



# Lattice Boltzmann modeling of buoyant rise of single and multiple bubbles

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## ABSTRACT

Buoyant rise of bubbles is investigated using the lattice Boltzmann method (LBM) based Gunstensen's color model. An external force/sink term is incorporated in the collision step to simulate buoyant rise of bubbles under gravitational force. The shape of a bubble is controlled by inertial, viscous and surface tension forces. The interplay between these forces is quantified using non-dimensional numbers such as Eötvös number (Eo), Morton number (Mo) and Reynolds number (Re). A set of results from numerical simulations are presented to demonstrate the ability of the proposed approach to simulate rise of single and multiple bubbles under buoyancy. The proposed modification is verified by comparing terminal velocity of bubbles in an infinite medium against the analytical solution. The shape of bubbles in various flow regimes characterized by the non-dimensional numbers is compared against the experimental data. The effect of surface tension and viscosity ratio on terminal velocity and shape of bubbles is investigated. The LBM results for topological change in the shape of bubbles or circularity of bubbles is compared against COMSOL. Co-axial and oblique coalescence of two gas bubbles are simulated and compared against the experimental data. The simulation results from LBM simulations were found to be in good agreement with the analytical solution, the experimental data and the COMSOL simulation.

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## 1. Introduction

Multiphase flow system is commonly observed in several natural and industrial processes such as ink-jet printing [1,2], spray cooling [3,4], carbon sequestration [5], soil-vapor extraction [6–8] and nuclear waste management [9,10]. Buoyant rise of bubbles under gravitational force has been a common area of interest for experimental and numerical researchers. Rise of bubbles in viscous fluid is characterized by non-dimensional numbers such as the Eötvös number  $Eo = \frac{d_0^2 g \Delta \rho}{\sigma}$ , Morton number  $Mo = \frac{\rho_l^2 v_l^4 g \Delta \rho}{\sigma^3}$  and Reynolds number  $Re = \frac{v_l d_0}{\nu_l}$ ; where  $d_0$  is diameter of bubble,  $\rho_l$  is density of suspended liquid, and  $\rho_g$  is density of gas or bubble,  $\nu_l$  is kinematic viscosity of liquid,  $\Delta \rho = \rho_l - \rho_g$  is the density difference between the liquid ( $\rho_l$ ) and the gas/bubble ( $\rho_g$ ),  $g$  is gravitational acceleration,  $V$  is terminal velocity and  $\sigma$  is surface tension. Eötvös number (Eo) and Morton number (Mo) represent the ratio between surface tension force and buoyant force acting on a suspended bubble. Reynolds number (Re) indicates the balance between viscous drag and inertial force. Buoyant force lifts the bubble against the gravity whereas the viscous drag tends to retard the flow of a

bubble. Surface tension force tries to maintain the spherical shape of a bubble.

Different numerical methods have been applied to simulate multiphase flow (see Prosperetti and Tryggvason [11]). Fuster, Agbaglah [12] used a volume of fluid (VOF) method, balanced-force surface tension and quad/octree adaptive mesh refinement (AMR) to simulate bubble dynamics. van Sint Annaland et al. [13] presented an interface reconstruction technique based on piecewise linear interface representation in volume of fluid (VOF) method to simulate co-axial and oblique coalescence of two gas bubbles. van Sint Annaland et al. [14] used a 3-D front tracking method employing a new surface tension model to simulate single and multiple bubble dynamics in dispersed fluid. Olsson and Kreiss [15–17] used a level set method to simulate bubble dynamics. COMSOL Multiphysics [18] is a commercial software that applies level set method to simulate multiphase flow system.

The numerical simulation of multiphase flow is a challenging class of problems because of the inherent difficulty in tracking the fluid interfaces, mass conservation, and the correct treatment of the surface tension forces [19]. In recent years, the lattice Boltzmann method (LBM) has emerged as a very promising numerical approach for simulation of complex multiphase flow [20–26]. LBM based immiscible multiphase flow model can be divided into three types: Rothman–Keller (R–K) model [20,27,28], the Shan–Chen (SC) model [22], and the free energy (FE) approach

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[24,29]. Huang et al. [30] compared performance and stability of three approaches to simulate immiscible multiphase flow; the FE method was found to be better than the other two approaches for high density and viscosity contrast between two fluid components.

Sankaranarayanan et al. [31] presented comparison between LBM and front-tracking finite-difference methods for bubble simulations and found that both numerical schemes are qualitatively similar and within a few percent quantitatively. Several variants of LBM based multiphase flow model [19,32–39] have been applied to simulate bubble dynamics in recent years. The successes of LBM-based simulations are mainly due to their mesoscopic and kinetic nature, which enables the simulation of their macroscopic interfacial dynamics with their underlying microscopic nature.

In this work, we adopted the Rothman–Keller (R–K) type binary color model introduced by Gunstensen [20,27] for the LBM to simulate immiscible multiphase flow. The Gunstensen's binary color model recovers Galilean invariance with proper assignment of immobile equilibrium particle, and the model can adjust the surface tension independent of the density and the viscosity contrast between binary fluid components [40]. However, the model works well only for negligible density ratios [39,41], and is computationally less efficient than the Shan–Chen model [22] due to an additional collision step for perturbation (see detail in the following section). Grunau et al. [42] introduced two real valued parameters in the original binary color model to account for density contrast between two fluid components. Tölke [33] applied Gunstensen's color model with modification suggested by Grunau et al. [42] to simulate multicomponent multiphase flow in porous media with variable density and viscosity ratios between multiple binary fluids. It was found that the model is not stable for large-scale real-life problems where binary fluids have significant density or viscosity contrast. The binary color model has been applied to demonstrate the effect of geometry and viscosity contrast on flow regimes at high capillary numbers [34,41]. Farhat et al. [43] applied binary color model to simulate deformation and velocity of red blood cell (RBC) while streaming through capillaries whose diameters are smaller than the RBC size. The interfacial surface tension was made non-uniform as a function of surfactant concentration on RBC. Leclaire et al. [44] modified the original recoloring step proposed by Latva-Kokko and Rothman [45] in Gunstensen's binary color model to improve efficiency and accuracy of estimate for surface tension. The modified model is able to simulate viscosity contrast as high as 10,000. Tölke et al. [40] applied Gunstensen's color model on multiple relaxation time (MRT) scheme in LBM to simulate multi-phase flows on non-uniform adaptive grids. Li et al. [46] modified Gunstensen's color model on the MRT scheme by decoupling the interfacial tension and the viscosity-related relaxation time, and adding another MRT diffusion step to eliminate the anti-diffusion effect of the recoloring step.

Bubble dynamics have been studied using different variants of LBM-based multiphase flow model. Sankaranarayanan et al. [47] used both the Shan and Chen [22] and the Shan and Doolen [23] multiphase models to simulate bubble dynamics for a density ratio of 100 with  $Bo < 5$  and  $Mo > 1 \times 10^{-6}$  [19,32] have used the Shan–Chen model to simulate bubble dynamics. A non-ideal equation of state is generally assumed in this model to implement the interfacial surface tension, and an external forcing term [47] was used to implement buoyancy effect in the multiphase flow model. Yu and Fan [48] applied the adaptive mesh refinement (AMR) method on the Shan–Chen model to simulate buoyant rise of bubbles and found that LBM combined with AMR can significantly improve accuracy and reduce computational cost [36,37] have applied free energy (FE) method [24] to study dynamics of single bubbles for moderate Reynolds number [21,49,50] used the projection method in the free energy (FE) method to simulate buoyant rise of bubble

for high density ratio. Zheng et al. [51] included external forcing term [37] in the free energy (FE) method to simulate bubble dynamics with large density ratio. Farhat et al. [39] have combined 3-D migrating multi-block algorithm with Gunstensen's color model to study bubble dynamics. The Grunau et al. [42] method was adopted in this model to simulate density contrast; however, the highest density contrast applied was  $O(10)$  due to thick interface between the two fluids and stability issues.

The objective of this paper is to present a modification in the LBM-based Gunstensen's color model [20] to simulate buoyant rise of bubbles. An effective force term is included during the collision step in the model to account for buoyant force due to density contrast between the fluid components; hence, the buoyancy was not directly simulated as an effect of pressure gradients in the flow, but was introduced from an analytical understanding of buoyancy effects. Therefore, density contrast was not explicitly introduced in the model. Mohamad and Kuzmin [52] explored three different schemes to implement external force in LBM to simulate physical processes such as density dependent flow, as well as spatially and/or temporally varying body force with non-zero gradients. Buick and Greated [53] also analyzed the implementation of body force in LBM and concluded that better accuracy in LBM can be achieved by adding external force in the collision step. This work verifies the shape regime obtained with the proposed modification at various  $Eo$  and  $Mo$  numbers against the experimental data. The terminal velocity for bubbles from LBM simulation was verified against the analytical solution, and the LBM results were also compared against COMSOL simulation for circularity of bubble and terminal  $Re$ . The simulation results from LBM for oblique and co-axial coalescence of two bubbles were compared against the experimental data.

## 2. Lattice Boltzmann model

Lattice Boltzmann method (LBM) is a numerical scheme to simulate hydrodynamic systems governed by the Navier–Stokes equations (NSE) for isothermal compressible fluid flow [1,54,55]. LBM's are based on kinetic theory of gas at microscopic scale and have proven to recover the Navier–Stokes solution at macroscopic scales through Chapman–Enskog expansion of the Boltzmann equation at low frequency, long wavelength limits, and at a low Mach number [56]. Mach number ( $Ma$ ) is a non-dimensional number that represents velocity of fluid ( $V$ ) relative to speed of sound ( $c_s$ ). Unlike traditional numerical methods, the LBM does not discretize the governing equations at macroscopic scale in space and time; instead, it solves the dynamics of hypothetical particles governed by the Boltzmann equation. The Boltzmann equation governs the time rate of change of the particle distribution function ( $f_j$ ). The particle distribution function ( $f_j$ ) represents the dynamic state of a hypothetical group of particles in terms of its location ( $\mathbf{x}$ ) and momentum at any time ( $t$ ). The  $f_j$  streams on discrete lattices and is updated by a collision mechanism.

The linearized discrete Boltzmann equation as shown in Eq. (1) is solved on discrete lattices [56]:

$$\underbrace{f'_j(\mathbf{x} + \mathbf{e}_j \Delta t, t + \Delta t)}_{\text{Streaming}} = \underbrace{f_j(\mathbf{x}, t) - \frac{f_j(\mathbf{x}, t) - f_j^{eq}(\mathbf{x}, t)}{\tau}}_{\text{Collision}} + \varphi_j \quad (1)$$

where  $\mathbf{e}_j$  is the microscopic velocity of particle groups,  $f_j^{eq}$  is equilibrium distribution function and  $\tau$  is a relaxation parameter that indicates the rate at which the system approaches equilibrium through a series of collisions and streaming.  $\varphi_j$  is a sink term that will be

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