SIMULATION OF PHASE SEPARATION PHENOMENON USING LATTICE BOLTZMANN METHODS

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for the award of Bachelor of Mechanical Engineering with Automotive Engineering

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SUPERVISOR'S DECLARATION

We hereby declare that we have checked this project report and in our opinion this project is satisfactory in terms of scope and quality for the award of the degree of Bachelor of Mechanical Engineering with Automotive Engineering.

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STUDENTS DECLARATION

I hereby declare that the work in this report is my own expect for quotations and summaries which have been duly acknowledged. The report has not been accepted for any degree and is not concurrently submitted for award of other degree.

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ABSTRACT

This thesis deals with the simulation of the phase separation of two phase flow. The lattice Boltzmann methods is one of the alternative technique to solve multiphase problem such as phase separation of two-phase flow. A derivation of the Lattice Boltzmann scheme from the classical Boltzmann equation is discussed in detail. According to the problems, a single component multiphase (SCMP) LBM is used or involved in the equation in order to solve more phase of fluids. Before that, investigation on non ideal fluid is discussed using Van der Waals fluids where the critical constant of pressure, volume and temperature is solved. By doing this, it will tell the characteristic of the liquid and gas phase. From the Maxwell equal area construction, the value of macroscopic variables, density of fluids is determined which will be code in the algorithm. The source code of the phase separation generate by considering certain criteria. The result of simulation generate from the code prove the precise of the LBM. The 101x101 lattice was used and it is proven that the phase separation formed within the time increased. It is separated into two parts of colour that described the different properties of fluid phase. This project proven the LBM is the best way to simulate phase separation.

ABSTRAK

Tesis ini adalah bertujuan untuk mengkaji pengasingan fasa bagi aliran dua fasa menggunakan kaedah LBM. LBM ini mempunyai banyak kelebihan berbanding kaedah tradisional. Dalam proses kajian ini, banyak perkara perlu diambil kira bagi mendapat keputusan yang tepat dan jitu. Objektif utama adalah pemprograman data didalam perisian FORTRAN. Dalam proses pemprograman ini, banyak persamaan telah digunakan bagi mewujudkan satu persamaan baru berdasarkan persamaan 'lattice Boltzmann'. Daripada persamaan ini, nilai awal bagi kedudukan, warna, saiz dan masa berlakunya proses ini telah dikira. Kesemua nilai-nilai awal ini telah dimasukkan kedalam program komputer bagi menghasilkan keputusan kajian ini. Setelah diteliti dan diamati, keputusan kajian ini membuktikan bahawa pengasingan fasa akan berlaku secara perlahan pada kadar peningkatan tempoh tertentu. Cecair-cecair ini akan terasing secara sendiri berdasarkan ketupatan cecair masing-masing dan ini boleh dilihat daripada pengasingan warna daripada keputusan kajian. Daripada kajian ini, pembuktian tentang keberkesanan menggunakan LBM berbanding kaedah tradisional telah diketahui berdasarkan keputusan yang tepat dan jitu.

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LIST OF SYMBOL

ρ	Density
e_i	Lattice vector
c	Lattice velocity
w_i	Weighting factor
f, g	Distribution functions
Ω_i	Collision operator
k	Phase (k=β or k=α)
τ	Relaxation parameter
v	Kinematic viscosity
p	Pressure
f^{eq}	Equilibrium distribution function
u	Velocity
r_i	Coefficients for $\rho_\beta \neq \rho_\alpha$
s_i	Surface tension force (color-fluid model)
κ	Local curvature (color-fluid model)
σ	Surface tension coefficient
VOF	Volume of fluid function
δ	Fluid-separation coefficient
λ	Coefficient-two-relaxation-time collision
V_{inter}	Velocity on the outer side of the interface
n_k	Number density $n_k = \rho_k / m_k$
m_k	Initial density
u^{eq}	Modified equilibrium velocity
$F_k(x)$	Interactive force
μ	Chemical potential
P_{kl}	Pressure tensor
n	Total number density

φ	Number density difference between the two fluids
ϕ	Order parameter
ϕ^*	Expected order parameter
F_s	Surface tension force
T	Bulk temperature
R	Gas constant
μ	Dynamic viscosity
Re	Reynolds number

LIST OF ABBREVIATION

LBM	Lattice Boltzmann method
CFD	Computational Fluid Dynamics
LBE	Lattice Boltzmann Equations
BGK	Bhatnagar-Gross-Krook (collision operator)
VOF	Volume of fluid
LSM	Level set method
LGA	Lattice-gas automata
CSF	Continuum surface force
EOS	Equation of state
TRT	Two-relaxation-time
TC	Test of coherence
PA	physical test-case compared with an analytical solution

CHAPTER 1

INTRODUCTION

1.1 Introduction

Fluid dynamics is one of the science branches and it is very important in our daily lives because it touches every aspect. It will show us about the flow of the fluid and the property of the fluids in the universe. Otherwise, it is also an important knowledge for the engineering study. Power generation, automotive, aerospace and air conditioning are the example of the technology that related to the fluid dynamics.

The dynamics behavior of fluid flow can now be investigated by researchers using computers with certain software. The advances of computer programming have also helped them to do experiment repeatedly without having to install real apparatus. This has saved time and energy consumption.

Computational method has years been used to investigate the fluid flow behavior. One of the most popular methods used is the Computational Fluid Dynamics (CFD). CFD is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. Lattice Boltzmann Methods (LBM), the parts of the CFD is best used to simulate the fluid behavior.

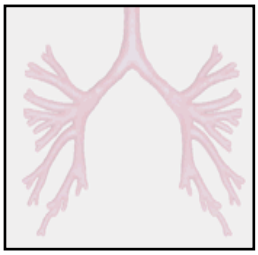
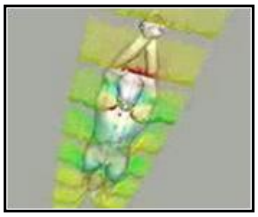
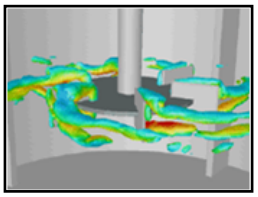
1.2 Computational Fluid Dynamics (CFD)

Computational fluid dynamics (CFD) is a computational technology that enables you to study the dynamics of things that flow. Using CFD, you can build a computational model that represents a system or device that you want to study. Then you apply the fluid flow physics and chemistry to this virtual prototype, and the software will output a prediction of the fluid dynamics and related physical phenomena.

Therefore, CFD is a sophisticated computationally-based design and analysis technique. CFD software gives you the power to simulate flows of gases and liquids, heat and mass transfer, moving bodies, multiphase physics, chemical reaction, fluid-structure interaction and acoustics through computer modeling. Using CFD software, you can build a 'virtual prototype' of the system or device that you wish to analyze and then apply real-world physics and chemistry to the model, and the software will provide you with images and data, which predict the performance of that design.

The fundamental basis of almost all CFD problems is the Navier-Stokes equations, which define any single-phase fluid flow. These equations can be simplified by removing terms describing viscosity to yield the Euler equations. Further simplification, by removing terms describing vorticity yields the full potential equations. Finally, these equations can be linearized to yield the linearized potential equations. There are three compelling reasons to use CFD software: insight, foresight, and efficiency.

Table 1.1: Compelling reason to used CFD

Insight 	CFD analysis is able to virtually crawl inside the design and see how it performs. There are many phenomenons that can witness through CFD, which wouldn't be visible through any other means, gives a deeper insight into the designs [15].
Foresight 	Because CFD is a tool for predicting what will happen under a given set of circumstances, it can quickly answer many' questions. This CFD will give the outcomes or results of the numerical set of boundary conditions. All of this can be done before physical prototyping and testing [15].
Efficiency 	The foresight that is gain from CFD helps engineer to design better and faster, save money, meet environmental regulations and ensure industry compliance. CFD analysis leads to shorter design cycles and the products get to market faster. In addition, equipment improvements are built and installed with minimal downtime. CFD is a tool for compressing the design and development cycle allowing for rapid prototyping [15].

Source: Yuan, P. et al., 2006

1.3 Lattice Boltzmann Methods (LBM)

LBM is a relatively new simulation technique for complex fluid systems and has attracted interest from researchers in computational physics. Unlike the traditional CFD methods, which solve the conservation equations of macroscopic properties (i.e., mass, momentum, and energy) numerically, LBM models the fluid consisting of fictive particles, and such particles perform consecutive propagation and collision processes over a discrete lattice mesh. Figure 1.1 shows the explanation of the basic concept of the LBM. Due to its particulate nature and local dynamics, LBM has several advantages over other conventional CFD methods, especially in dealing with complex boundaries, incorporating of microscopic interactions, and parallelization of the algorithm. A different interpretation of the lattice Boltzmann equation is that of a discrete-velocity Boltzmann equation. The numerical methods of solution of the system of partial differential equations then gives rise to a discrete map, which can be interpreted as the propagation and collision of fictitious particles [1] [2].

Simulating multiphase flows has always been a challenge to conventional CFD because of the moving and deformable interfaces. More fundamentally, the interfaces between different phases (liquid and vapor) or components (e.g., oil and water) originate from the specific interactions among fluid molecules. Therefore it is difficult to implement such microscopic interactions into the macroscopic Navier–Stokes equation. However, in LBM, the particulate kinetics provides a relatively easy and consistent way to incorporate the underlying microscopic interactions by modifying the collision operator. Several LBM multiphase models have been developed [3]. Phase separations are generated automatically from the particle dynamics and no special treatment is needed to manipulate the interfaces as in traditional CFD methods. Successful applications of multiphase LBM models can be found in various complex fluid systems, including interface instability, bubble/droplet dynamics, wetting on solid surfaces, interfacial slip, and droplet electro hydrodynamic deformations.

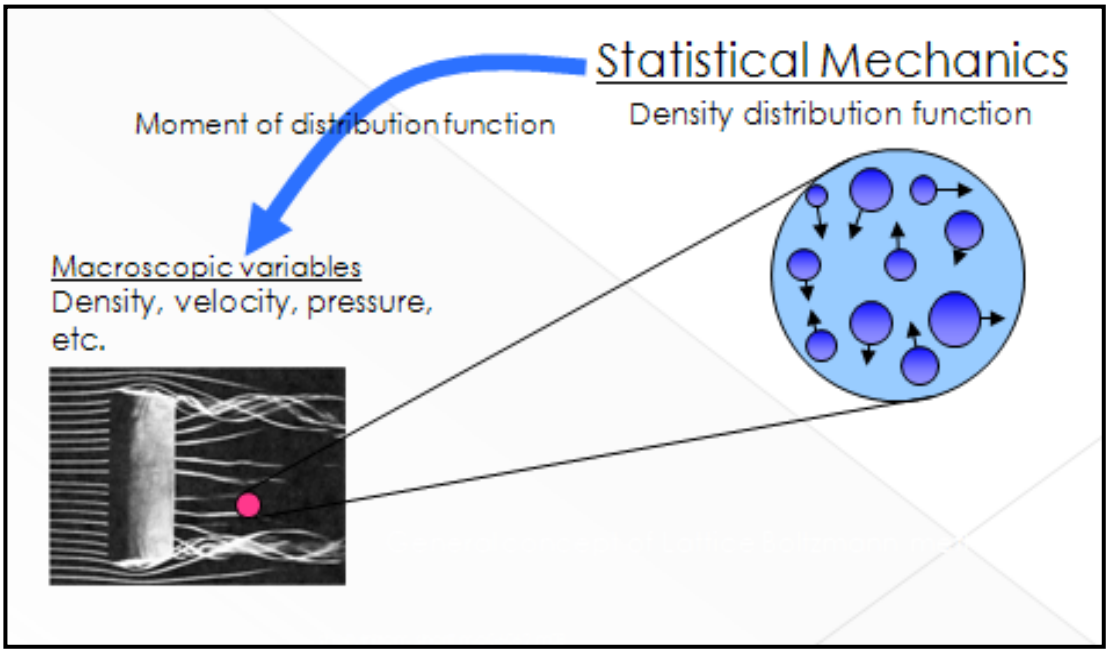


Figure 1.1: General concept of LBM

Source: Nik Mohd Izual, 2009

1.4 Problem Statement

The problem statement regarding this project is stated below:

- Most complex fluid dynamics problems cannot be solved analytically but can be analyze by using code of LBM.

1.5 Objective

The objective of this project is to simulate phase separation phenomenon using Lattice Boltzmann Methods (LBM).

1.6 Scopes

1. Literature review of lattice Boltzmann method (LBM).
2. Use free energy (FE) parameters proposed by Nik Mohd Izual [28].
3. Simulate the phase separation of LBM.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

Lattice Gas Cellular Automata (LGCA) and Lattice Boltzmann Method (LBM) are relatively new and promising methods for the solution of nonlinear partial differential equations and simulation of fluid flows. In the last few years, a remarkable development has been taken place in (LBM) [1-6]. Lattice Boltzmann models have ability to simulate single and multi-phase flows of single and multicomponent fluids. Historically the LBM evolves from LGCA which belongs to the class of cellular automata that are used for simulation of the fluid flow phenomena. It represents an idealization of the physical system in which space and time both are discrete. In 1986, Frisch, Hasslacher, and Pomeau and Wolfram proposed the first two-dimensional lattice gas automaton model for the specific purpose of computational fluid dynamics [7].

In 1988, a proposal to use the lattice Boltzmann equation to simulate fluid flow problems was made for the first time [6]. The kinetic nature of LBM has several distinct features different from other computational fluid dynamics (CFD) approaches that are used to solve the Navier Stokes equations. The convection operator in LBM is linear in phase space, similar to that of the Boltzmann kinetic equation, but different than the Euler or the Navier Stokes equations and pressure is obtained through an equation of state, instead of solving a Poisson equation as in the incompressible Navier Stokes equations. LBM uses minimum set of discrete velocities so that the conserved quantities remain preserved throughout the simulation.

Researchers have used LGCA and LBM for a variety of fluid flow problems and geometries. A rich variety of behaviors including unsteady flows, phase separation, evaporation, condensation, cavitations, porous media flows, blood flow simulation, solute and heat transport, buoyancy, multiphase flows, compressible flows and interactions with surfaces can readily be simulated [8-25]. Various fluid flow problems have been simulated using LGCA and results have been compared with experimental investigations [8]. LGCA has been used to investigate flow through geometrically irregular media [11].

An LGCA model with non-ideal equation of state has been presented to simulate the transition from solid to gas phase [12]. LBM has been used to numerically analyze the turbulent shear flows [13]. Results obtained for three-dimensional low Reynolds number flows, using LBM, demonstrate the viability of the method for such flows in complex geometries [14]. LBM is equally applicable for simulation of multiphase flows. LB Models have been formulated for two-dimensional multiphase flows in porous media [15]. Many researchers have formed thermal models to investigate heat conduction process and convective flows by using LBM [20, 23]. LBM has even been used to simulate shock wave phenomena [25].

2.2 Classical Boltzmann Equation

LBM is relatively recent technique that has been shown to be as accurate as traditional CFD methods having the ability to integrate arbitrarily complex geometries at a reduced computational cost. Lattice Boltzmann models vastly simplify Boltzmann's original conceptual view by reducing the number of possible particle spatial positions and microscopic momenta from a continuum to just a handful and similarly discretizing time into discrete steps. Figure 2.1 shows that particle positions are confined to the node of a lattice. Variations in momenta that could have been due to a continuum of velocity directions and magnitudes and varying particle mass are reduced to eight directions leading to a D2Q9 model.

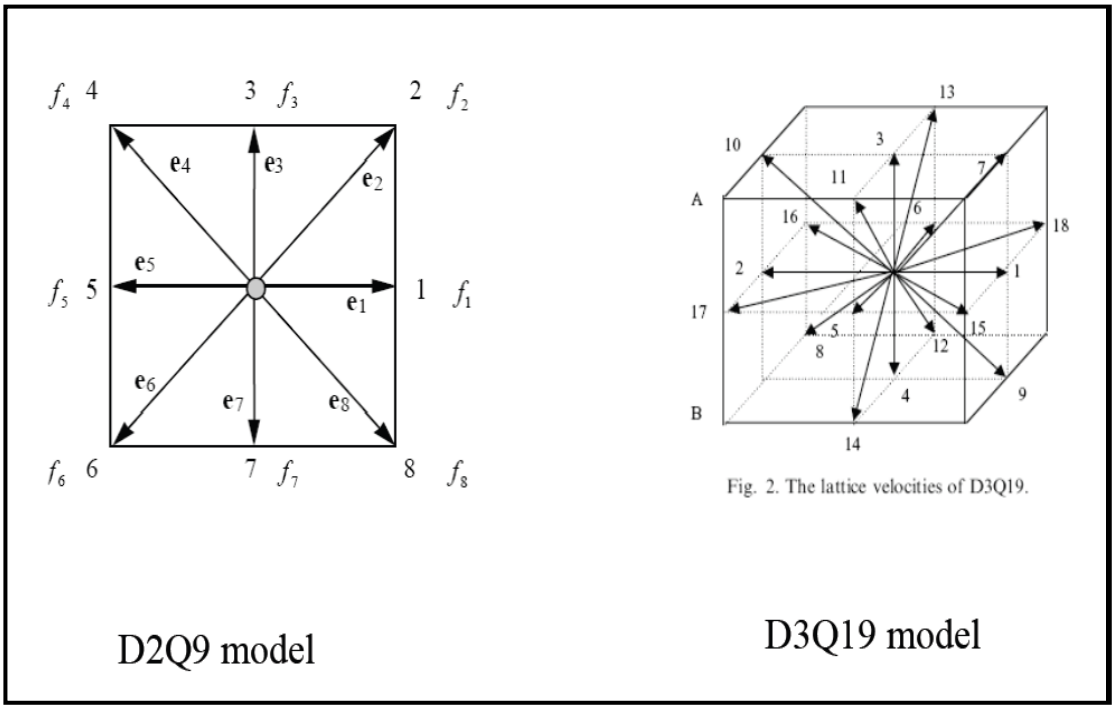


Fig. 2. The lattice velocities of D3Q19.

Figure 2.1: Discrete lattice velocity model

Source: Grunau, D., et al., 1993

Lattice Boltzmann equation can be obtained directly from the lattice gas automata by taking ensemble average with the assumption of random phase, leading to the following equation [26];

$$f(x + c\Delta t, c + a\Delta t, t + \Delta t) - f(x, c, t) = \Omega_\alpha(f) \qquad (2.1)$$

Where $\Omega_\alpha(f)$ is the Lattice Boltzmann collision operator and $f(x, c, t)$ is the single particle distribution functions with discrete velocity *c*.

There are two conditions that are related to the distribution function, without collisions and with collisions [27][28]. The distribution function of $f(x, c, t)$ describes the number of particles in the situation where it is at the position of *x*, move with velocity *c* at time *t*.

At the short duration of time Δt , each particle changing the velocity from c to $c + a\Delta t$ to move from x to $x + c\Delta t$, where a is an acceleration due to the external forces. The number of molecules for both $f(x, c, t)\, dx\, dc$ and $f(x + c\Delta t, c + a\Delta t, t + \Delta t)\, dx\, dc$ are same in the condition of distribution without collision. Therefore;

$$f(x + c\Delta t, c + a\Delta t, t + \Delta t)\, dx\, dc - f(x, c, t)\, dx\, dc = 0 \qquad (2.2)$$

In the condition where collision occurs, there will be a net different number of molecules between these two functions that can be express by;

$$f(x + c\Delta t, c + a\Delta t, t + \Delta t)\, dx\, dc - f(x, c, t)\, dx\, dc = \Omega_\alpha(f)\, dx\, dc\, dx\, dt \qquad (2.3)$$

After dividing this equation with *cdt*, *dt* tends to zero (*dt*~0), give the Boltzmann equation of *f*

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial c_\alpha} + a \frac{\partial f}{\partial c_\alpha} = \Omega(f) \qquad (2.4)$$

2.3 Boltzmann Collision Operator

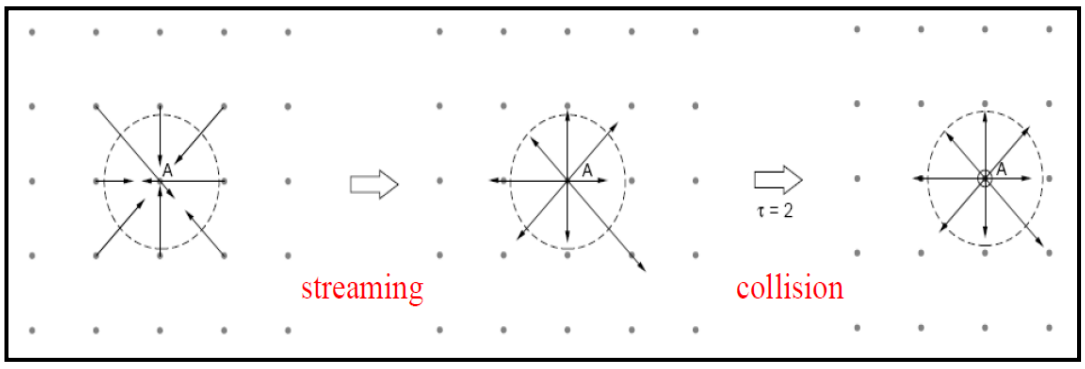


Figure 2.2: Streaming and collision of LBM

Source: Zhang, R., et al., 1999

An expression of the collision operator is required for any solution of Boltzmann equation.

$$\int \begin{bmatrix} 1 \\ c \\ c^2 \end{bmatrix} \Omega(f)\, dc \tag{2.5}$$

By the way, collision operator can change the distribution function $f(x, c, t)$ in two ways;

1. After the collision, the velocities of the particle will be different from the initial velocity and this circumstances causing the decrease in $f(x, c, t)$

2. The particles that have the velocities of others will have the velocity after collision, increasing $f(x, c, t)$

2.4 Bhatnagar-Gross-Krook Collision Model

From the previous derivation of Boltzmann equation, assuming that a gas consist of hard-sphere and undergoing the binary collision [15]. There is the derivation of Boltzmann equation without external force shows that the change in distribution functions per unit time due to collision;

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{\partial c_\alpha} = \frac{\partial f}{\partial t} = \left.\frac{\partial f}{\partial t}\right|_{collision} \tag{2.6}$$

where;

$$\left.\frac{\partial f}{\partial t}\right|_{collision} = \Omega(f) \tag{2.7}$$

Through the second Order Taylor's series expansion, the distribution function f can be attached to the equilibrium function f^{eq} .

$$f^{eq} = (x, c, t) \approx f(x, c, t) + \frac{\partial f}{\partial t} collision(\delta t) + 0(\delta t)^2 \tag{2.8}$$

$$\frac{\partial f}{\partial t} collision = \frac{f^{eq}(x, c, t) - f(x, c, t)}{\delta t} = \frac{f^{eq}(x, c, t) - f(x, c, t)}{\tau_f} \tag{2.9}$$

After replacing the δt with the characteristic time between collision τ_f , it will become BGK collision model.

2.5 The Lattice Boltzmann Equation

There is the expression of the Boltzmann equation with BGK collision model;

$$\frac{\partial f}{\partial t} + c_\alpha \frac{\partial f}{x_\alpha} = \frac{f - f^{eq}}{\tau_f} \tag{2.10}$$

The Maxwell-Boltzmann equilibrium distribution function can be defined as;

$$f^{eq} = \rho \left(\frac{1}{2\pi RT}\right)^{\frac{D}{2}} exp\left\{\frac{(c-u)^2}{2RT}\right\} \tag{2.11}$$

The BGK lattice Boltzmann equation can be derived by further discretization using an Euler time step in conjunction with an upwind spatial discretization and setting the grid spacing divided by the time step equal to the velocity [26];

$$\frac{f(x, t + \Delta t) - f(x, t)}{\Delta t} + c\frac{f(x + \Delta x, t + \Delta t) - f(x, t + \Delta t)}{\Delta t} = \frac{f - f^{eq}}{\tau_f} \tag{2.12}$$

$$\frac{f(x, t + \Delta t) - f(x, t)}{\Delta t} + c\frac{f(x + c\Delta x, t + \Delta t) - f(x, t + \Delta t)}{\Delta t} = \frac{f - f^{eq}}{\tau_f} \tag{2.13}$$

Resulting in;

$$f(x + c\Delta x, t + \Delta t) - f(x,t) = -\Delta t\left(\frac{f - f^{eq}}{\tau_f}\right) \tag{2.14}$$

There is a basic explanation in which the collision term is evaluated locally and there is only one streaming step operation per lattice velocity. The lattice spacing is the distance travel by the particles during a time step and this is the explanation for the stream and collide particles [28].

The macroscopic variables such as the density, ρ and flow velocity, u can be evaluated as the moment to the distribution function as follow

$$\sum f = \sum f^{eq} = \rho \text{ or } \int f\, dc = \int f^{eq}\, dc = \rho \tag{2.15}$$

$$\sum cf = \sum f^{eq} = \rho u \; or \; \int cf\, dc = \int cf^{eq}\, dc = \rho u \tag{2.16}$$

2.6 Isothermal Lattice Boltzmann Models

The LBM model is constructed on lattice space that contains fluid particles and each particle is force to travel from one node on the grid to another by giving them discrete velocity. Each of the particles is spread to each node according to a set of rules that administrate the collision process.

In order to apply the lattice Boltzmann scheme into the digital computer, the lattice Boltzmann BGK equation needs to delicate in velocity space which escalating the Boltzmann-Maxwell equilibrium distribution function up to u^2. According to the Boltzmann equation which is discrete in space-time stated that the distribution function evolves the single relaxation-time Bhatnagar-Gross-Krook (BGK) operator.

$$f^{eq} = \rho\left(\frac{1}{2\pi RT}\right)^{\frac{D}{2}} \exp\left\{-\frac{c^2}{2RT}\right\}\left[1 + \frac{c.u}{RT} + \frac{(c.u)^2}{2(RT)^2} - \frac{u^2}{2RT}\right] \tag{2.17}$$

In general

$$I_f(c) = \int c^m f^{eq}\, dc \tag{2.18}$$

Where I_f must be satisfies for $m = 0,1,2,3$. $\emptyset_f$ can be defined as follows;

$$\emptyset_f = c^m \rho \left(\frac{1}{2\pi RT}\right)^{\frac{D}{2}} \exp\left\{-\frac{c^2}{2RT}\right\}\left[1 + \frac{c.u}{RT} + \frac{(c.u)^2}{2(RT)^2} - \frac{u^2}{2RT}\right] \tag{2.19}$$

By substituting eq. (2.18) into eq. (2.19) will produced the equation below;

$$I_f(c) = \int \emptyset_f(c) \exp\left\{-\frac{c^2}{2RT}\right\} dc \tag{2.20}$$

Insert the microscopic velocity, $c = \sqrt{2RT}\vec{\xi}$

$$I_f\left(\sqrt{2RT}\vec{\xi}\right) = \int \emptyset_f\left(\sqrt{2RT}\vec{\xi}\right) \exp\left\{-\vec{\xi}^2\right\} \sqrt{2RT}\vec{\xi} \tag{2.21}$$

In order to get the result for quadrature of zero-to-fifth-order of velocity moment of f^{eq} , the Gauss-Hermite quadrature was used. So, the result of I_f is;

$$I_f\left(\sqrt{2RT}\vec{\xi}\right) = \int \emptyset_f(\sqrt{2RT}\left(\zeta_1, \zeta_2, \dots \zeta_{I_D}\right)) \exp\left\{-\zeta_{I_D}^2\right\} \dots \exp\left\{\zeta_{I_D}^2\right\}\left(\sqrt{2RT}\right)^D d\zeta_{I_1}, d\zeta_{I_2}, \dots d\zeta_{I_D}$$

$$= (2RT)^{\frac{D}{2}} \sum_{I_D}^{N} \dots \sum_{I_2}^{N} \sum_{I_1}^{N} W_{I_D} .. W_{I_2} W_{I_1} \emptyset_f \left(\sqrt{2RT}\left(\zeta_1, \zeta_2, \dots \zeta_{I_D}\right)\right) \tag{2.22}$$

where W_k is a weight coefficient, N is a number of abscissas and ζ_k is the Gaussian abscissas. For 2D, D=2, N=2 and the output equation for W_k and ζ_k will be;

$$\zeta_1 = -\sqrt{\frac{3}{2}}, \zeta_2 = 0, \zeta_3 = \sqrt{\frac{3}{2}}, W_1 = \frac{\sqrt{\pi}}{6}, W_2 = \frac{2\sqrt{\pi}}{3}, W_3 = \frac{\sqrt{\pi}}{6} \tag{2.23}$$

The result of the expression for the dicretised density equilibrium distribution function is obtained as follow

$$f_i^{eq} = \rho\omega_i \left[1 + 3\frac{c_i u}{c^2} + \frac{9(c_i.u)^2}{2c^4} + \frac{3u^2}{2c^2}\right] \tag{2.24}$$

where $c = \sqrt{2RT}$ and weights are $w_1 = \frac{4}{9},\ w_2 = w_3 = w_4 = w_5 = \ w_6 = w_7 = w_8 = \frac{1}{9}$

2.7 Boundary Conditions

Distribution function is one of the important characters before computing any meaningful result. After each streaming process, the distribution function at the boundary nodes is unknown and the boundary conditions are responsible for this problem. But, the appropriate selection is significant and it depends on the type of boundary conditions to be applied. In other words, LBM is the best solution because it has several boundary conditions for selection.

2.7.1 Periodic Boundary Conditions

Periodic boundary condition can be classified as the simplest boundary condition which is used to isolate bulk phenomena from the actual boundaries of the real physical system [27]. So, they are satisfactory for physical phenomena where surface effect play an insignificant role. The periodic boundary condition is the other type of boundary condition used in this paper along with bounce back boundary condition that can be explained by bringing the distribution function that leaves the outlet to the inlet which can be shown in the figure 2.2 below. Particles will arrive at node A and will go to node B.

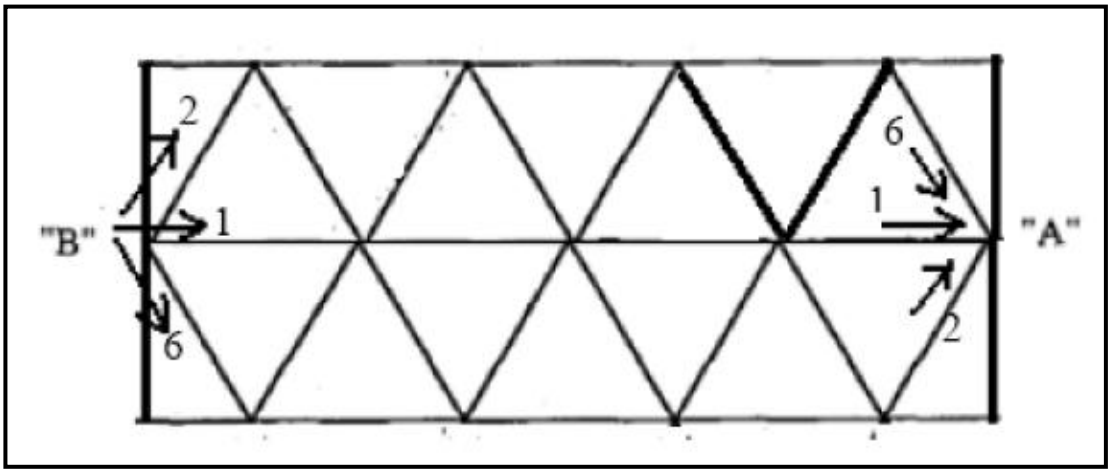


Figure 2.3: Periodic boundary condition

Source: Nor Azwadi, 1997

2.7.2 Free Slip Boundary Condition

Free slip is applied to the case of smooth boundaries with insignificant of resistance exerted upon the flowing gas or liquid. Free slip boundary condition reflecting the distribution function at the boundaries to the neighboring position in lattice in the case where the tangential motion of fluid flow on the wall is free and no momentum is to be exchanged with the wall along the tangential component [28].

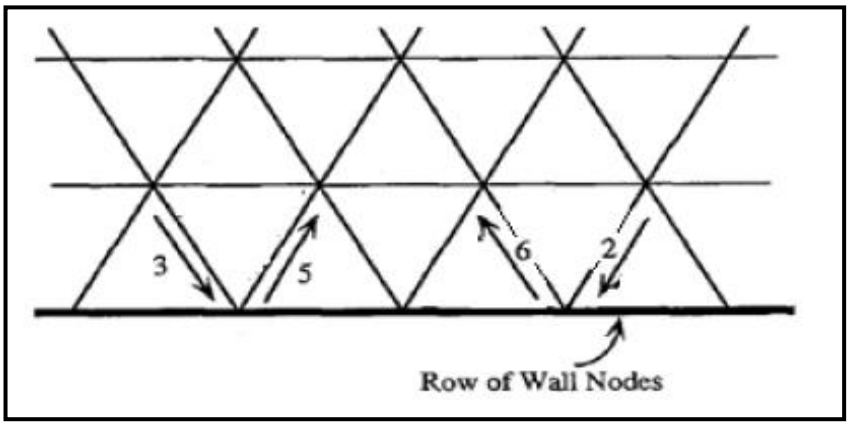


Figure 2.4: Free slip boundary condition

Sorce: Nor Azwadi, 1997

2.7.3 Bounce Back Boundary Condition

Bounce back or non-slip boundary condition is the most popular and simplest boundary condition that important in simulating fluids in domains characterized by complex geometries such as those found in porous media. In LBM, it defines the velocity at the wall to be zero by averaging the velocity before and after the collision around the wall.

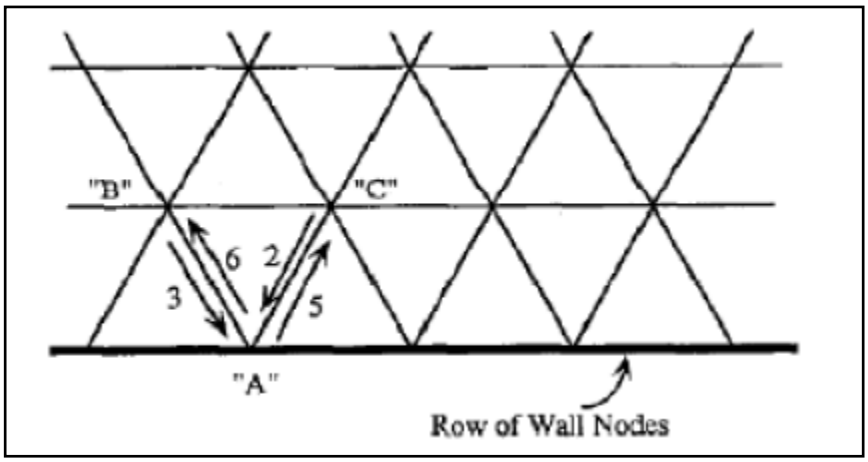


Figure 2.5: Bounce back boundary condition

Source: Nor Azwadi, 1997

2.8 Relaxation Time

In BGK collision model, time relaxation, τ can be explained as the time taken to reach a steady state solution for transient fluid flow problem. the equilibrium state is needed to converge the numerical stability and iteration which means that manipulating the time relaxation to be closer than 1, lots of particles exchange to the equilibrium state

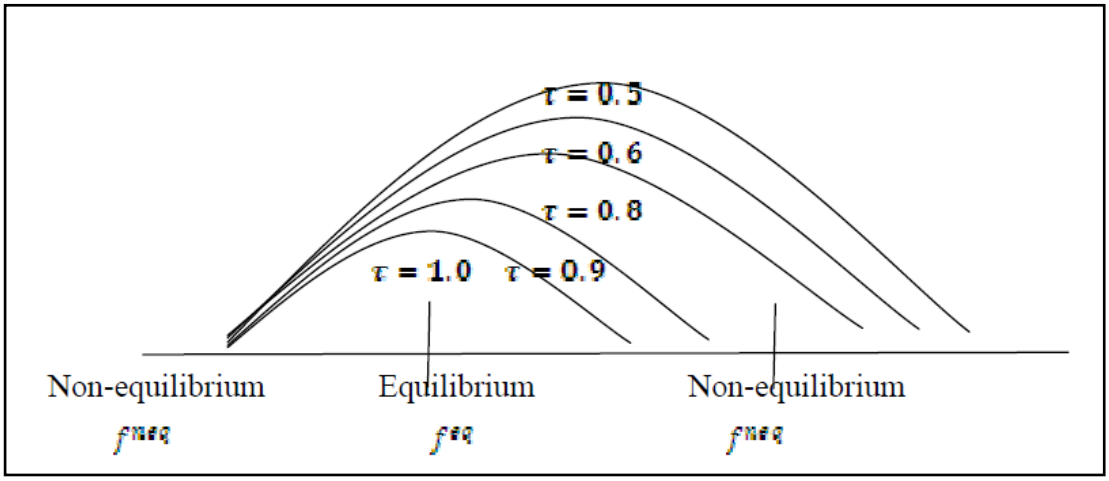


Figure 2.6: Time relaxation concept

Source: Nik Mohd Izual, 2009

From the figure 2.5 above, at $\tau = 0.5$, all the particles initially non equilibrium exchanged to non equilibrium state and resulting instability. The iteration cannot be converge at this condition and the value of $\tau = 0.5$ is the limit of the tome relaxation [27].

CHAPTER 3

MULTIPHASE

3.1 Introduction

The limitation of the theoretical solution availability is one of the factors that lots of complex multiphase flow problem still cannot be answer. The experimental solution for the multiphase flow is very expensive and costly. It is because multiphase flow experiment is required expensive apparatus just because this apparatus have high sensitivity and precise.

There are few traditional methods that can solved the problem of multiphase flow and this methods can be categorized into two types, front capturing method and front tracking method. The first method, front capturing method is specially used to capture the interface afterwards and capture the movement of the fluids. This method is using two fluids modeled as a single continuum with discontinuous properties of the interface. More specifically this method is tracking the interface of these two fluids making the result more accurate and precise.

Lately, LBM got much attention due to its greatness compared to traditional methods. The interaction force between the particles creating phase segregation and surface tension which means that traditional method is not capable to analyze this problem and only LBM is capable to incorporating this interparticles.

3.2 Van Der Waals Fluids

The Van Der Waals real gas equation of state is;

$$\left(P + \frac{n^2}{V^2}\right)(V - nb) = nRT \tag{3.1}$$

where *P, V, T* can be describe as usual pressure, volume and temperature, *a* and *b* are the constant characteristics of a particular gas. *R* is the gas constant and *n* is the mole number. A point of the reflection on the isotherm that corresponding to the critical point of the gas can be seen when the isotherms of Van Der Waals gas of a *p-v* is plotted. It can be describe as follows,

$$\left(\frac{\partial P}{\partial V}\right)_{T=Tc} \tag{3.2}$$

$$\left(\frac{\partial^2 P}{\partial V}\right)_{T=Tc} \tag{3.3}$$

For the convenience, *n*=1 is sated. The other form of Van Der Waals equation can be performed as below,

$$P = \frac{RT}{V - b} - \frac{a}{b^2} \tag{3.4}$$

By applying first and second derivation for Van Der Waals equation above, it will be

$$\left(\frac{\partial P}{\partial V}\right)_{T=T_c} = -\frac{RT_c}{(V_c - b)^2} - \frac{2a}{V_c^3} \tag{3.5}$$

$$\left(\frac{\partial^2 P}{\partial V}\right)_{T=T_c} = -\frac{2RT_c}{(V_c - b)^3} - \frac{6a}{V_c^3} \tag{3.6}$$

After rearranging Eq. (3.5) and Eq. (3.6) and set the RT_c as the main purpose of both equations.

$$RT_c = \frac{2a(V_c - b)^2}{V_c^3} \tag{3.7}$$

$$RT_c = \frac{3a(V_c - b)^3}{V_c^4} \tag{3.8}$$

By making an assumption the equations are equal for both sided,

$$2a = 3a\frac{V_c - b}{V_c} \tag{3.9}$$

Finally,

$$V_c = 3b \tag{3.10}$$

Substituting this V_c into Eq. 3.7 will produced equation below,

$$T_c = \frac{8a}{27bR} \tag{3.11}$$

By substituting eq. (3.10) and (3.11) into eq. (3.7), the equation generated as below;

$$P_c = \frac{8a}{27b^2} \tag{3.12}$$

Define the following 'reduced' quantities

$$\tilde{P} = \frac{P}{P_c}; \tilde{V} = \frac{V}{V_c}; \tilde{T} = \frac{T}{T_c} \tag{3.13}$$

Thus the Van Der Waals equation becomes

$$\left(\tilde{P} + \frac{3}{V^2}\right)(3\tilde{V} - 1) = 8T \tag{3.14}$$

Figure 3.1 shows the graph of pressure versus specific volume, $(\tilde{P} - \tilde{V})$ for the various $\tilde{T}$. When the temperature is higher than critical temperature ($T > T_c$), the plot is very similar to the ideal gas isotherm. When $T < T_c$, the graph shows that there is a curve which is separate the system into two phase, liquids and gasses. There are two different values of specific volume that related to both phases when there is the same pressure value P_{LG}, V_L stand for liquids and V_G stands for gasses. The value of V_L and V_G can be determined by using Maxwell equal area construction, by recalling that equilibrium condition with equilibrium chemical potentials for both phases.

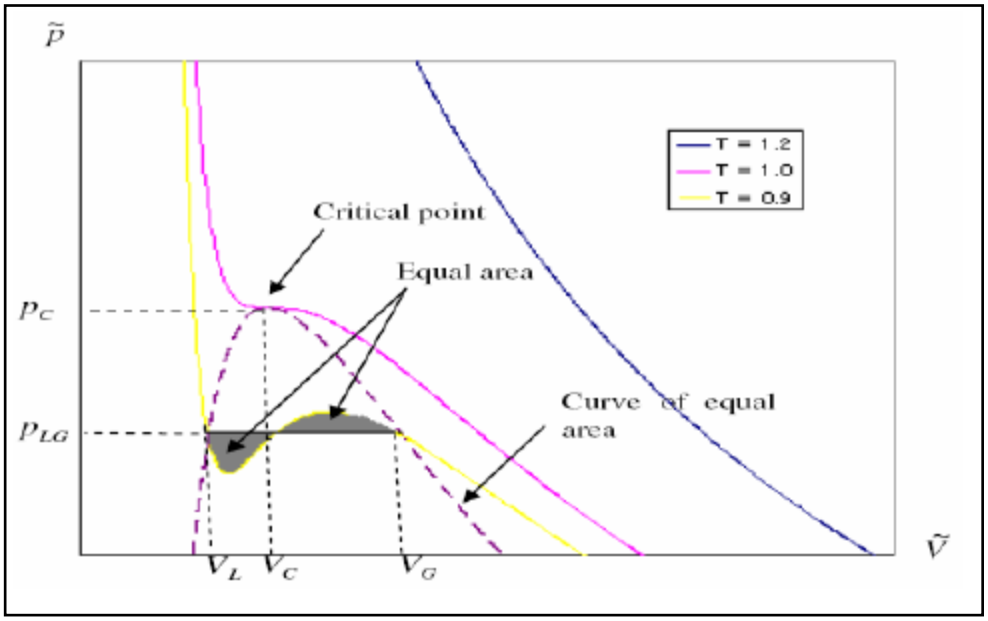


Figure 3.1: Isotherm plot of p-v

Source: Nik Mohd Izual, 2009

There are three temperatures that are considered for this graph, T=0.9, 1.0, 1.2. The volume of liquid and gas at T=0.55 are $V_l = 0.2043$ ($\rho_l = 4.895$) and $V_g = 0.4523$ $(\rho_g = 2.221)$.

3.3 The Lattice Boltzmann Model

In the section 3.3.1, there will be an explaination of the basic scheme of the free energy lattice Boltzmann model by showing the used the lattice Boltzmann equation, detailaing the collision term and equilibriun distribution, preenting the Navier-strokes level equation and finally introducing the collision and streaming steps needed for numerical computation [7]. In the section 3.3.2 informing about the free energy for the liquid-gas system, by a model of two bulk phases at different densities and interfaces of finite width between phases.

3.3.1 Free energy Lattice Boltzmann

The lattice Boltzmann methods is used to simulate the time evaluation of the density function $f_{\sigma i}(x,t)$ which is representing the particles at the position of *x* at the time *t* and moving with velocity $e_{\sigma i}$. There are the function of fluid density *n* and velocity *u* that are related to distribution function [9].

$$\sum_{\sigma,i} f_{\sigma i} = n \tag{3.15}$$

$$\sum_{\sigma,i} f_{\sigma i} e_{\sigma i\alpha} = n u_{\alpha} \tag{3.16}$$

where $e_{\sigma i\alpha}$ is the vector velocity $c_{\sigma i}$ for the α component. *A* can be recognize as the lattice direction *x* and *y*. After making an assumption that single relaxation time was estimated, the distribution function was evolved according to the lattice Boltzmann equation.

$$f_{\sigma i}(x + e_{\sigma i}\Delta t, t + \Delta t) - f_{\sigma i}(x,t) = \frac{1}{\tau_f}\left(f_{\sigma i} - f_{\sigma i}^{eq}\right) \tag{3.17}$$

where $f_{\sigma i}^{eq}$ stands for the equilibrium distribution function while τ_f is the non-dimensional relaxation time. From the equation (3.17), the right hand side reprisenting the Bhatnagar-Gross-Krook collision operator. This is the overview over early model form and dictates that $f_{\sigma i}$ relaxes towards the local equilibrium distribution $f_{\sigma i}^{eq}$ with a single characteristic time, τ_f [19]. The equilibrium distribution determines the physics natural in the simulation.

$$f_{\sigma i}^{eq} = A_\sigma + B_\sigma e_{\sigma i\alpha} u_\alpha + C_\sigma u^2 + D_\sigma e_{\sigma i\alpha} e_{\sigma i\beta} u_\alpha u_\beta + G_{\sigma\alpha\beta} e_{\sigma i\alpha} e_{\sigma i\beta} \tag{3.18}$$

The value of the coefficient $A_\sigma, B_\sigma, C_\sigma, D_\sigma$ and $G_{\sigma\alpha\beta}$ were determined from the process of placing constrains on the moment of $f_{\sigma i}^{eq}$. The first two moments of $f_{\sigma i}^{eq}$ were constrained in order that the collision term in equation before conserve mass and momentum.

$$\sum_{\sigma,i} f_{\sigma i}^{eq} = n \tag{3.19}$$

$$\sum_{\sigma,i} f_{\sigma i}^{eq} e_{\sigma i\alpha} = n u_\alpha \tag{3.20}$$

The hydrodynamics of a one-component, non-ideal fluid is described correctly from the next moment of is chosen such that the continuum macroscopic equations approximated by the evolution scheme (3.17) which resulting in

$$\sum_{\sigma i} f_{\sigma i}^{eq} e_{\sigma i\alpha} e_{\sigma i\beta} = P_{\alpha\beta} + n u_\alpha u_\beta + v\left[u_\alpha \partial_\beta(n) + u_\beta \partial_\alpha(n) + u_\gamma \partial_\gamma(n)\delta_{\alpha\beta}\right] \tag{3.21}$$

The pressure tensor can be shown by $P_{\alpha\beta}$ and kinetic shear viscosity can be derive by $v = c^2\left(\tau_f - \frac{1}{2}\right)\left(\frac{\Delta t}{3}\right)$. The first formulation of the model omitted the third term in (3.21) and was not Galilean invariant. The coefficients $A_\sigma, B_\sigma, C_\sigma, D_\sigma$ and $G_{\sigma\alpha\beta}$ are needed in order to fully constrain a fourth condition which is

$$\sum_{\sigma i} f_{\sigma i}^{eq}\, e_{\sigma i\alpha} e_{\sigma i\beta} = \frac{nc^2}{3}\left(u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_{\gamma\delta_{\alpha\beta}}\right) \tag{3.22}$$

The values of the coefficients can be determined using a well established procedure. For constraints (3.19)-(3.22) one possible choice of coefficients is:

$$A_2 = \frac{P_o}{8c^2} + \frac{v}{4c^2}\left(u_x \partial_x n + u_y \partial_y n\right) \tag{3.23}$$

$$A_1 = 2A_2, A_o = n - 12A_2 \tag{3.24}$$

$$B_2 = \frac{n}{12c^2}, B_1 = 4B_2 \tag{3.25}$$

$$C_2 = -\frac{n}{16c^2}, C_1 = 2C_2, C_o = 12C_2 \tag{3.26}$$

$$D_2 = -\frac{n}{8c^4}, D_1 = 4D_2 \tag{3.27}$$

$$G_{2xx} = \frac{\kappa}{16c^4}\left[(\partial_x n)^2 - \left(\partial_y n\right)^2\right] + \frac{v}{8c^4}\left(u_x \partial_x n - u_x \partial_y n\right) \tag{3.28}$$

$$G_{2xy} = G_{2yx} = \frac{\kappa}{8c^4}\left[(\partial_x n)\left(\partial_y n\right)\right] + \frac{v}{8c^4}\left(u_x \partial_x n - u_x \partial_y n\right) \tag{3.29}$$

$$G_{2yy} = -G_{2xx} \tag{3.30}$$

$$G_{1\alpha\beta} = 4G_{2\alpha\beta} \text{ for all } \alpha \text{ and} \beta \tag{3.31}$$

From the above analysis, the evolution scheme (3.17) approximates the continuity equations

$$\partial_t \rho + \partial_\alpha(\rho u_\alpha) = 0 \tag{3.32}$$

The Navier-Stokes level equation is as follows:

$$\begin{aligned}\partial_t(\rho u_\alpha)\partial_\beta\left(\rho u_\alpha u_\beta\right) = &-\partial_\beta p_{\alpha\beta} + v\partial_\beta\left[\left\{\partial_\beta u_\alpha + \partial_\alpha u_\beta + \delta_{\alpha\beta}\partial_\gamma u_\gamma\right\}\right] \\ &-\frac{3v}{c^2}\partial_\beta\left[u_\alpha\partial_\gamma p_{\beta\gamma} + u_\beta\partial_\gamma p_{\alpha\gamma} + \partial_\gamma\left(\rho u_\alpha u_\beta u_y\right)\right] \\ &-\frac{3v}{c^2}\partial_\beta\left[\left(\partial_\rho p_{\alpha\beta}\right)\partial_\gamma\left(\rho u_\gamma\right)\right] \\ &-\frac{3v}{c^2}\partial_\beta\left[u_\alpha\partial_\gamma\left(u_\beta\partial_\gamma\rho + u_\gamma\partial_\beta\rho + \partial_{\gamma\beta}u_\lambda\partial_\lambda\rho\right)\right] \\ &-\frac{3v}{c^2}\partial_\beta\left[u_\alpha\partial_\gamma\left(u_\beta\partial_\gamma\rho + u_\gamma\partial_\beta\rho + \partial_{\alpha\gamma}u_\lambda\partial_\lambda\rho\right)\right] \\ &-\frac{3v}{c^2}\partial_\beta\left[u_t\partial_\gamma\left(u_\alpha\partial_\beta\rho + u_\beta\partial_\alpha\rho + \partial_{\alpha\beta}u_\lambda\partial_\lambda\rho\right)\right] \qquad (3.33)\end{aligned}$$

The first line shows the compressible Navier-Stokes equation while the subsequent lines are error terms. The evolution equation (3.17) for the computational purpose is sepaarated into two distinct steps, which can be considered as a streaming and collision. For the purpose of facilitating the equation, a new field at each lattice site was introduced in order to define the collision step as follows:

$$f^*_{\sigma i}(x,t) = f_{\sigma i}(x,t) + \frac{1}{\tau_f}\left(f^{eq}_{\sigma i} - f_{\sigma i}\right) \qquad (3.34)$$

The streaming step:

$$f_{\sigma i}(x, t+\Delta t) == f^*_{\sigma i}(x - c_{\sigma i}\Delta t, t) \qquad (3.35)$$

Each site of the lattice Boltzmann equation represents the collision and streaming step that can be considered as a framework for a one component free energy lattice Boltzmann. For coexisting phases, the properties of the fluids are determined by the pressure tensor [28]. **Figure 3.2** until figure 3.4 show that the initial condition, streaming (translate) and collision process of the particles.

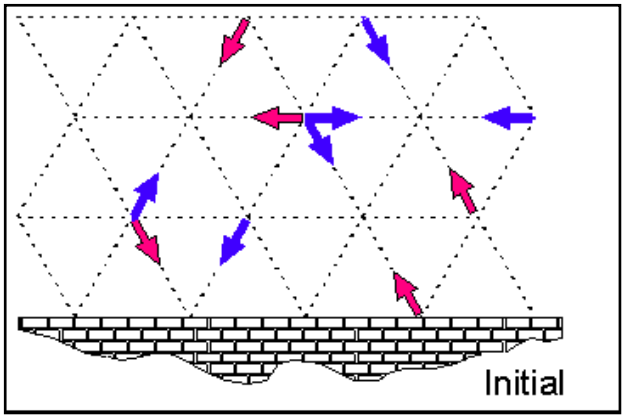


Figure 3.2: Initial condition of the particles

Source: Zhang, R., et al., 1999

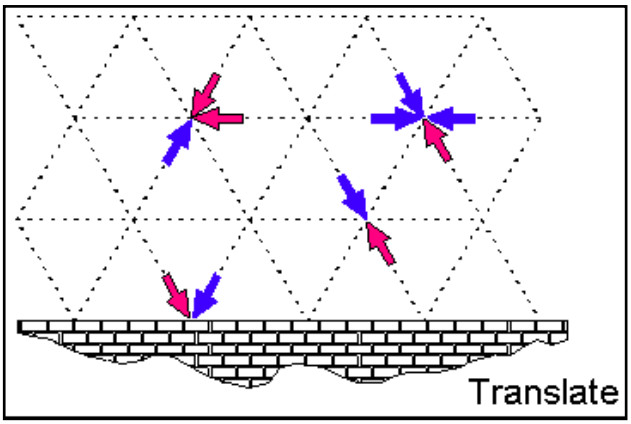


Figure 3.3: Translation or streaming of particles

Source: Zhang, R., et al., 1999

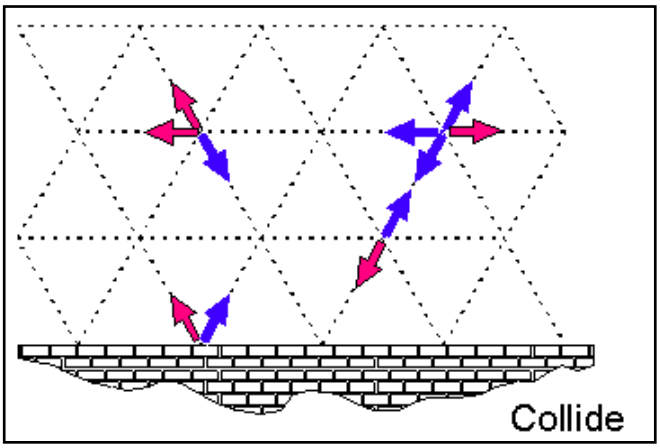


Figure 3.4: collision of particles

Source: Zhang, R., et al., 1999

3.3.2 Thermodynamics of the fluids

The thermodynamics of the fluid enters the lattice Boltzmann simulation through the pressure tensor $P_{\alpha\beta}$. A Landau free energy functional is used to describe the equilibrium properties of a system with no surfaces such as periodic boundaries.

$$\psi_b = \int dV \left[\psi(T,n) + \frac{\kappa}{2}(\partial_\alpha n)^2\right] \tag{3.36}$$

The above equation is subjected to the constraint

$$M = \int dV\, n \tag{3.37}$$

Where, $\psi(T,n)$ = the free energy density of bulk phase

κ = constant related to the surface tension

M = total mass of fluid

The free energy contribution from density gradients in an inhomogeneous system can be shown as the second term in the equation (3.36). The below equilibrium condition is getting from minimizing the equation (3.36) by using a constant Langrange multiplier, μ.

$$\frac{\partial\psi}{\partial\rho} - \mu - \kappa\nabla^2 n = 0 \tag{3.38}$$

Then, this equilibrium condition equation (3.38) was multiple by $\frac{\partial n}{\partial x}$ and integrate once with respect to *x*. As a result, the first integral shown below

$$\psi - \mu n - \frac{\kappa}{2}(\partial_\alpha n)^2 = \text{constant} \tag{3.39}$$

The below equations are from equation (3.38) and (3.39) after defining $W(n,T) = \psi - \mu n - constant.$

$$\frac{\partial W}{\partial n} = \kappa \nabla^2 n \tag{3.40}$$

And

$$W = \frac{\kappa}{2}(\partial_\alpha n)^2 \tag{3.41}$$

Presume that there is a density constant in the bulk phases, $W(n) = 0\ and\ \frac{\partial W}{\partial n} = 0$. The next process is specifying the excess of free energy function W (or equivalent ψ) to obtained two phase coexistence. For two bulk phases with positive density, the function of $W = \frac{\partial W}{\partial n} = 0$ was chosen and its shows clearly by;

$$W(v,\tau) = p_c(v^2 - \beta\tau)^2 \tag{3.42}$$

where $v = \frac{(n-n_c)}{n_c}$ and $\tau = \frac{(T_c-T)}{T_c}$ are reduced density and temperature ratio. The other parameter $T_c, p_c\ and\ n_c$ are stand for critical temperature, pressure and density respectively while β is a constant. The free energy related to the selected W is

$$\psi = p_c(v+1)^2(v^2 - 2v + 3 - 2\beta\tau) \tag{3.43}$$

There are two bulk phases with densities for $T < T_c$,

$$n_l = n_c\left(1 + \sqrt{\beta\tau}\right) \tag{3.44}$$

$$n_g = n_c\left(1 - \sqrt{\beta\tau}\right) \tag{3.45}$$

In addition to uniform phases $n = n_g$ or n_l, equation (3.40) allows a solution with an interface between two phases. In order to see how this works, specialize to one-dimension equation and rewrite equation (3.40) as

$$\frac{4p_c}{n_c^2} v(v^2 - \beta\tau) - \kappa \frac{d^2 v}{dx^2} = 0 \tag{3.46}$$

This gives a solution of

$$v(x) = \sqrt{\beta\tau} \tanh\left(\frac{x}{\sqrt{2}\xi}\right) \tag{3.47}$$

The width of the interface region can be measure as ξ,

$$\xi = \sqrt{\frac{\kappa n_c^2}{4\beta\tau p_c}} \tag{3.48}$$

The surface tension of the interface as shown below

$$\sigma = \kappa \int dx \left(\frac{dn}{dx}\right)^2 \tag{3.49}$$

Changing the variable of integration to *n*, using equation (3.42)

$$\sigma = \int_{n_g}^{n_l} dx \sqrt{2\kappa W} \tag{3.50}$$

So, the final result for *W* is

$$\sigma = \frac{4}{3}\sqrt{2\kappa p_c}(\beta\tau)^{\frac{3}{2}} n_c \tag{3.51}$$

Therefore ψ and W are used to determine the equilibrium properties of the model and the pressure tensor,$p_{\alpha\beta}$ is used by the free energy to enter the lattice Boltzmann. The conservation of momentum can be taken from eq. (3.52) which follows the Noether's theorem. This is possible since the free energy function and total mass constraint are independent of position.

$$\partial_\beta p_{\alpha\beta} = 0 \tag{3.52}$$

The pressure tensor, $p_{\alpha\beta}$ is given by

$$p_{\alpha\beta} = \frac{\partial F}{\partial(\partial_\alpha n)}\left(\partial_\beta n\right) - F\delta_{\alpha\beta} \tag{3.53}$$

where $F = \psi - \mu + \kappa\frac{\left(\partial_\gamma n\right)^2}{2}$. For ψ this gives

$$p_{\alpha\beta} = p(x)\delta_{\alpha\beta} + \kappa(\partial_\alpha n)\left(\partial_\beta n\right) \tag{3.54}$$

with

$$p(x) = p_o - \kappa\nabla^2 n - \frac{\kappa}{2}\left(\partial_\gamma n\right)^2 \tag{3.55}$$

where $p_o = n\partial_n\psi - \psi$ is the equation of the state of the fluid

CHAPTER 4

METHODOLOGY

4.1 Introduction

This chapter can be subdivided into two sections; the flow chart and simulation algorithm. These parts will explain the details of the overall process or tasks. In the diagram of flow chart, there are lots of important steps that need to consider ensuring that this project can be done on time. The initial process until the end of the project is stated in the flow chart diagram. The step from literature previous study of LBM, collecting the data will tells the detailed about LBM and phase separation process. While the simulation algorithm details about process need to be done for getting the result of phase separations.

4.2 The Flow Chart

Figure 4.1 shows that there are seven main steps or procedure from start until end of the project. The first procedure is literature review about previous people study of LBM and phase separation. This is the guide for overall project regarding to the scopes. Next, the identification of the parameters that used in the equation related to the phase separation is most important process need to be done. After identified this parameters, the initial values were set up because all of these parameters and initial values will be used in the code of phase separation. Then, the code of phase separation was generated based on the scopes which mean that all the data and information used in generating coding. After that, the code of phase separation was run using FORTRAN software. The results of this simulation were compared to the theoretical result and previous result and the expected result was discussed based on

the certain criteria. Then, the overall summary had been concluded and some ideas for the further study had been recommended.

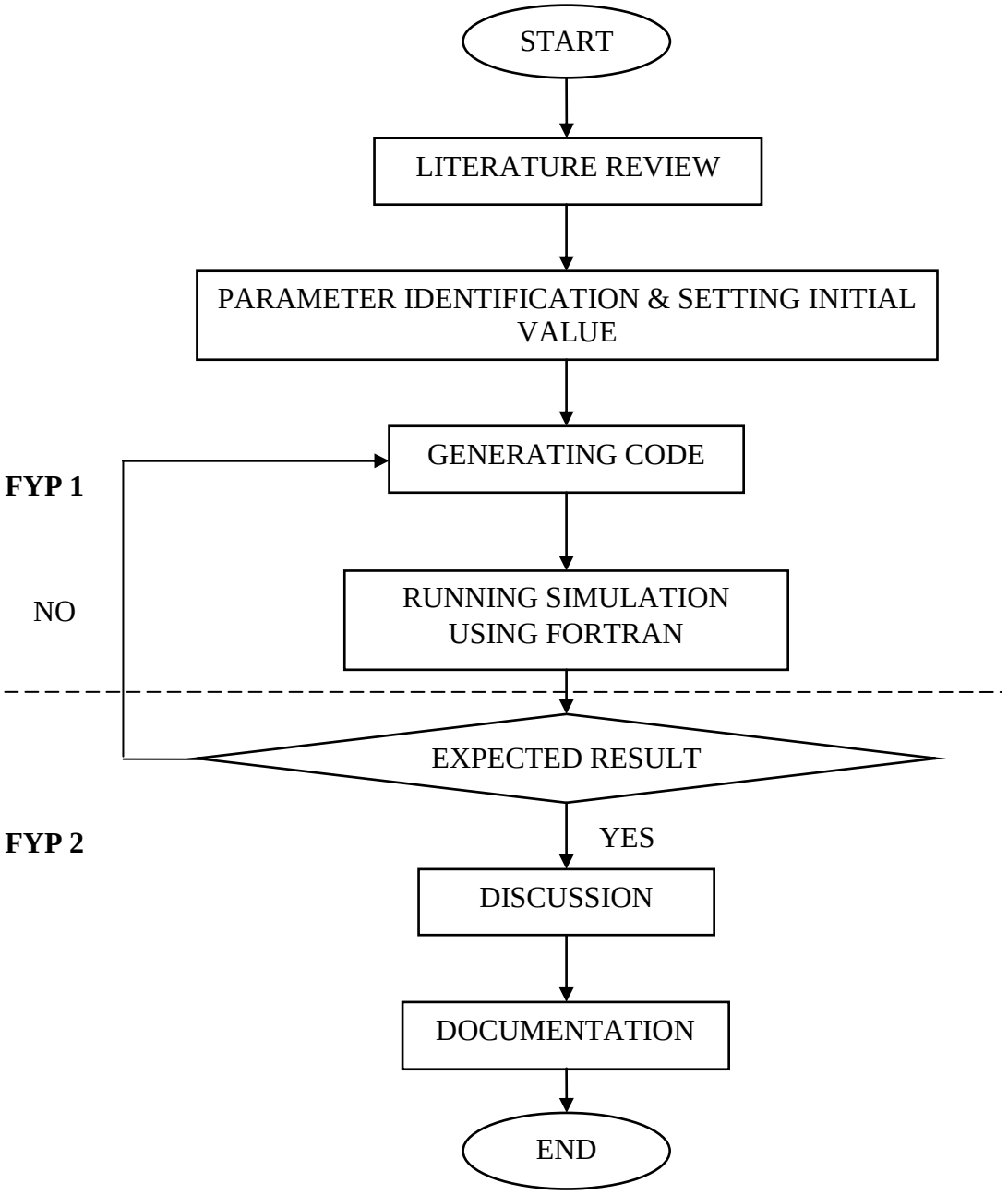


Figure 4.1: The flow chart of the project

4.3 Simulation Algorithm

Simulation algorithm plays the main rule for this project of the phase separation phenomenon which includes the calculation of the multiphase flow. Lattice Boltzmann equation is used for calculating the important parameters that will use in further calculation. After that, the initial values are set up for finding the solution of the streaming and collision process. **Figure 4.2** will describe the overall algorithm of LBM for multiphase flow.

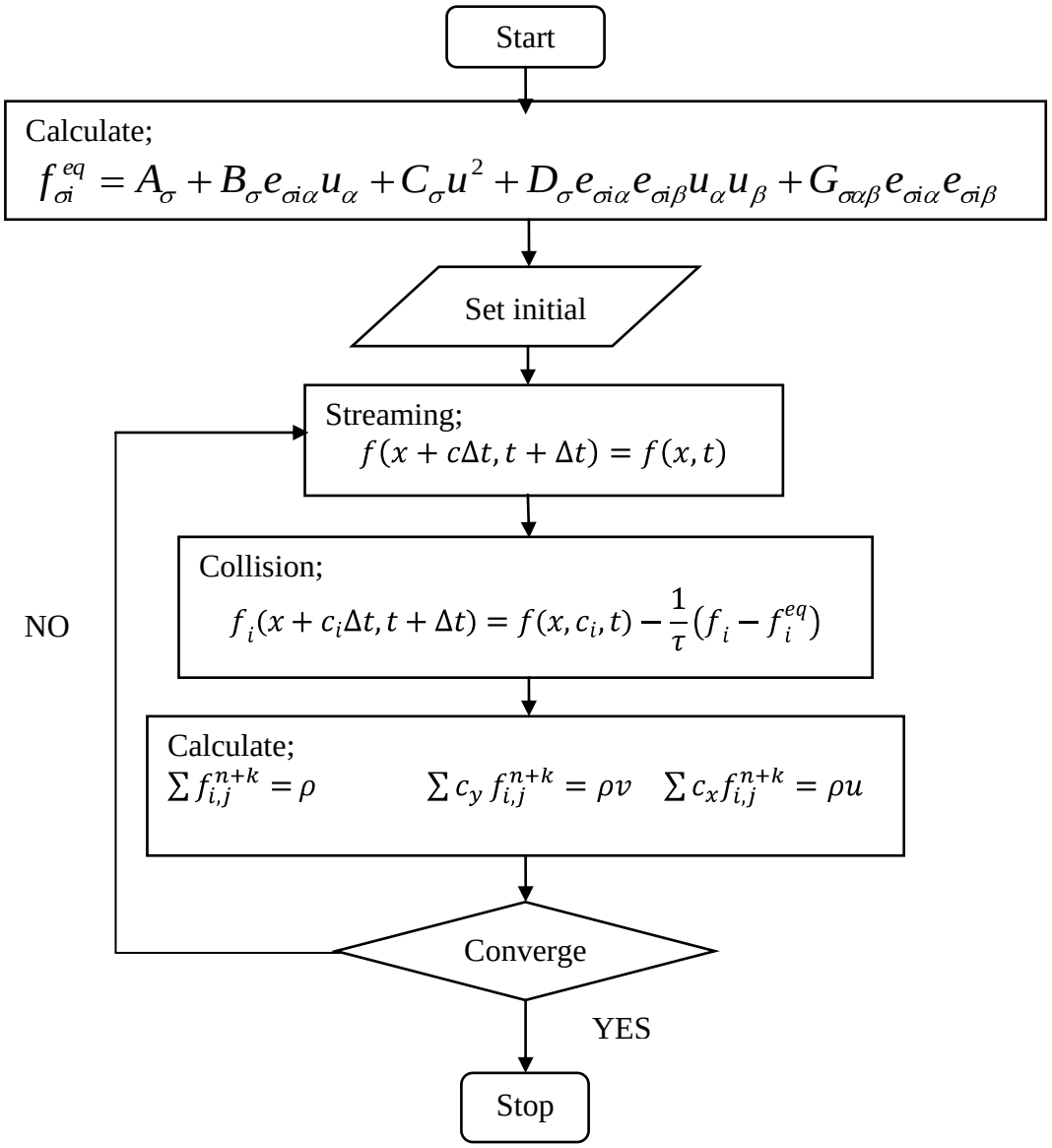


Figure 4.2: Algorithm of LBM for multiphase

CHAPTER 5

RESULT AND DISCUSSION

5.1 Introduction

The main objective of this project is to simulate the phase separation phenomenon for two-phase fluid flow using LBM. This chapter will describe the results for the better understanding on the lattice Boltzmann methods in the situation of isothermal. The size of lattice used in this simulation is about 101x101 lattices. Section 5.2 will described the overall result from the simulation.

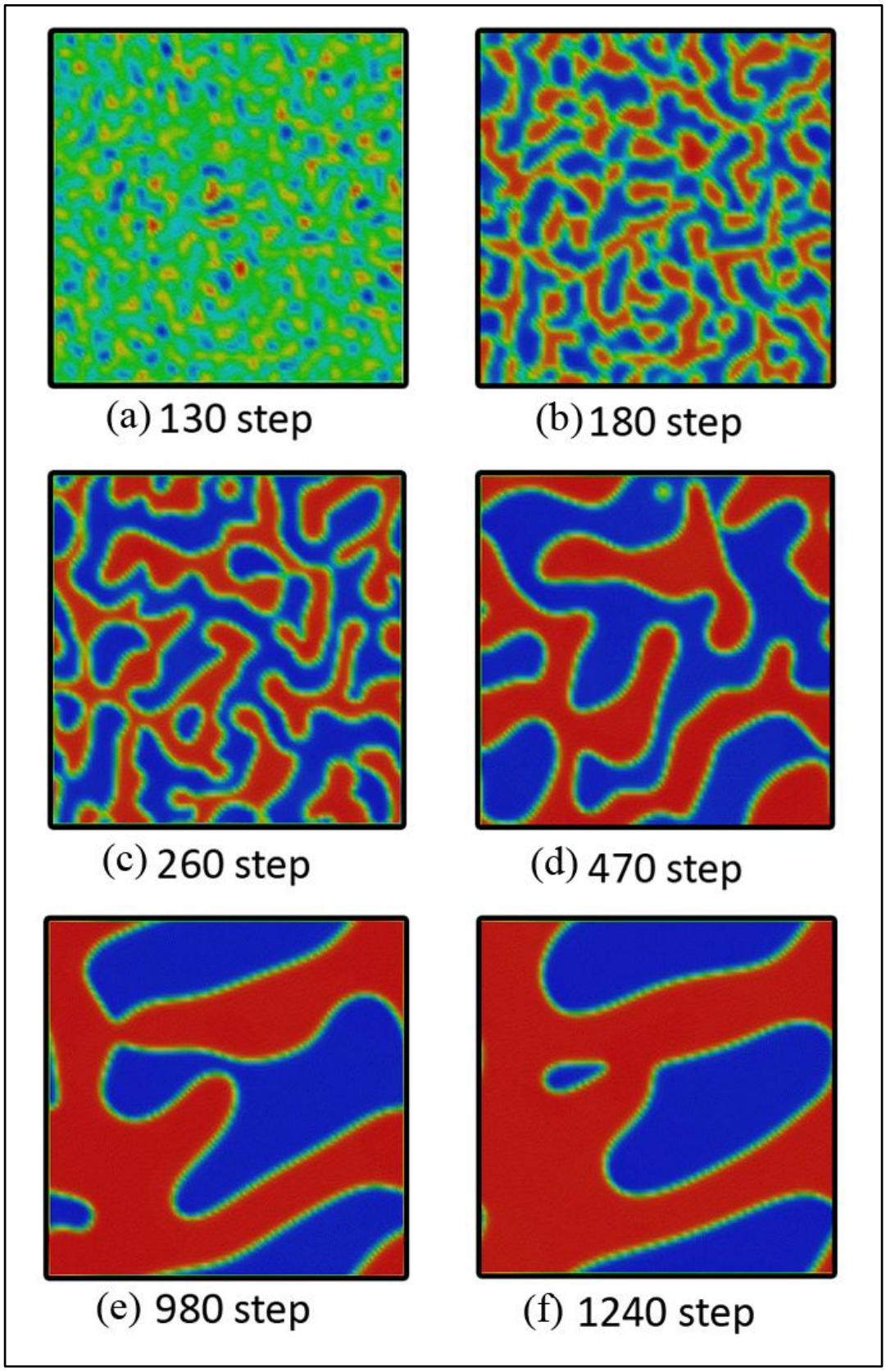
5.2 Result and Discussion

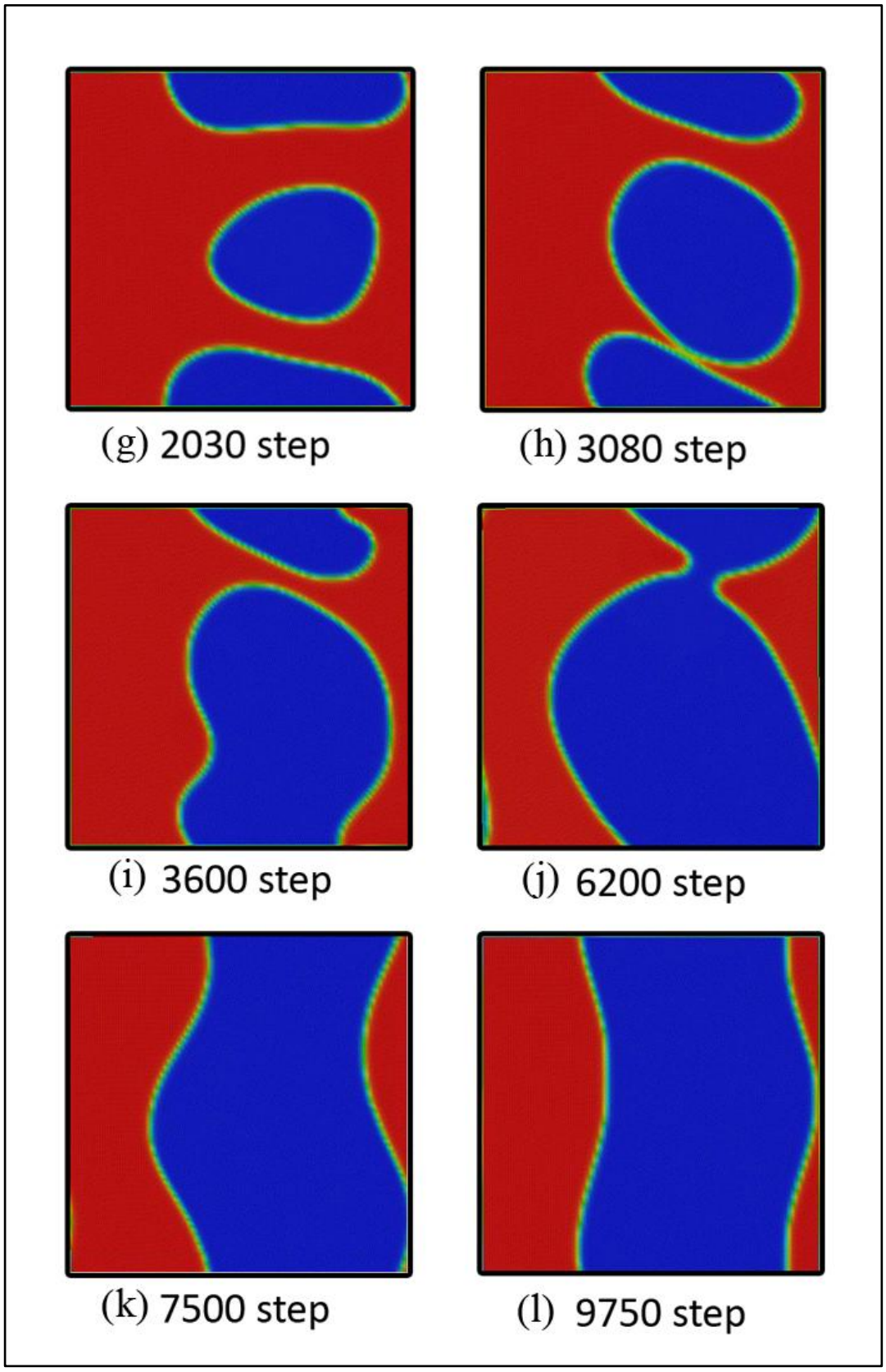
5.2.1 Two-phase flow LBM model

The phase separation which is based on thermodynamic instability of the Van Der Waals fluid was simulated in order to test the validity of existing FE model. The D2Q9 model with the size of 101x101 lattice is used in this simulation test with the temperature, T=0.55. **Table 5.1** shows the other parameters that been used in the test**.**

Table 5.1: Parameters used for simulate phase separation

Δx	Δy	Δt	τ	κ	T
1.0	1.0	1.0	1.00	0.0075	0.55


(a) 130 step
(b) 180 step
(c) 260 step
(d) 470 step
(e) 980 step
(f) 1240 step


(g) 2030 step
(h) 3080 step
(i) 3600 step
(j) 6200 step
(k) 7500 step
(l) 9750 step

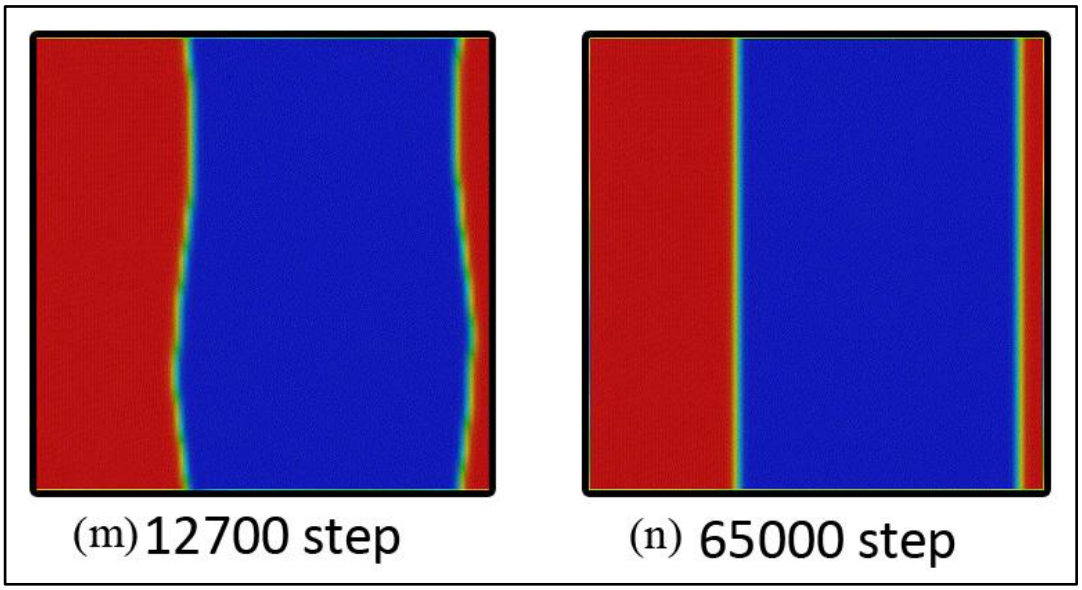


Figure 5.1: Time evaluation of density distribution

Figure 5.1 shows the evaluation of density distribution for the phase separation of 101x101 lattices. Figure 5.1(a) shows that the combination of the fluids with different properties can coexist in one phase condition. The small grain color start to form and this situation can be seen on figure 5.1(b). These small grains color start to combine with each other forming a big grain. This grain was separate with two different colors with different fluid property. After few time steps, the separation was fully happen creating two phase color, red and blue as shown in figure 5.1(n). The blue color is describing the fluid that has low density which means that this blue region is gasses. The red region is for the high density fluid, which means it is liquids.

CHAPTER 6

CONCLUSION AND RECOMMENDATION

6.1 Introduction

Starting from the process of the literature review, calculating the parameter of fluids, and running the simulation, this project is proving that the theory of the Lattice Boltzmann Methods is correct and it is applicable to the previous study.

6.2 Conclusion

There are six main chapter that are consists in this thesis. First, we can conclude that the first chapter is an introduction of LBM and CFD. This introduction is the main guide for the project flow. This chapter also consist the objective of the project, project scope and the problem statement. All of these are the most important thing need to know before starting the project. The second part of the thesis is chapter two. In this chapter, we make some literature review on the theory of Lattice Boltzmann Methods and any equation or formula that is related to LBM. Next, chapter three focuses on the single component of multiphase fluid flow. Lots of multiphase properties and formulas are stated under this chapter. In chapter four, methodology that is focus on the process flow chart from the beginning of the project until the end of the project. It also including the simulation algorithm used in this study of phase separation algorithm. After that, chapter five is the result and conclusion for this study. The result of the phase separation of two phase fluid flow was discussed by presenting the diagram of the process of phase separation. The last chapter, chapter six that is about the conclusion of the case study and the recommendation for further study base on the LBM.

The result of the project proved that the LBM is very useful and effective for simulating the phase separation of the fluid phase. The separation shows the detailed about the fluids with different properties coexist in one condition and this phrase was proved by the result generated which shows the red and blue fluids slowly separated into two different sections. As a conclusion, there are lots of advantages of using LBM for phase separation process compare to the old methods of CFD. The result generated by using LBM is precise and accurate.

6.3 Recommendation

The study of phase separations gives tons of advantages for science and technology. All of this advantages and information will use either by an engineer or scientist for creating goods to all human. Bio-science is one of the science branches that related to this study. The investigation and experimentation of the phase separation, for example, the process of separating red blood and platelet in the human blood vein will improve human live by creating new vaccine for lots of diseases.

The further study of LBM is needed in order to have a detail understanding about phase separation. There are few recommendations for the further study of LBM;

(i) Model moving solid particles in flow
(ii) Add external forces to flow
(iii) Incorporate Immersed Boundary Method into LBM
- Fluid Filled Particles
- Deformable Boundary

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Appendices

Appendix A: Gantt Chart / Project Schedule for Final Year

Gantt Chart FYP 1

	W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12	W13	W14	W15
1.0 PROPOSAL CONFIRMATION	★	★													
2.0 DEFINE PROBLEM STATEMENT															
2.1 BACKGROUND WRITING		★	★	★	★	★									
2.2 INTRODUCTION WRITING		★	★	★	★	★									
2.3 LITERATURE REVIEW	★	★	★	★	★	★	★	★	★	★	★	★	★	★	★
3.0 METHODOLOGY															
3.1 GENERATING CODING					★	★	★	★	★	★	★	★	★	★	★
3.2 RUNNING SIMULATION							★	★	★	★	★	★	★	★	★

Gantt Chart FYP 2

	W1	W2	W3	W4	W5	W6	W7	W8	W9	W10	W11	W12	W13	W14
4.0 RESULT														
4.1 MEASUREMENT INSTALLATION			★	★	★	★	★	★	★	★	★			
4.2 RESULT DOCUMENTATION					★	★	★	★	★	★	★	★		
5.0 DISCUSSION														
5.1 RESULT DISCUSS							★	★	★	★	★	★	★	
5.2 RECOMMENDED RESULT								★	★	★	★	★	★	
5.3 FUTURE WORK										★	★	★	★	★
6.0 DRAFT & THESIS PREPARATION														
6.1 DRAFT WRITING							★	★	★	★	★	★	★	★
6.2 FULL MANUSCRIPT PREPARATION											★	★	★	★

Appendix B

SOURCE CODES

```
PARAMETER (LX = 101, LY = 101, CD = 8)
                REAL*8 RHO(1:LX,1:LY), U(1:LX,1:LY), V(1:LX,1:LY)
                REAL*8 F(1:LX,1:LY,0:CD),
FEQ(1:LX,1:LY,0:CD),FNEW(1:LX,1:LY,0:CD)
                REAL*8 CX(0:CD),CY(0:CD)
                REAL*8 KAPPA, A, B, T, R, NL, NG, TAU, NU

                KAPPA = 0.0075D0
                A = 9.0D0/49.0D0
                B = 2.0D0/21.0D0
                T = 0.55D0
                R = 1.0D0
                NL = 4.895D0
                NG = 2.211D0
!               TAU = 0.3708D0
                TAU = 1.0D0
                NU = (TAU+0.5)/3.0D0

                CX(0) =  0.0D0
                CY(0) =  0.0D0

                CX(1) =  1.0D0
                CY(1) =  0.0D0

                CX(2) =  0.0D0
                CY(2) =  1.0D0

                CX(3) = -1.0D0
                CY(3) =  0.0D0
```

```
                CX(4) =  0.0D0
                CY(4) = -1.0D0

                CX(5) =  1.0D0
                CY(5) =  1.0D0

                CX(6) = -1.0D0
                CY(6) =  1.0D0

                CX(7) = -1.0D0
                CY(7) = -1.0D0

                CX(8) =  1.0D0
                CY(8) = -1.0D0

                DO J = 1,LY
                        DO I = 1,LX

                        RHO(I,J) = 3.0d0 + rand()
                        u(i,j) = 0.0d0
                        v(i,j) = 0.0d0
                        END DO
                END DO

!               CALL MACRO(lx,ly,cd,rho,f,u,v)

                CALL EQUILIBRIUM
(LX,LY,CD,U,V,CX,CY,RHO,KAPPA,NU,A,B,T,FEQ)

                DO I = 1,LX
                DO J = 1,LY
                DO K = 0,CD
```

```
                F(I,J,K)=FEQ(I,J,K)
                END DO
                END DO
                END DO

                DO ITER = 1, 1000000
                CALL COLLIDE(lx,ly,cd,f,feq,fnew,TAU)
                CALL MOVE(lx,ly,cd,f,fnew)
                CALL MACRO(lx,ly,cd,rho,f,u,v)
                CALL EQUILIBRIUM
(LX,LY,CD,U,V,CX,CY,RHO,KAPPA,NU,A,B,T,FEQ)
                IF(MOD(ITER,10) .EQ.0)THEN
                WRITE(*,*)ITER

                CALL fileoutput(lx,ly,u,v,rho,ITER)
                END IF
                END DO
!               CALL fileoutput(lx,ly,u,v,rho,ITER)
                do i = 1,lx
                write(100,*) rho(i, ly/2)
                end do
                END PROGRAM

                !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
        subroutine fileoutput(lx,ly,u,v,rho,ITER)
        real*8 x(10201),y(10201)
        integer nbool(4,10000)
        real*8 U(1:LX,1:LY),V(1:LX,1:LY),RHO(1:LX,1:LY)

        nnode = lx*ly
        ne = (lx-1)*(ly-1)

        do j=1,ly
```

```
                do i = 1,lx
      ID=lx*(j-1)+i
      x(ID)=DFLOAT(I-1)+1
      Y(ID)=DFLOAT(J-1)+1
      IF(I.EQ.1) X(ID)=1
      IF(I.EQ.lx) X(ID)=lx
      IF(J.EQ.1) Y(ID)=1
      IF(J.EQ.ly) Y(ID)=ly
                end do
        end do

        IE=0
   do J=1,ly-1
                do I=1,lx-1
     IE=IE+1
     NBOOL(1,IE)=(J-1)*lx+i
     NBOOL(2,IE)=NBOOL(1,IE)+1
     NBOOL(4,IE)=NBOOL(1,IE)+lx
     NBOOL(3,IE)=NBOOL(4,IE)+1
                END DO
   END DO

!       open(unit=iter+100,file='OUTPUT.inp',status = 'REPLACE',action =
'write',iostat = ierror)



        WRITE(iter+100,*) NNODE,NE,3,0,0
     DO I=1,NNODE
      WRITE(iter+100,900) I,X(I),Y(I),0.0D0
     END DO
     DO IE=1,NE
      WRITE(iter+100,901) IE,'1  quad',(NBOOL(NA,IE), NA=1,4)
     END DO
```

```
      WRITE(iter+100,*) 3,1,1,1
      WRITE(iter+100,*) 'uvel , _'
      WRITE(iter+100,*) 'vvel , _'
      WRITE(iter+100,*) 'density, _'
!           WRITE(16,*) 'U velocity , _'
 !     WRITE(16,*) 'V velocity , _'
!           WRITE(16,*) 'Temperature, _'

             do j=1,ly
                   do i = 1,lx
        ID=lx*(j-1)+i
       WRITE(iter+100,902) ID,u(I,j),v(I,j),rho(I,j) !,temp(i),U(i),V(i)
      END DO
             end do
  900 FORMAT(I6,3E17.8)
  901 FORMAT(I6,A10,4I6)
  902 FORMAT(I6,3E17.8)
  903 FORMAT(I6,E17.8)
           CLOSE(iter+100)


           return
           end

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!1
                   subroutine
EQUILIBRIUM(LX,LY,CD,U,V,CX,CY,RHO,KAPPA,NU,A,B,T,FEQ)
                   REAL*8 FEQ(1:LX,1:LY,0:CD)
                   REAL*8 RHO(1:LX,1:LY)
                   REAL*8 U(1:LX,1:LY),V(1:LX,1:LY),CX(0:CD),CY(0:CD)
                   REAL*8 KAPPA,NU,A,B,T
                   REAL*8 D_RHO_DX, D_RHO_DY,
LAPLACIAN,A2,A3,A1,B2,B3,C2,C3,D1,D2,D3,A0,B0,C0,D0
```

```
REAL*8 G2XX,G2YY,G2XY,G2YX,G3XX,G3YY,G3XY,G3YX
REAL*8 UX,UY,TMP,UU

do i = 1,lx
idown = i-1
iup = i + 1
if(i .eq. lx) iup = 1
if(i .eq. 1) idown = lx

do j = 1,ly
jup = j + 1
jdown = j-1
if(j .eq. ly) jup = 1
if(j .eq. 1) jdown = ly
UX = U(I,J)
UY = V(I,J)
      D_RHO_DX = 0.5D0*(RHO(IUP,J) - RHO(IDOWN,J))
      D_RHO_DY = 0.5D0*(RHO(I,JUP) - RHO(I,JDOWN))
      LAPLACIAN = RHO(IUP,J) -2.0D0*RHO(I,J)+
RHO(IDOWN,J)+ RHO(I,JUP) -2.0D0*RHO(I,J)+ RHO(I,JDOWN)
      G2XX = (KAPPA*D_RHO_DX*D_RHO_DX +
2.0D0*NU*UX*D_RHO_DX)/8.0D0
      G2YY = (KAPPA*D_RHO_DY*D_RHO_DY +
2.0D0*NU*UY*D_RHO_DY)/8.0D0
      G2XY = (KAPPA*D_RHO_DX*D_RHO_DY +
NU*UX*D_RHO_DY + NU*UY*D_RHO_DX) /8.0D0  !MODIFIED TANAKA
      G2YX = G2XY
      G1XX = 4.0D0*G2XX
      G1YY = 4.0D0*G2YY
      G1XY = 4.0D0*G2XY
      G1YX = 4.0D0*G2YX
```

```
                PO = (RHO(I,J)*T/(1.0D0-B*RHO(I,J))) -
A*RHO(I,J)*RHO(I,J)
                A2 = (1.0D0/12.0D0)*(PO-KAPPA*RHO(I,J)*LAPLACIAN-
KAPPA*(D_RHO_DX+D_RHO_DY)*(D_RHO_DX+D_RHO_DY))
                A1 = 4.0D0*A2
                A0 = RHO(I,J)-4.0D0*(A1+A2)-
3.0D0*(2.0D0*NU*(UX*D_RHO_DX+UY*D_RHO_DY)+KAPPA*(D_RHO_DX
+D_RHO_DY)*(D_RHO_DX+D_RHO_DY))/2.0D0
                B2 = RHO(I,J)/12.0D0
                B1 = 4.0D0*B2
                B0 = 0.0D0
                C2 = RHO(I,J)/8.0D0
                C1 = 4.0D0*C2
                C0 = 0.0D0
                D2 = -RHO(I,J)/24.0D0
                D1 = 4.0D0*D2                    ! MODIFIED
TANAKA
                D0 = -2.0D0*RHO(I,J)/3.0D0

                feq(i,j,0) = A0 + D0*(UX*UX+UY*UY)
                do k = 1,4
                TMP = CX(K)*UX+CY(K)*UY
                UU = UX*UX+UY*UY
                FEQ(I,J,K) = A1 + B1*TMP+C1*TMP*TMP+d1*UU +
G1XX*CX(k)*CX(k)+G1XY*CX(K)*CY(K)+G1YX*CY(k)*CX(k)++G1YY*CY(
k)*CY(k)
                end do
                do k = 5,8
                TMP = CX(K)*UX+CY(K)*UY
                UU = UX*UX+UY*UY
                FEQ(I,J,K) = A2 + B2*TMP+C2*TMP*TMP+d2*UU +
g2xx*CX(k)*CX(k)+G2XY*CX(k)*CY(k)+G2YX*CY(k)*CX(k)++G2YY*CY(k)*
CY(k)
```

```
                end do
            END DO
            END DO

            RETURN
            END

            !!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
        subroutine MACRO(lx,ly,cd,rho,f,u,v)
        real*8 F(1:LX,1:LY,0:CD)
        real*8 RHO(1:LX,1:LY),U(1:LX,1:LY),V(1:LX,1:LY)

        do i = 1,lx
            do j = 1,ly
                u(i,j) = 0.0d0
                v(i,j) = 0.0d0
            end do
        end do

        do i = 1,lx
            do j = 1,ly
                rho(i,j) =
f(i,j,1)+f(i,j,2)+f(i,j,3)+f(i,j,4)+f(i,j,5)+f(i,j,6)+f(i,j,7)+f(i,j,8)+f(i,j,0)
                u(i,j) = f(i,j,1)+f(i,j,5)+f(i,j,8)-f(i,j,3)-f(i,j,7)-f(i,j,6)
                v(i,j) = f(i,j,5)+f(i,j,6)+f(i,j,2)-f(i,j,7)-f(i,j,8)-f(i,j,4)

                u(i,j) = u(i,j)/rho(i,j)
                v(i,j) = v(i,j)/rho(i,j)
            end do
        end do

        return
        end
```

```
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
      subroutine colliDE(lx,ly,cd,f,feq,fnew,TAU)
      real*8 F(1:LX,1:LY,0:CD),FEQ(1:LX,1:LY,0:CD),FNEW(1:LX,1:LY,0:CD)
      real*8 TAU
      real*8 tfrac

      do i = 1,lx
            do j = 1,ly
            tfrac = 1.0d0/TAU
            fnew(i,j,1) = tfrac*feq(i,j,1)+(1.0d0-tfrac)*f(i,j,1)
            fnew(i,j,2) = tfrac*feq(i,j,2)+(1.0d0-tfrac)*f(i,j,2)
            fnew(i,j,3) = tfrac*feq(i,j,3)+(1.0d0-tfrac)*f(i,j,3)
            fnew(i,j,4) = tfrac*feq(i,j,4)+(1.0d0-tfrac)*f(i,j,4)
            fnew(i,j,5) = tfrac*feq(i,j,5)+(1.0d0-tfrac)*f(i,j,5)
            fnew(i,j,6) = tfrac*feq(i,j,6)+(1.0d0-tfrac)*f(i,j,6)
            fnew(i,j,7) = tfrac*feq(i,j,7)+(1.0d0-tfrac)*f(i,j,7)
            fnew(i,j,8) = tfrac*feq(i,j,8)+(1.0d0-tfrac)*f(i,j,8)
            fnew(i,j,0) = tfrac*feq(i,j,0)+(1.0d0-tfrac)*f(i,j,0)
            end do
      end do

      return
      end

!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
      subroutine move(lx,ly,cd,f,fnew)
      real*8 F(1:LX,1:LY,0:CD),FNEW(1:LX,1:LY,0:CD)

      do i = 1,lx
      idown = i-1
      iup = i + 1
      if(i .eq. lx) iup = 1
```

```
if(i .eq. 1) idown = lx

do j = 1,ly
jup = j + 1
jdown = j-1
if(j .eq. ly) jup = 1
if(j .eq. 1) jdown = ly

f(i,j,0) = fnew(i,j,0)
f(i,j,1) = fnew(idown,j,1)
f(i,j,2) = fnew(i,jdown,2)
f(i,j,3) = fnew(iup,j,3)
f(i,j,4) = fnew(i,jup,4)
f(i,j,5) = fnew(idown,jdown,5)
f(i,j,6) = fnew(iup,jdown,6)
f(i,j,7) = fnew(iup,jup,7)
f(i,j,8) = fnew(idown,jup,8)

end do
end do

return
end
```