operated by controlling the pulsing frequency and duration, the sequence of injection plates and gas pressure. Low equipment cost, high durability, easy decontamination and low operating costs are some of the advantages of pulsed-air mixers over other waste mixing technologies.

The pulsed-air technology is commercially available and its effectiveness has been demonstrated at Pacific Northwest National Laboratory [1,2,3], however, understanding the physical nature of the mixing phenomena by injection of air bubbles and the effects of the air release process to the tank environment need to be studied by considering various waste conditions. Such an analysis can be made possible by

developing a numerical method that can simulate the process of air bubble generation inside tanks filled with liquid. The final computational program would serve as a tool for the site engineers to predict various mixing scenarios and improve operational procedures of pulsed-air mixing efficiently.

In this paper, a numerical method, lattice Boltzmann method, is reviewed that can model multiphase flows accurately and efficiently. Lattice Boltzmann method is advantageous over traditional Navier-Stokes [4] based computational models since surface forces are handled more effectively in lattice Boltzmann method [5]. Lattice Boltzmann method has been mostly employed using the Bhatnagar-Gross-Krook collision operator [6] with a single relaxation time to simulate multiphase flows. This has brought a limitation when the fluid viscosity is low which makes the lattice Boltzmann method simulations unstable. In order to avoid instability issues, multiple-relaxation-time lattice Boltzmann models are proposed that use a collision operator that can adjust the bulk and shear viscosities independently. Feasibility of multiple-relaxation-time lattice Boltzmann method for multiphase flow simulations is investigated in this paper. A thorough literature review is presented with successful verification cases related to bubbly flows in tanks.

Special attention will be given to two-phase flows with high density ratios since this brings another challenge in terms of instabilities to lattice Boltzmann method simulations for multiphase flows with density ratios larger than 10. The instability is considered to be generated as a result of large density gradients in the interfacial region between two phases. Possible solutions found in the literature are discussed in the paper.

The outline of the report is given as the following: first an overview of numerical modeling approaches to multiphase flows is presented. Secondly, the lattice Boltzmann method using the single relaxation time for the collision term is introduced in relation to the multiphase flows. Later, multiple relaxation time based lattice Boltzmann methods for multiphase flows are discussed. Applications to model multiphase flows with a large density ratio between different phases are shown. Finally, conclusions are drawn and discussions for future work plan are presented.

MULTIPHASE COMPUTATIONAL FLUID DYNAMICS METHODS

There are two major computational fluid dynamics methods used to study multiphase flows, which are front capturing methods and front tracking methods.

In front capturing methods the exact location of the interface separating two fluids is not determined exactly but approximated. The Marker-and-Cell and Volume-of-Fluid methods are the most popular front capturing methods. In the Marker-and-Cell method, the Navier-Stokes equations are solved for the whole domain as a single fluid using a stationary Eulerian grid and different phases are simulated by adjusting the local fluid properties (Fig. 1.(a)). The interface is tracked using Lagrangian markers that are used to interpolate the fluid properties such as viscosity and density. In order to represent the fluid properties accurately, a large number of markers need to be employed which makes the method computationally intensive. Challenges regarding the determination of the interface from the markers, grid resolution dependence of the accuracy of the solution and macroscopic representation of the surface tension make the method disadvantageous for multiphase flow simulation.

Volume-of-Fluid method replaces the need to allocate a large number of markers in the Marker-and-Cell method by calculating volume fractions at each grid cell (Fig. 1.(b)). However, surface tension still has to be calculated as it is in Marker-and-Cell method. Volume-of-Fluid also suffers from inability to capture the exact location of the interface and still has problems in solving cases with liquid break-up and coalescence. Level set method is another front capturing method which uses two sets of equations in contrast to the Marker-and-Cell and Volume-of-Fluid methods. In addition to the Navier-Stokes equation, a convection equation is solved to calculate the level set function that changes sign depending on the position with respect to the interface. The surface tension is calculated similar to Volume-of-Fluid;

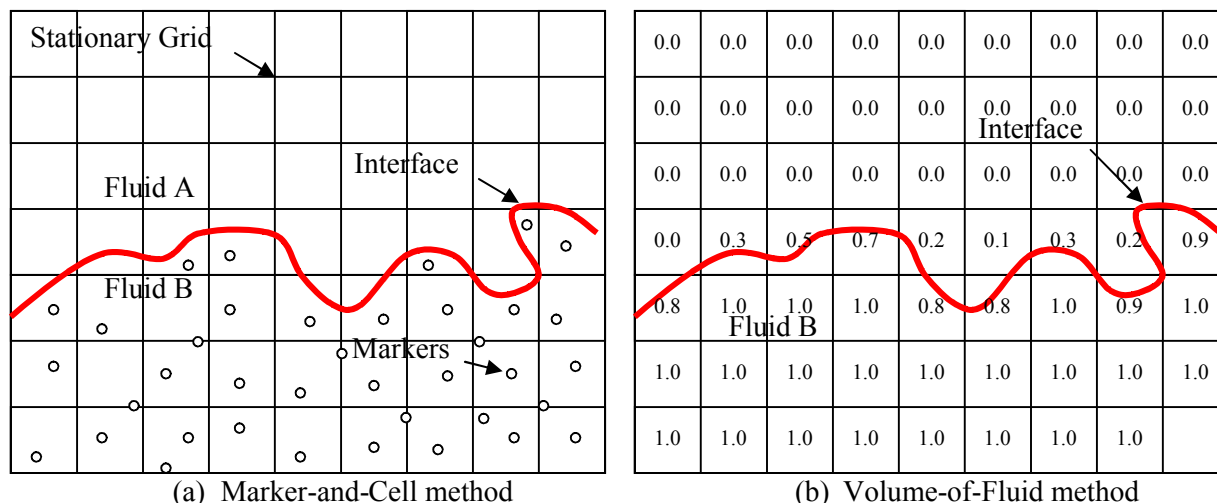


Fig. 1. Schematic presenting the representation of the interface in front capturing methods.

however, the interface is determined more easily as compared to the Volume-of-Fluid method. Mass conservation is an issue with the level set method due to the non-conservative convection equation solved for the index function.

Front tracking methods, on the other hand, capture the location of the interface exactly since the interface is tracked directly. There are different approaches used in front tracking methods. In the boundary-fitted grid method, the interface is fit on the grid and the Navier-Stokes equations are solved for both sides of the interface. Surface tension is applied on the interface as a boundary condition where the Laplace's law [7] is used to determine the pressure in cells surrounding the interface. At each time step in the iteration the new location of the interface is moved according to the velocity of the field. In this method the grid must be fine enough to represent the interface properly and liquid break-up is difficult to simulate. Unverdi and Tryggvason (1992) have developed a hybrid method that uses two sets of grids at the same time [8]; a stationary grid for the fluid flow and a lower dimension grid for the interface. In this method, which is presented in detail in [9], a single Navier-Stokes equation is used for the whole domain as in front capturing methods while the exact location of the interface is still tracked. Gokaltun *et al.* (2003) have used the front tracking method coupled with a finite volume solver to extend the method to multiphase flows in complex geometries [10]. Representing the geometry of the interface independent from the grid reduces the grid resolution requirement in this method as compared to the boundary-fitted method. On the other hand, the criterion used for break-up or coalescence of liquids in this method does not have a physical base but rather depends on the distance between interfaces.

MULTI PHASE LATTICE BOLTZMANN METHOD BHATNAGAR-GROSS-KROOK MODELS

Due to its capability to inherently capture interfacial flows, lattice Boltzmann method multiphase models has been investigated in the past two decades by many researchers [11,5,12]. The lattice Boltzmann method has advantages in simulating multiphase flows where the intermolecular attraction between different phases can be modeled easily. The interface between two liquids is not required to be determined as in Volume of Fluids approach, but liquid break-up can still be predicted using front capturing methods. In addition to this, the information is passed on to the neighboring nodes locally that allow the lattice Boltzmann method computations to be highly parallelizable.

Gunstensen *et al.* (1991) has developed a multiphase lattice Boltzmann method [13] called the 'color method' that was based on a two-component lattice gas automata model [14]. This model used two distribution functions, red and blue, in order to represent two different fluids. The interface was maintained by introducing a re-coloring step in order to force different phases towards the fluids with

same colors. The drawback of this model was that it was computationally expensive to re-distribute the colored density at each lattice node. In addition to that, anisotropic surface tension could cause vortices near interfaces [15]

Another multiphase lattice Boltzmann method, typically referred to as the ‘potential method’, was proposed by Shan and Chen (1993) that automatically generated the surface interface by modifying the surface tension related terms in the collision operators using the inter-particle potentials [16]. The isotropy of the surface tension was improved, however, this model was observed to create spurious currents near interfaces which was due to the deficiency of the surface tension related collision operator to conserve local momentum [15]

Swift *et al.* (1995) developed a multiphase lattice Boltzmann method based on the free-energy approach [17]. The equilibrium distribution was modified so that the pressure tensor was consistent with the tensor derived from the free-energy function of non-uniform fluids. The method lacked Galilean invariance that the temperature would depend on the density gradient even for isothermal fluids resulting in an incorrect energy balance equation.

He *et al.* (1999) introduced an incompressible multiphase lattice Boltzmann method where interfacial dynamics were modeled by incorporating molecular interactions and the interfaces between different phases were tracked using an index function [18]. Two sets of distribution functions were used; one for tracking the pressure and velocity fields and the other for the variable called the index function which is used to obtain density and viscosity. The model was extended by Premnath (2004) to incorporate axisymmetric coordinates [15]. Two-dimensional Rayleigh-Taylor instabilities were simulated and the results for initial linear growth rate and the terminal bubble velocity were verified comparing against previous theoretical and numerical results for the single mode instability.

The methods listed above represented the interface between two fluids as a transition layer, whose evolution was either not described explicitly as in the color method [13] and the potential method [16], or the physics of the interface capturing equation was not clearly stated as in the index method of He *et al.* [18]. The density gradient was calculated in the whole flow field and the interface was captured where the gradient was non-zero. Only in the free energy method [17] a convection-diffusion equation was used to capture the interface that captured the evolution equation of the interface, Cahn-Hilliard equation, when the Chapman-Enskog expansion was used.

LATTICE BOLTZMANN METHOD FOR HIGH-DENSITY RATIO MULTIPHASE FLOWS

One common limitation of the multiphase lattice Boltzmann method described so far was that their applications were limited to low density ratios between phases. The density ratio obtained by the Swift’s free-energy method was less than 10, which was also the limit for the index-function method of He *et al.* (1999). Attempts to improve Gunstensen’s color method to higher density ratios were only successful to achieve density ratios up to 4 [19] and 20 [20]. Lishchuk *et al.* (2008) have claimed to extend the color method to density ratios up to 500 however they have reported simulations with density ratios less than 10 due to computational expense of the method at larger density ratios [21]. The exact reasons of this low-density-ratio limit in lattice Boltzmann method multiphase models have not yet been explained clearly, however the inherent compressible characteristic of the lattice Boltzmann method is considered to be one of the reasons.

Inamuro *et al.* (2004) proposed a method based on the free energy method to extend its capability to incorporate fluids with large density ratios up to 1000 [22]. They used a pressure correction step in order to enforce the continuity equation after the collision and streaming step. The projection step required solving the Poisson’s equation for the whole flow field and has reduced the computational efficiency of the method and problems with assigning a cut-off value for the order parameter, evolved by the Cahn-Hilliard interface evolution equation, and a lack of analytical expression of the surface tension coefficient

has been brought forward as deficiencies of the method [23,24]. In addition, the additional terms that show up in the recovered interface evolution equation caused the method to lack Galilean invariance.

Lee and Lin (2005) have used the index function method of He *et al.* [18] in order to develop a stable version for multiphase flows with large density ratios up to 1000 and viscosity ratio varying from 40 to 100 [25]. A modified pressure was introduced in order to avoid the large pressure fluctuations across the interface causing the scheme to be unstable at high density ratios in the index function model by He *et al.* (1999). The forcing term in the pre-streaming collision step and post-collision step were treated differently in order to improve the stability of the method. The results were verified for a stationary drop using the Laplace's law and their method was observed to have a high degree of isotropy. Using a D3Q19 lattice model, a 3D droplet oscillation case is solved for a density ratio of 1000 and a viscosity ratio of 100. The oscillation periods for droplets with various radius size and thicknesses were verified against analytical results with maximum errors being less than 5%. Droplet splashing on a thin liquid film was also analyzed where the density ratio was 1000, maximum viscosity ratio was 40 and the Weber number was 8000. However, their model was criticized for not recovering the lattice Boltzmann equation (LBE) for the interface to the Cahn-Hilliard equation [23].

Based on the free-energy model, Zheng *et al.* (2006) used a modified lattice Boltzmann method [26] that recovered the lattice Boltzmann equation for the interface to the Cahn-Hilliard equation with the second order of accuracy. They also employed a D2Q5 lattice structure that improved the efficiency compared to the other models using D2Q9. Their model was Galilean invariant and the potential form of the surface tension related term was used to reduce the spurious currents. Their model was verified by comparing the surface tension for a stationary liquid cylinder with a density ratio of 1000 against the Laplace law. Oscillating capillary wave motion of an interface with density ratio of 1000 was also simulated and verified against theoretical results for angular frequencies. Buoyancy driven rising bubbles were simulated in comparison to Volume-of-Fluid and lattice Boltzmann method simulations of Takada *et al.* using the Swift's free energy method [27] with maximum errors of 3.89% and 4.35% respectively for the terminal velocities at a density ratio of 2.5. Rising bubble shapes and wake formations at a density ratio of 1000 were found to be in agreement with experimental findings [28]. The interface capturing method was recently extended into three-dimensions using a D3Q15 and D3Q7 lattices [29]. Numerical tests for translation, rotation and stretching with tear showed better performance than Volume-of-Fluid method and the approach of Inamuro *et al.* (2004).

Cheng *et al.* (2009) used the 3D model of Zheng *et al.* (2008) to simulate multiple bubbles rising under buoyancy in a viscous and incompressible fluid at rest [30]. They used a nineteen-velocity model (D3Q19) for the momentum phase and a seven-velocity model (D3Q7) for the fluid phase. Viscosity ratio was found to have a negligible effect on terminal bubble shape and velocity as compared to the ratio of density that is why the simulations were carried out for two phases with uniform viscosity. Terminal bubble shapes at a density ratio of 1000 was found to be in good agreement with experimental images at different Morton numbers ($M=266, 41.1$ and 5.51) where the Eotvos number was 116. Oblique coalescence of two rising bubbles and a evolution of a cloud of rising bubbles were investigated numerically.

An alternative method was introduced by Mehravaran and Hannani (2008) where a hybrid level-set lattice Boltzmann method was used to solve for incompressible two-phase immiscible fluids with large density ratios up to 1000 and viscosity ratios up to 100 [31]. The velocity field was solved using the lattice Boltzmann method and were input to the level-set solver in order to determine the new position of the interface. Poiseuille two-phase flow, oscillation of two colliding droplets and Rayleigh-Taylor instability were solved as numerical test cases.

MULTIPLE-RELATION-TIME MULTIPHASE LATTICE BOLTZMANN METHOD

The multiphase lattice Boltzmann method presented so far used the Bhatnagar-Gross-Krook single relaxation time collision operator. Using the Bhatnagar-Gross-Krook collision model, the distribution

functions are relaxed to the local equilibrium values at a rate determined by a single relaxation time parameter which is related to kinematic viscosity. lattice Boltzmann method using the Bhatnagar-Gross-Krook model becomes numerically unstable at low values of fluid viscosity. This is primarily due to the linear relation of bulk viscosity and the kinematic viscosity in lattice Bhatnagar-Gross-Krook models. When the kinematic viscosity is reduced at high Reynolds numbers, the bulk viscosity is also reduced which creates spurious density fluctuations due to insufficient dissipation. The causes of numerical instabilities are also attributed to the nonexistence of an H theorem [32]. There have been two main approaches introduced in order to find a remedy to the stability problem at low viscosities; entropic methods [32] and multiple-relaxation-time methods. A non-polynomial equilibrium distribution function is used in the entropic methods. Increased computational requirements, non-constant transport coefficients depending on the velocity field are some of the disadvantages of these methods in practical computer simulations with lattice Boltzmann method. The multiple-relaxation-time model permits adjustment of kinematic and bulk viscosities separately. This is achieved by using a scattering matrix for the collision term that relaxes the distribution functions to their local equilibrium values at characteristic time scales. This allows keeping the bulk viscosity large enough to dissipate density fluctuations while lowering the shear viscosity at the same time for high Reynolds numbers. The multiple-relaxation-time method was developed by D'Humieres (1994) at the same time when the Bhatnagar-Gross-Krook method was first proposed [33]. Bhatnagar-Gross-Krook method obtained more popularity due to its simplicity compared to the multiple-relaxation-time method. D'Humieres *et al.* (2002) recently reviewed the multiple-relaxation-time method [34] and optimal boundary conditions were reported in the literature [35]. Single-phase multiple-relaxation-time method has been verified by Du *et al.* (2006) for steady Poiseuille flow, driven cavity flow with $2000 < Re < 10,000$ and double shear flow at $Re = 7500$ and $100,000$ [36].

Prof. Abraham's group in Purdue University has produced multiple-relaxation-time based multiphase lattice Boltzmann method using He *et al.*'s index-function approach [18] to study simulation of liquid jets [37], drop impingement on dry and wet walls [38] in two-dimensional planar and axi-symmetric coordinates and binary drop collisions in three dimensional coordinates [15]. The multiphase model that was used in their multiple-relaxation-time method depended on the kinetic theory of dense fluids proposed by He *et al.* (1999). McCracken and Abraham (2005) showed that the multiphase multiple-relaxation-time method using the index-function model can capture the pressure change across a two-dimensional liquid cylinder due to surface tension within 12% accuracy when compared with the Laplace's law [39]. It was also shown that the index function multiple-relaxation-time model was able to solve an oscillating liquid cylinder problem where a liquid cylinder of initial elliptical cross section with a density ratio of 10 oscillates in time until it reaches equilibrium. The oscillation frequencies for various surface tension values were captured within 3% of the analytical solution given by Lamb [40]. Simulations for oscillating capillary waves with an initial sinusoidal perturbation showed 8% error in the oscillation frequency and the decay rate when compared with the analytical solutions where the multiple-relaxation-time model was observed to yield accurate results with viscosities 16 times lower than of a Bhatnagar-Gross-Krook solution.

The benchmark test cases given above were also verified with the same multiple-relaxation-time model in three-dimensions by Premnath and Abraham (2007) where Laplace-Young relation was predicted within 8% accuracy, three dimensional drop oscillations were solved with 5% error for oscillation time periods with a density ratio of 4 [41]. In another study by Premnath and Abraham (2005), both axisymmetric and three dimensional representation of multiple-relaxation-time lattice Boltzmann method with the index function model were used to investigate drop collisions with density ratios up to 4 [42]. It was reported that the multiple-relaxation-time collision model does not improve numerical stability of the lattice Boltzmann method simulations at high density ratios.

Others have also tried to extend the multiple-relaxation-time lattice Boltzmann method into multiphase flows. Tolke *et al.* (2006) have presented a multiple-relaxation-time lattice Boltzmann method using the

color method [13] in order to simulate rising bubble motion with local grid refinement employed around the interface [43]. Li *et al.* (2005) carried out three-dimensional investigations of viscous coupling effects for two-fluid flow in a porous media [44] using multiple-relaxation-time lattice Boltzmann method with the potential approach of Shan and Chen [16]. Lallemand *et al.* (2007) have combined the multiple-relaxation-time lattice Boltzmann method with the front-tracking method to simulate interfacial dynamics with surface tension in two-dimensions [45].

MULTIPLE-RELAXATION-TIME LATTICE BOLTZMANN METHOD FOR HIGH-DENSITY RATIO MULTIPHASE FLOWS

Using multiple-relaxation-time collision model in the lattice Boltzmann method improves the stability at lower viscosities however the instabilities still are observed when the density ratio between the two liquids are large. In order to obtain an multiple-relaxation-time lattice Boltzmann method that is stable at high density ratios, Mukherjee (2006) has extended the multiple-relaxation-time lattice Boltzmann method to the higher density-ratio multiphase model developed by Lee and Lin (2005). Compared to the previous multiphase multiple-relaxation-time lattice Boltzmann method from the same group [37,15], the multiple-relaxation-time pressure distribution equation was developed for a smoothly varying pressure function rather than the actual pressure. This aimed to reduce the large pressure fluctuations across the interface in the multiple-relaxation-time using He's model [18]. The density was also computed directly from the density distribution function while an index function was used to interpolate density previously.

In order to verify the model, the Laplace's law was reproduced using the axisymmetric high density-ratio multiple-relaxation-time lattice Boltzmann method for a spherical liquid drop that is in equilibrium with the surrounding fluid [46]. The pressure difference between the two phases was solved within 3% of the analytical equation for a density ratio of 1000 and a viscosity ratio of 40. Using the same density and viscosity ratios, the multiple-relaxation-time lattice Boltzmann method solution for the dynamic problem of liquid drop oscillation was also found to be within 8% of the analytical solution of Lamb (1932) for the period of oscillations. Drop impingements on a wet wall were also simulated at the same density and viscosity ratios and power-law growth of the corona until the break-up was successfully captured. Similar benchmark cases at high density and viscosity ratios were also verified with comparable accuracies in planar two-dimensional coordinates by the same authors separately [47]. Drop impingement on walls with a pre-existing liquid film was further investigated using the axisymmetric multiple-relaxation-time lattice Boltzmann method in order to investigate the influence of wall liquid film thickness and surrounding gas density and viscosity on crown behavior [48]. It was observed that the rate of crown radius and height increases with increase in the thickness of the liquid film. An increase in surrounding gas density was found to delay the break-up of the crown whereas an increase in viscosity speeds up the break up process.

There have been a few other studies published in the literature trying to extend multiple-relaxation-time lattice Boltzmann method to multiphase flows with a high density and viscosity ratios [49,50,51]. Niu *et al.* (2009) have used the multiple-relaxation-time lattice Boltzmann method multiphase model presented by McCracken and Abraham (2004) in order to investigate water-gas transport processes in the gas-diffusion-layer (GDL) of a proton exchange membrane fuel cell system [49]. The multiphase multiple-relaxation-time lattice Boltzmann method model was validated for a static droplet on a wetting wall and the contact angle was tested. The density and viscosity ratios between the gas and the liquid was 1000 and 100 respectively. The variation of the calculated contact angles with the wetting potential was found to be in good comparison with the theoretical solution. Water-gas transportation in a three-dimensional GDL structure was simulated to investigate the effects of the pressure drop, wettability and viscosity ratio on the relative permeability that was found to show agreement with previous numerical and experimental works. The multiple-relaxation-time lattice Boltzmann method method was reported to be a viable tool for the simulation of multiphase flows in fuel cells.

Kuzmin and Mohaman (2009) have attempted to extend interparticle potential model into multiple-relaxation-time lattice Boltzmann method by combining the Shan-Chen force with an expanded equilibrium distribution function [51]. They were able to simulate the Young's law benchmark case with a density ratio of 160; however the theoretical foundation of their method was not yet established. Knutson and Noble (2009) have followed a different approach [50] compared to the multiphase models described so far. The multiphase flow lattice Boltzmann method models proposed for high-density-ratio problems [22,25,23] that describe the interface using a finite width of 3 or more lattice sites were criticized to be problematic for a number of flows such as flow through narrow pores and flows with significant shear stresses. They have used the multiple-relaxation-time method and the expansion method which does not assume the interface to have a finite width but represents it as a sharp separation between the fluids. They have simulated a Poiseuille-Couette flow with a phase separation at the vertical center where the density ratio between the fluids at the top and bottom of the interface was 100. The location of the interface was fixed and they have captured the velocity profile accurately. The presented method still needs to be improved to simulate more complex shapes of interfaces.

CONCLUSIONS AND FUTURE WORK

The literature review has shown that, specifically for high Reynolds number flows with buoyant bubbles rising in a liquid at a higher density compared to the gas, the multiple-relaxation-time models developed by Prof. Abraham's group at Purdue University incorporating the index-function approach has great potential to be applicable for modeling multiphase flows related to Department of Energy operations such as bubble generations and pulsed-air mixing in tanks. This model is well published and three Ph.D dissertations are available that explain the procedures in detail in addition to the journal publications by the same research group. However, the free-energy based model that was recently proposed by researchers from Singapore (Zheng *et al.*, 2006) have claimed that the model used in Prof. Abraham's group does not have a clear physical background for the evolution of the interface between different phases. Instead they proposed a multiphase Bhatnagar-Gross-Krook method with the capability to handle large density ratios that can recover the lattice Boltzmann method to the Cahn-Hilliard equation which is the evolution equation for the interface using the Chapman-Enskog expansion. This research group has extended the method to three dimensions and showed that the performance of the interface tracking is superior to the Volume of Fluid and Layer-Set methods used in classical computational fluid dynamics methods. Extending the free-energy based method into fluids with low viscosities using the multiple-relaxation-time collision term has not been published yet and would be a novel contribution to the scientific field.

For the purpose of obtaining a numerical method based on high-density-ratio multiple-relaxation-time lattice Boltzmann method that can be used to simulate practical multiphase flow test cases such as bubble generations, rising bubbles, free-surface break-up and bubble coalescence, the multiple-relaxation-time lattice Boltzmann method developed at Prof. Abraham's research group that uses the modified index-function model will be used in our future work. Applications using this multiphase model, both with the Bhatnagar-Gross-Krook and the multiple-relaxation-time collision operators, have shown that the multiphase model by Lee and Lin (2005) is suitable for our research purposes.

Future work will include implementing a two dimensional multiple-relaxation-time single-phase lattice Boltzmann method that will be used as the base for the multiphase flow solver. Application of boundary conditions and the accuracy of the solver will be tested for benchmark cases such as the Poiseuille flow and the cubic cavity flow at various Reynolds numbers. Once the single-phase flow multiple-relaxation-time lattice Boltzmann method is verified, the multiphase flow model by Lee and Lin (2005) will be added to the lattice Boltzmann equation. Benchmark cases to verify the multiphase flow solver will be the Laplace's law for surface tension, oscillation of capillary waves and oscillation of a droplet. The verified multiple-relaxation-time multiphase lattice Boltzmann method will be used to solve the dynamics of rising bubbles in tanks. The purpose of this test case will be to compare whether the shape of the rising

bubble will be captured accurately by the multiple-relaxation-time multiphase lattice Boltzmann method as compared to previous numerical results. Special attention will be given to the circulation caused around the bubbles and the mixing effectiveness of the process of injecting bubbles in tanks.

REFERENCES

- [1] Tanks Focus Area, "Pulsed-Air Mixer," U.S. Department of Energy, Innovative Technology Summary Report DOE/EM-0462, August 1999.
- [2] M.R. Powell and C. R. Hymas, "Retrieval Process Development and Enhancements FY96 Pulsed-Air Mixer Testing and Deployment Study," Pacific Northwest National Laboratory, Richland, PNNL-11200 1996.
- [3] J.A. Bamberger, "An Assessment of Technologies to Provide Extended Sludge Retrieval from Underground Storage Tanks at the Hanford Site," Pacific Northwest National Laboratory, Richland, PNNL-13048 2000.
- [4] C. L. M. H. Navier, "Memoire sur les lois du mouvement des fluides," *Mem. Acad. Sci. Inst.*, vol. 6, pp. 389-440, 1822.
- [5] S Chen and G.D. Doolen, "Lattice Boltzmann Method for Fluid Flows," *Annual Review of Fluid Mechanics*, vol. 30, pp. 329-364, 1998.
- [6] P.L. Bhatnagar, E.P. Gross, and M. Krook, "A Model for Collision Processes in Gases. I. Small Amplitude Processes in Charged and Neutral One-component Systems," *Physical Review*, vol. 94, pp. 511-525, 1954.
- [7] Thomas Young, "An Essay on the Cohesion of Fluids," *Philosophical Transactions of the Royal Society of London*, vol. 95, pp. 65-87, 1805.
- [8] S.O. Unverdi and G. Tryggvason, "A Front-Tracking Method for Viscous, Incompressible, Multi-fluid Flows," *Journal of Computational Physics*, vol. 100, p. 25, 1992.
- [9] G. Tryggvason et al., "A Front-Tracking Method for the Computations of Multiphase Flow," *Journal of Computational Physics*, vol. 169, p. 708-759, 2001.
- [10] S. Gokaltun, H. Saygin, and M. Muradoglu, "Implicit Multigrid Computations of Unsteady Multiphase Flows in Varying Cross-Sectional Area Channels," in *IUTAM Symposium on Integrated Modeling of Fully Coupled Fluid Structure Interactions Using Analysis, Computations and Experiments*, New Brunswick, 2003, pp. 509-519.
- [11] S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond.*: Clarendon Press, 2001.
- [12] D Yu, R Mei, L.-S. Luo, and W Shyy, "Viscous flow computations with the method of lattice Boltzmann equation," *Progress in Aerospace Sciences*, vol. 39, pp. 329-367, 2003.
- [13] A. K. Gunstensen, D. H. Rothman, S. Zaleski, and G. Zanetti, "Lattice Boltzmann model of immiscible fluids," *Physical Review A*, vol. 43, p. 4320, 1991.
- [14] D.H. Rothman and J.M. Keller, "Immiscible cellular-automaton fluids," *Journal of Statistical Physics*, vol. 52, pp. 1119-1127, 1988.
- [15] K. N. Premnath, "Lattice Boltzmann Models for Simulations of Drop-Drop Collisions," Purdue University, West Lafayette, IN, Ph.D Dissertation 2004.

- [16] X. Shan and H. Chen, "Lattice Boltzmann model for simulating flows with multiple phases and components," *Phys. Rev. E*, vol. 47, no. 3, pp. 1815-1819, 1993.
- [17] M.R. Swift, W.R. Osborn, and J.M. Yeomans, "Lattice Boltzmann simulation of non-ideal fluids," *Physical Review Letters*, vol. 75, pp. 830-833, 1995.
- [18] X. He, S. Chen, and R. Zhang, "A lattice Boltzmann scheme for incompressible multiphase flow and its application in simulation of," *Journal of Computational Physics*, vol. 152, no. 2, pp. 642-663, 1999.
- [19] J. Tolke, M. Krafczyk, M. Schulz, and E. Rank, "Lattice Boltzmann simulations of binary fluid flow through porous media," *Royal Society of London Philosophical Transactions Series A*, vol. 360, p. 535, 2002.
- [20] T. Reis and T. N. Phillips, "Lattice Boltzmann model for simulating immiscible two-phase flows," *Journal of Physics A*, vol. 40, pp. 4033-4053, 2007.
- [21] S. V. Lishchuk and I. & Care, C. M. Halliday, "Multicomponent lattice Boltzmann method for fluids with a density contrast," *Physical Review E*, vol. 77, p. 036702, 2008.
- [22] T. Inamuro, T. Ogata, S. Tajima, and N. Konishi, "A lattice Boltzmann method for incompressible two-phase flows with large density," *Journal of Computational Physics*, vol. 198, pp. 628-644, 2004.
- [23] H.W. Zheng, C. Shu, and Y.T. Chew, "A lattice Boltzmann model for multiphase flows with," *Journal of Computational Physics*, vol. 218, pp. 353-371, 2006.
- [24] H. W. Zheng, C. Shu, and Y. T. Chew, "Lattice Boltzmann interface capturing method for incompressible flows," *Physical Review E*, vol. 72, p. 056705, 2005.
- [25] T. Lee and C.-L. Lin, "A stable discretization of the lattice Boltzmann equation for simulation of incompressible two-phase flows at high," *Journal of Computational Physics*, vol. 206, pp. 16-47, 2005.
- [26] A. Lamura and S. Succi, "A lattice Boltzmann for disordered fluids," *International Journal of Modern Physics B*, vol. 17, pp. 145-148, 2003.
- [27] N. Takada, M. Misawa, A. Tomiyama, and S. Hosokawa, "Simulation of bubble motion under gravity by Lattice Boltzmann Method," *Journal of Nuclear Science and Technology*, vol. 38, no. 5, pp. 330-341, May 2001.
- [28] D. Bhaga and M.E. Weber, "Bubbles in viscous liquids: shapes, wakes and velocities," *Journal of Fluid Mechanics*, vol. 105, pp. 61-85, 1981.
- [29] H. W. Zheng, C. Shu, and Y. T. & Sun, J. H. Chew, "Three-dimensional lattice Boltzmann interface capturing method for incompressible flows," *International Journal for Numerical Methods in Fluids*, vol. 56, pp. 1653-1671, 2008.
- [30] M. Cheng and J. & Lou, J. Hua, "Simulation of bubble-bubble interaction using a lattice Boltzmann method," *Computers & Fluids*, 2009, In Press.
- [31] M. Mehravaran and S. K. Hannani, "Simulation of incompressible two-phase flows with large density differences employing lattice Boltzmann and level set methods," *Computer Methods in Applied Mechanics and Engineering*, vol. 198, pp. 223-233, 2008.

- [32] B. M. Boghosian, J. Yezpez, and P. V. & Wager, A. Coveney, "Entropic lattice Boltzmann methods," *Proceedings of the Royal Society of London. Series A*, vol. 457, pp. 717-766, 2001.
- [33] D. D'Humieres, "Generalized lattice Boltzmann equations.," in *Rarefied gas dynamics*, Vancouver, 1994, pp. 450-458.
- [34] D. D'Humières, I. Ginzburg, M. Krafczyk, and P. & Luo, L.-S. Lallemand, "Multiple-relaxation-time lattice Boltzmann models in three dimensions," *Royal Society of London Philosophical Transactions Series A*, vol. 360, p. 437, 2002.
- [35] I. Ginzbourg and P. M Adler, "Boundary flow condition analysis for the three-dimensional lattice Boltzmann model," *J. Physique II France*, vol. 4, p. 191-214, 1994.
- [36] R. Du and B. & Chen, X. Shi, "Multi-relaxation-time lattice Boltzmann model for incompressible flow," *Physics Letters A*, vol. 359, pp. 564-572, 2006.
- [37] M. E. McCracken, "Development and Evaluation of Lattice Boltzmann Models for Investigations of Liquid Break-Up," Purdue University, West Lafayette, IN, Ph.D Dissertation 2004.
- [38] S. Mukherjee, "Numerical Simulation of Wall Impinging Drops," Purdue University, West Lafayette, IN, Ph.D Dissertation 2006.
- [39] M. E. McCracken and J. Abraham, "Multiple-relaxation-time lattice-Boltzmann model for multiphase flow," *Physical Review E*, vol. 71, pp. 036701/1 - 036701/9, 2005.
- [40] Lamb, *Hydrodynamics*. Cambridge, England: Cambridge University Press, 1932.
- [41] K. N. Premnath and J. Abraham, "Three-dimensional multi-relaxation time (MRT) lattice-Boltzmann models for multiphase flow," *Journal of Computational Physics*, vol. 224, pp. 539-559, 2007.
- [42] K. N. Premnath and J. Abraham, "Simulations of binary drop collisions with a multiple-relaxation-time lattice-Boltzmann model," *Physics of Fluids*, vol. 17, pp. 122105-1-122105-21, 2005.
- [43] J. Tolke and S. & Krafczyk, M. Freudiger, "An adaptive scheme using hierarchical grids for lattice Boltzmann multi-phase flow simulations," *Computers & Fluids*, vol. 35, pp. 820 - 830, 2006.
- [44] H. Li and C. & Miller, C. T. Pan, "Pore-scale investigation of viscous coupling effects for two-phase flow in porous media," *Physical Review E*, vol. 72, p. 026705, 2005.
- [45] P. Lallemand, L.-S. Luo, and Y. Peng, "A lattice Boltzmann front-tracking method for interface dynamics with surface tension in two dimensions," *Journal of Computational Physics*, vol. 226, pp. 1367 - 1384, 2007.
- [46] S. & Abraham, J. Mukherjee, "Lattice Boltzmann simulations of two-phase flow with high density ratio in axially symmetric geometry," *Physical Review E*, vol. 75, pp. 026701/1-026701/13, 2007.
- [47] S. Mukherjee and J. Abraham, "A pressure-evolution-based multi-relaxation-time high-density-ratio two-phase lattice-Boltzmann model," *Computers and Fluids*, vol. 36, pp. 1149-1158, 2007.
- [48] S. Mukherjee and J. Abraham, "Crown behavior in drop impact on wet walls," *Physics of Fluids*, vol. 19, p. 052103, 2007.
- [49] X.-D. Niu, T. Munekata, and S.-A. & Suga, K. Hyodo, "An investigation of water-gas transport

processes in the gas-diffusion-layer of a PEM fuel cell by a multiphase multiple-relaxation-time lattice Boltzmann model," *Journal of Power Sources*, vol. 172, pp. 542-552, 2007.

- [50] C. E. Knutson and D. R. Noble, "Embedding sharp interfaces within the lattice Boltzmann method for fluids with arbitrary density ratios," *The European Physical Journal*, vol. 171, pp. 21-29, 2009.
- [51] A. Kuzmin and A. Mohamad, "Multirange multi-relaxation time Shan-Chen model with extended equilibrium," *Computers & Mathematics with Applications*, 2009, In Press.