A Lattice Boltzmann Simulation of Gas Bubbles in Multiphase Flows with High Density Ratios - 11304

Seckin Gokaltun and Dwayne McDaniel
Applied Research Center, Florida International University
10555 West Flagler Street, Suite 2100, Miami, FL 33174

ABSTRACT

Multiphase flows involving gas and liquid phases can be observed in engineering operations at various Department of Energy sites, such as pulsed-air mixing and hydrogen gas generation in slurries. The dynamics of the gas phase in the liquid domain play an important role in the circulation created by pulsed-air mixers or the gas pressure build-up in tanks. To understand such effects, computational analysis can be utilized that can simulate the process of gas motion inside tanks filled with liquid.

In this paper, the lattice Boltzmann method (LBM), is presented that can model multiphase flows accurately and efficiently. LBM is favored over traditional Navier-Stokes based computational models since surface forces are handled more effectively in LBM. The LBM is easier to program, more efficient to solve on parallel computers, and has the ability to capture the interface between different fluid phases intrinsically. The LBM used in this paper can solve for the incompressible and viscous flow field, while at the same time, solve the Cahn-Hillard equation to track the position of the gas-liquid interface specifically when the density ratio between the two fluids are high. This feature is of primary importance since the previous LBM models proposed for multiphase flows become unstable when the density ratio is larger than 10. The ability to provide stable and accurate simulations at large density ratios become important when the simulation case involves real fluids such as air and water that have a density ratio around 1000 that can be observed in many engineering problems.

In order to verify the capability of the LBM method used in this paper at high density ratios a static bubble simulation was conducted to solve for the pressure difference between inside and outside of the bubble. The results show that the method was in agreement with the Laplace law. Once the method was verified for static bubbles, rising bubble simulations were conducted for various flow conditions characterized by the non-dimensional Eotvos (Eo) and Morton (M) numbers. According to the value of the Eo and M numbers, the bubble obtained different shapes that were found agree with the benchmark solution. It was observed that the LBM presented in this paper can be used to predict bubble dynamics accurately across a wide range of multiphase flow regimes.

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 (DOE) sites. DOE 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 (PNNL), 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 (LBM), is presented that can model multiphase flows accurately and efficiently.

Special attention was given to two-phase flows with high density ratios since this brings another challenge in terms of instabilities to LBM 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. The current LBM presented in this paper is able to provide stable and accurate simulations at large density ratios between the fluid and the gas phases.

The outline of the report is given as the following: first an overview of numerical modeling approaches to multiphase flows is presented. Second, 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.

LBM FOR HIGH-DENSITY RATIO MULTIPHASE FLOWS

One common limitation of the multiphase LBM is that its 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 [3] and 20 [4]. 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 [5]. The exact reasons of this low-density-ratio limit in LBM multiphase models have not yet been explained clearly, however, the inherent compressible characteristic of the LBM is considered to be one of the reasons.

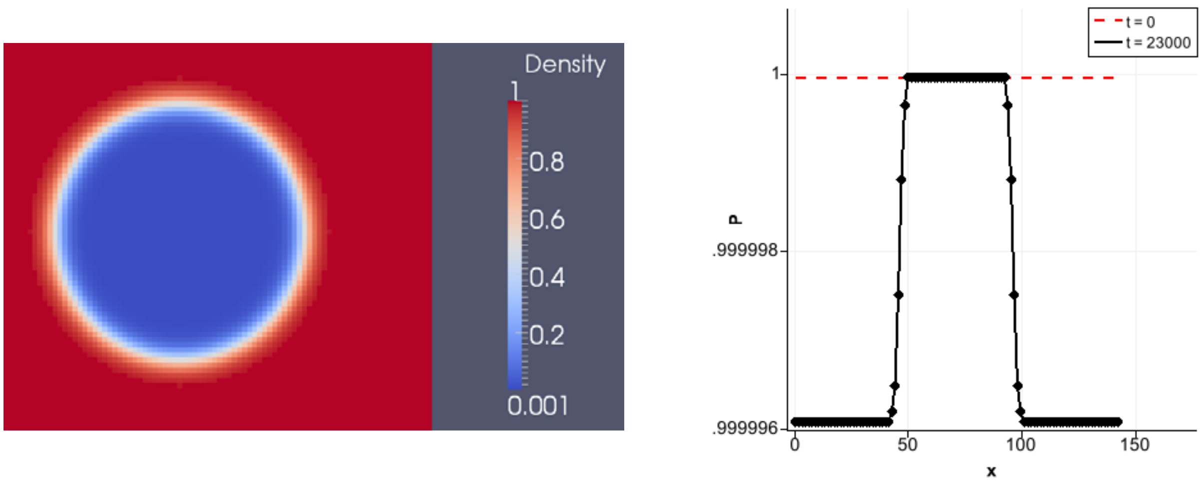
Inamuro et al. (2004) proposed a method based on the free energy method to extend its capability to incorporate fluids with large density ratios up to 1000 [6]. They used a pressure correction step in order to enforce the continuity equation after the collision and streaming step. The projection step 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 [7, 8]. 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. [8] 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 [9]. 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 [7].

STATIC BUBBLE SIMULATIONS

The multiphase model proposed by Lee and Lin (2005) simulates the Navier-Stokes equations for the hydrodynamics and the Cahn-Hillard equation for tracking the evolution of the interface. This is achieved by solving a set of lattice Boltzmann equations that yields pressure and velocity fields represented by the *f* distribution function and the density field represented by the *g* distribution function. The multiphase mode allows simulating two-phase systems with arbitrary fluid density and viscosity ratios.

In the first numerical test case presented here, a circular two-dimensional bubble was initially generated in a fluid domain by assigning a density profile. The fluid domain was 101x101 lattice units (lu) in size and the bubble radius was 25 lu. The surface tension was imposed as an input parameter. The density ratio was set to 1000 and the viscosity ratio between the fluids was 100. The initial pressure field in the fluid domain was uniform; however, as the system converged to an equilibrium state, a pressure difference between the fluid domain and the gas domain was created as shown in Figure 1.



(a) (b)

Figure 1. (a) Initial density distribution of the bubble. (b) Initial and final pressure distribution across the bubble cross section.

The relaxation of the interface between the two fluids were tested against the Laplace's law that expresses the pressure difference between the inside and the outside of a bubble as a function of the surface tension and the radius as given in two-dimensions by, $\Delta P = \frac{\sigma}{R}$. The difference of pressure between the inside and the outside of the bubble, P_{diff}, was computed at every time step and the relative error against the exact value is calculated as, $P_{err} = \frac{P_{diff} - \Delta P}{\Delta P}$. The convergence of P_{err} was measured at every 10 iterations by $Conv(t) = [(P]_{err}(t) - P_{err}(t-1))$ and the simulation was assumed to converge to a steady state result when $\varepsilon = 0.1 \sum_{i=1}^{10} Conv(t) < 0.005$. Figure 2 shows that this convergence criteria was achieved in 23000 iterations for the example problem shown in Figure 1.

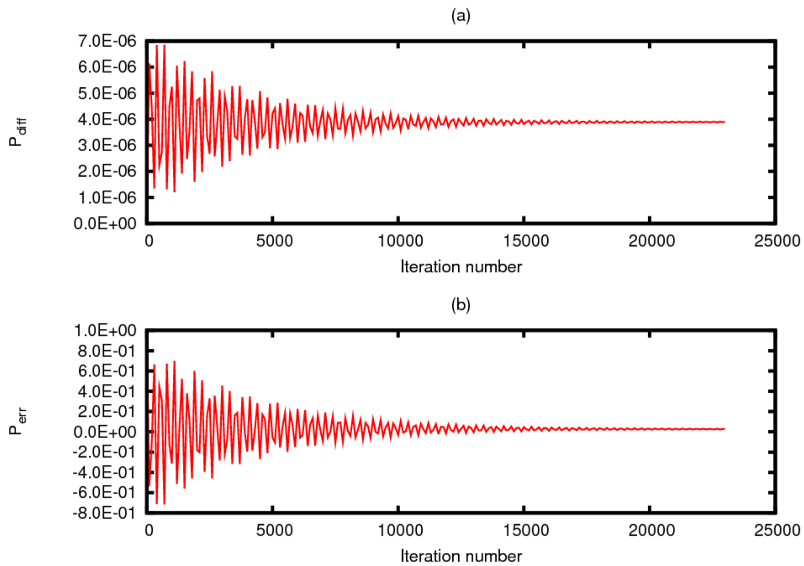


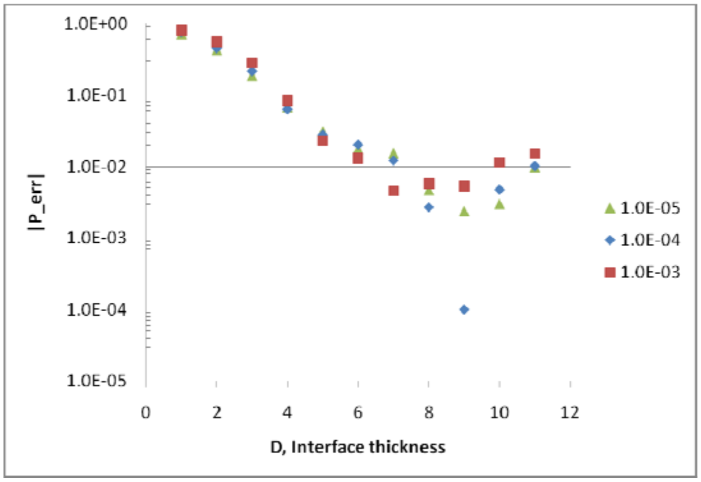
Figure 2. Convergence history of Pdiff (a) and Perr (b).

The LBM method described here is a diffuse interface method that represents the interface by a thin layer in which the properties of the fluids can mix. A parametric study was conducted in order to understand the effect of the interface thickness, *D*, on the solution accuracy.

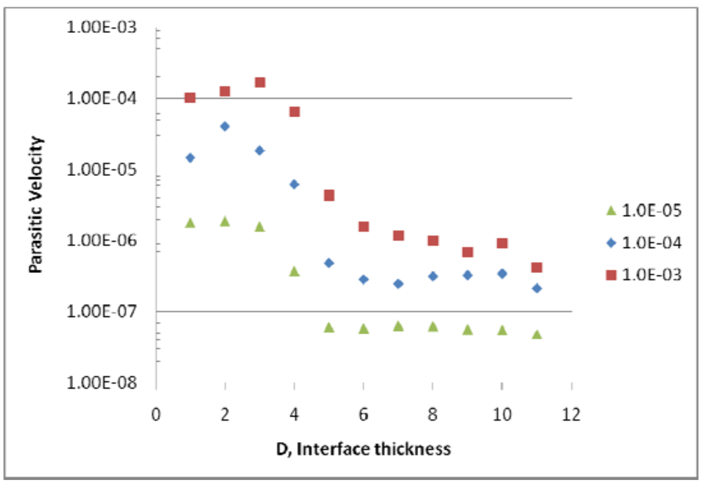
Error! Reference source not found. (a) shows that the relative error of the pressure difference between the gas and the liquid reduces as the interface thickness is increased for $1 < D < 8$; however, this error starts increasing for larger interface thicknesses. The pressure inside the bubble should always be larger than the outside pressure in order to balance the surface tension force, however, for interface thicknesses larger than 8, the pressure inside the bubble was observed to be less than the liquid pressure. Three different values of surface tension were tested and a similar trend was obtained in all of the simulations.

For static bubbles a spurious or parasitic velocity field is obtained along the interface of the bubble, which is an artifact of the numerical discretization error in the computational model that is used (Figure 3 (c)). For accurate simulations, the value of spurious velocities need to be kept small as compared the characteristic velocity of the problem.

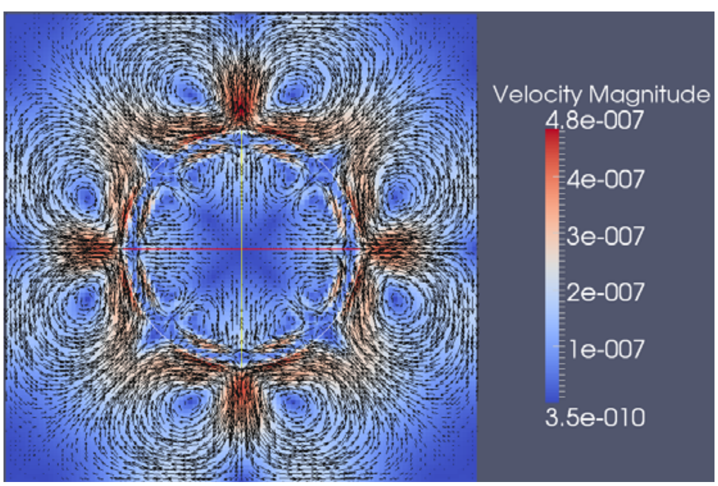
The parametric study presented here has shown that the maximum magnitude of parasitic velocity drops significantly with an increase in interface thickness (i.e. when $3 < D < 6$, Figure 3 (b)). For thicker interface thicknesses a significant reduction in parasitic velocities was not detected.



(a)



(b)



(c)

Figure 3. Effect of interface thickness on the (a) magnitude of maximum parasitic velocity in the vicinity of the bubble interface at three different values of surface tension and (b) the pressure difference across the bubble interface at three different values of surface tension as given by different markers. (c) Spurious velocity field around the bubble.

DYNAMIC BUBBLE SIMULATIONS

The LBM was verified for static bubble cases where the buoyancy force applied on the bubble was ignored however for the engineering problems that the LBM is expected to be applicable to include the buoyancy force applied on the gas phase. In order to evaluate whether the LBM used in this study can successfully simulate multiphase flows with external body forces such as gravity applied on one phase of the system, a benchmark test case was simulated.

The benchmark problem is for a single circular bubble placed initially at rest in a vertical fluid column [10]. The bubble has a diameter that is equal to the half of the width of the channel. The top, bottom and side boundaries are set as wall surfaces in the benchmark solution. The density and viscosity of the fluids are important factors that determine the magnitude of the buoyancy force applied on the gas phase via three non-dimensional numbers. These are Eotvos number, $Eo = \frac{g(\rho_L - \rho_H)d^2}{\sigma}$, Reynolds number, $Re = \frac{\rho_L V_T d}{\mu}$ and Morton number, $M = \frac{g(\rho_L - \rho_G)\mu_L^4}{\rho^2 \sigma^3}$.

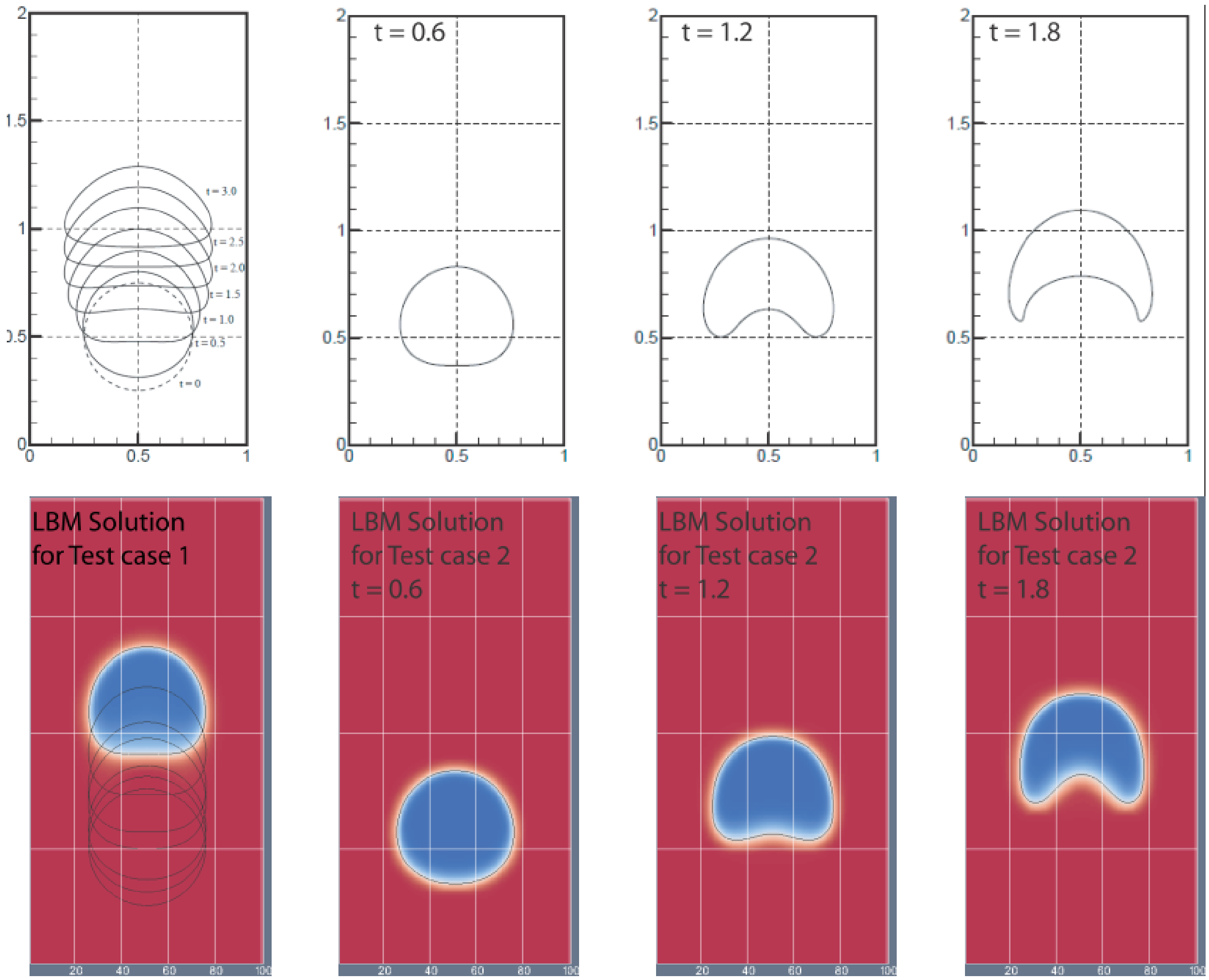
Two test cases were simulated that resulted in different terminal bubble shapes. These test cases were summarized in Table 1 below.

Table 1. Physical parameters and dimensionless numbers.

Test Case	*Re*	*Eo*	$\frac{\rho_L}{\rho_G}$	$\frac{\mu_L}{\mu_G}$
1	35	9	10	10
2	35	125	1000	100

Figure 4 shows the simulated cases using the LBM and the bubble shapes at different time frames as the bubble rises due to the effect of the buoyancy force. The results obtained for Test Case 1 is shown in Figure 4 (a) where the top figure is the benchmark solution for the bubble shapes during the rising motion of the bubble in the liquid column and the corresponding LBM simulation is given in color at the bottom. The results for test case 2 for non-dimensional time, t=0.6, t=1.2 and t=1.8 are given in Figure 4 (b-d).

It was observed that the LBM simulation agree with the benchmark solutions for both flow regimes. The benchmark solution was found to be more dimpled compared to the results obtained using the LBM however the location of the bubble at the corresponding time frames are comparable between two methods. This suggests that the overall velocity of the bubble was close in both the benchmark solution. One possible source of discrepancy between the two solutions can be the periodic boundary conditions applied in the LBM simulation which allowed injection of the fluid particles from the bottom of the domain as the fluid particles exited from the top. This could affect the flow structure around the bubble which may have resulted in a different shape.



(a) (b) (c) (d)

Figure 4. Comparison of simulations using the Lee and Lin (2005) method shown at the bottom in color with the benchmark solution given at the top.

CONCLUSIONS AND FUTURE WORK

In this summary document, the implementation of the LBM based on the Lee and Lin (2005) multiphase model was presented for static and bubbles at a density ratio of 1000 and a viscosity ratio of 100. The effect of the interface thickness and surface tension on the pressure and velocity field were investigated. Matching the Laplace's law was improved and the level of spurious currents was minimized when the interface thickness was around 6 lattice units. It was reported that the second-order discretization in LBM yields better accuracy when the interface thickness is larger than a minimum value (Lee & Lin, 2005). However the reduction in discretization error was not observed for values of *D* that were larger than 6. This may be due to the fact that the total diameter of the bubble approached the outer boundary of the computational domain when *D* was larger than 6 lu and the periodic boundary conditions were affected by the existence of the interface close to the boundary. The spurious currents and pressure error were observed to be less when the surface tension was reduced while the reduction in spurious velocity with the surface tension was more noticeable. The rising bubble simulations showed good agreement between the LBM simulations with the benchmark solution for two test cases where the *Eo* was 9 and 125. The bubble shape was predicted well and the location of the bubble at different time frames during the motion was also close to the benchmark solution. Further quantitative analysis is required to qualify that the LBM can be used as an alternative computational fluid dynamics solver for multiphase flows involving high density ratios.

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