Pressure-Driven Displacement Flow of a Non-Newtonian Fluid by a Newtonian Fluid

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in partial fulfillment of the requirements for the Degree of
MASTER OF TECHNOLOGY
in
Faculty of Engineering
by
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To my parents
DECLARATION

I declare that this written submission represents my ideas in my own words, and where ideas or words of others have been included, I have adequately cited and referenced the original sources. I also declare that I adhered to all principles of academic honesty and integrity and have not misrepresented or fabricated or falsified any idea/data/fact/source in my submission. I understand that any violation of the above will be cause for disciplinary action by the Institute and can also evoke penal action from the sources that have thus not been properly cited, or from whom proper permission has not taken when needed.

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This thesis entitled “Pressure-Driven Displacement Flow of a Non-Newtonian Fluid by a Newtonian Fluid” by Mr. Pinakinarayan A. P. Swain is approved for the degree of Master of Technology from IIT Hyderabad.

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Synopsis

The pressure-driven displacement of a non-Newtonian fluid by a Newtonian fluid in a two-dimensional channel is investigated via a multiphase lattice Boltzmann method using a non-ideal gas equation of state well-suited for two incompressible fluids. We validate the code by comparing the results obtained using different regularized models, proposed in the literature, to model the viscoplasticity of the displaced material. Then, the effects of the Bingham number, which characterises the behaviour of the yield-stress of the fluid and the flow index, which reflects the shear-thinning/thickening tendency of the fluid, are studied. We find that increasing the Bingham number and increasing the flow index increases the size of the unyielded region of the fluid in the downstream portion of the channel and the residual layer. This in turn decreases the interfacial instabilities and the speed of the propagating finger.
Refereed Publication

List of Figures

2.1 Schematic showing the geometry (not to scale) and initial flow configuration. The inlet and outlet are located at $x = 0$ and $x = L$, respectively. The aspect ratio of the channel, $L/H$, is 48. Initially the channel is filled with fluids ‘1’ and ‘2’ from $0 \leq x \leq 5$ and $5 \leq x \leq L$ of the channel, respectively. 5

2.2 $D2Q9$ model 6

3.1 Contours of the index function, $\phi$ for different mesh densities: (a) $3168 \times 66$, (b) $4704 \times 98$, (c) $6240 \times 130$. The rest of the parameters are $Re = 100$, $At = 0.2$, $Ri = 0.1$, $m = 2$, $\kappa = 0$, $Bn = 10$ and $n = 1.1$. The inset at the bottom represents the enlarged view of the contours at $t = 30$ obtained using $6240 \times 130$ grid. 14

3.2 (a) Temporal variation of volume fraction of the displaced fluid ($M_t/M_0$), (b) the average residual thickness of the bottom layer, $\bar{h}$, obtained using different mesh densities. The rest of the parameters are $Re = 100$, $At = 0.2$, $Ri = 0.1$, $m = 2$, $\kappa = 0$, $Bn = 10$ and $n = 1.1$. The dotted line in panel (a) represents the analytical solution of the plug-flow displacement given by $M_t/M_0 = 1 - tH/L$. 15

3.3 The effects of viscosity regularization parameter ($\epsilon$) on the spatio-temporal evolution of the $\phi$ contours obtained using the simple model: (a) $\epsilon = 10^{-6}$, (b) $\epsilon = 10^{-9}$ and (c) $\epsilon = 10^{-12}$. The rest of the parameter values are $Re = 100$, $Ri = 1$, $At = 0.2$, $m = 2$, $\kappa = 0.0075$, $Bn = 30$ and $n = 1.1$. 16

3.4 Spatio-temporal evolution of $\phi$ contours obtained using the (a) simple, (b) Bercovier and Engleman’s, and (c) Papanastasiou’s model. The rest of the parameter values are $Re = 100$, $Ri = 0.5$, $At = 0.2$, $m = 2$, $\kappa = 0.0075$, $Bn = 30$ and $n = 1.1$. 18

3.5 Spatio-temporal evolution of the unyielded domains obtained, shown in black, using (a) simple model, (b) Bercovier and Engleman’s model and (c) Papanastasiou’s model. The rest of the parameter values are the same as those used to generate Fig. 3.4. The insets at the bottom represent the corresponding enlarged view of the region shown by rectangles. 19
3.6 Contours of the index function, \( \phi \) for (a) \( Bn = 0 \), (b) \( Bn = 20 \), (c) \( Bn = 50 \) and (d) \( Bn = 100 \) at \( t = 20 \) and \( t = 30 \). The rest of the parameters are \( Re = 100 \), \( At = 0.2 \), \( Ri = 1 \), \( \kappa = 0.0075 \), \( m = 2 \) and \( n = 1 \).

3.7 Unyielded domains, shown in black, for \( Bn = 50 \) at \( t = 20 \) and \( t = 30 \). The rest of the parameters are values are the same as those used in Fig. 3.6.

3.8 (a) Temporal variation of volume fraction of the displaced fluid \( (M_t/M_0) \), (b) the rate of displacement, \( (M_t/M_0)' \), and (c) the average residual thickness of the bottom layer, \( \bar{h} \), for different values of \( Bn \). Here \( (') \) represents the the derivative with respect to time. The rest of the parameters values are the same as those used in Fig. 3.6.

3.9 Contours of the index function, \( \phi \) (top), and unyielded surface (bottom) for (a) \( n = 0.7 \), (b) \( n = 1 \) and (c) \( n = 1.3 \) at \( t = 20 \) and \( t = 30 \). The rest of the parameters are \( Re = 100 \), \( At = 0.2 \), \( Ri = 1 \), \( \kappa = 0.0075 \), \( m = 2 \) and \( Bn = 30 \).

3.10 (a) The rate of displacement, \( (M_t/M_0)' \), and (b) the average residual thickness of the bottom layer, \( \bar{h} \), for different values of \( n \). Here \( (') \) represents the the derivative with respect to time. The rest of the parameters values are the same as those used in Fig. 3.9.
Contents

Acknowledgements v

Synopsis vii

List of Figures xii

1 Introduction 1
  1.1 Miscible systems .................................................. 1
  1.2 Displacement of non-Newtonian fluids ........................... 2
  1.3 Immiscible systems ................................................ 2
  1.4 Buoyancy-driven flows ............................................ 3
  1.5 Present study ...................................................... 3
    1.5.1 GPU implementation .......................................... 4

2 Formulation 5
  2.1 Numerical method .................................................. 5
    2.1.1 D2Q9 model .................................................... 6
    2.1.2 Equilibrium distribution functions ........................... 7
    2.1.3 Calculation of variables ..................................... 7
    2.1.4 Carnahan-Starling equation of state ........................ 8
    2.1.5 Non-Newtonian fluid model .................................. 8
    2.1.6 Calculation of body and surface forces ...................... 8
2.2 Boundary conditions .......................................................... 9
2.3 Dimensionless numbers ...................................................... 11

3 Results and discussion .......................................................... 13
3.1 Grid convergence test ......................................................... 13
3.2 Effects of viscosity regularization parameter, \( \epsilon \) ................. 16
3.3 Effects of viscosity regularized models .................................. 17
3.4 Effects of \( Bn \) ................................................................. 20
3.5 Effects of \( n \) ................................................................. 23

4 Conclusions ....................................................................... 25

Appendices ............................................................................. 27

I Navier-Stokes equation from the Boltzmann equation ............ 27
   A Maxwell-Boltzmann equilibrium distribution function and some important identities ................................. 27
      A.1 Proof of Eq. (I.2) ......................................................... 28
      A.2 Proof of Eq. (I.3) ......................................................... 28
      A.3 Proof of Eq. (I.4) ......................................................... 29
      A.4 Proof of Eq. (I.5) ......................................................... 31
      A.5 Proof of Eq. (I.6) ......................................................... 31
   B Moments of Maxwell-Boltzmann equilibrium distribution function ......................................................... 33
      B.1 Zeroth moment of equilibrium distribution function .......... 33
      B.2 First moment of equilibrium distribution function ............ 33
      B.3 Second moment of equilibrium distribution function ........ 34
      B.4 Third moment of equilibrium distribution function .......... 34
   C Conservation of mass ........................................................ 35
   D Conservation of momentum .............................................. 36

xv
CHAPTER 1

Introduction

Pressure-driven displacement flows of one fluid by another having different fluid properties are common in many industrial processes, such as enhanced oil recovery [Taghavi et al. (2012)], the transportation of crude oil in pipelines [Joseph et al. (1997)], fixed bed regeneration, hydrology and filtration. In food processing industries, cleaning also involves the removal of highly viscous material from conduits via displacement by water streams. In flow through porous media or in Hele-Shaw cells, the displacement of a highly viscous fluid by a less viscous one is accompanied by viscous fingering [Homsky (1987)]. Thus achieving fundamental understanding of these flows became an active research area for decades [Govindarajan & Sahu (2013)].

The dynamics of displacement flows have been investigated both numerically and experimentally by several authors by considering miscible [Chen & Meiburg (1996); Goyal & Meiburg (2006); Mishra et al. (2012); Petitjeans & Maxworthy (1996); Rakotomalala et al. (1997); Sahu et al. (2009b); Taghavi et al. (2009, 2011)] as well as immiscible fluids [Chin et al. (2002); Dong et al. (2010); Grosfils et al. (2004); Joseph et al. (1984); Kang et al. (2004); Redapangu et al. (2012a)]. It is well known that the displacement flow is always stable when the invading fluid is more viscous than the resident fluid [Joseph et al. (1997)]. When the displacing fluid is less viscous, the flow becomes unstable and “roll-up” structures (in miscible flows [Sahu et al. (2009a); Taghavi et al. (2012)]) and sawtooth structures (in immiscible flows, [Redapangu et al. (2012a)]) appear at the interface separating the fluids. The linear instability in the three-layer/core-annular flow, which can be obtained when the elongated “finger” of the less viscous fluid penetrates into the bulk of the more viscous one, was also studied in immiscible [Sahu & Matar (2010); Yiantsios & Higgins (1988); Yih (1967)] and miscible [Govindarajan (2004); Malik & Hooper (2005); Sahu et al. (2009a); Sahu & Govindarajan (2011); Selvam et al. (2007)] systems.

1.1 Miscible systems

In a Hele-Shaw cell, Goyal & Meiburg (2006) studied numerically the miscible displacement flow of a highly viscosity fluid by a less viscous one. They observed that the two-dimensional instability patterns become three-dimensional at higher flow rates. The flow field obtained in their simulation was qualitatively similar to that observed in the experiment of Petitjeans & Maxworthy (1996) and the theoretical predictions of Lajeunesse et al. (1999). In the context of enhanced-oil recovery, Taghavi et al. (2009, 2011) studied experimentally the displacement flow of two miscible fluids and observed Kelvin-Helmholtz like instabilities at low imposed velocities in the exchange flow dominated regime. Sahu et al. (2009b) investigated the effects
of Reynolds number, Schmidt number, Froude number and angle of inclination in the pressure-driven flow of two miscible liquids of different densities and viscosities in an inclined channel. The behaviour of an infinitesimally small disturbance in such flows was also investigated by Sahu et al. (2009a) via a linear stability analysis.

The work discussed above considered only Newtonian fluids. In literature, to the best of our knowledge, very few studies has been carried out which investigated the displacement flow of viscoplastic materials. Below, we briefly review the previous work which studied the displacement flow of a non-Newtonian fluid by another Newtonian/non-Newtonian fluid.

1.2 Displacement of non-Newtonian fluids

Dimakopoulos & Tsamopoulos (2003) studied the displacement of a viscoplastic material by air in straight and suddenly constricted tubes. They have shown that unyielded material arises in front of the air bubble and in the case of a constricted tube, near the recirculation corner. Papaoannou et al. (2009), on the other hand, have studied the displacement of air by a viscoplastic fluid and revealed the conditions for the detachment of the viscoplastic material from the solid wall. Allouche et al. (2000) and Wielage-Burchard & Frigaard (2011) studied the displacement flow of Bingham fluid by another fluid in a plane channel. As the finger penetrates inside the channel a static residual layer of the displaced fluid is left behind the finger. They investigated the thickness of this residual layer for different Bingham numbers and compared their results with those obtained using the lubrication approximation. It is a difficult task to handle the viscoplastic behaviour of the fluid numerically as the problem becomes singular in the flow region of zero strain-rate. The complexity in using the discontinuous Bingham model increases because the yield surface is not known a priori but must be determined as part of the solution. Generally viscosity regularisation methods are used in order to overcome this difficulty. Frigaard & Nouar (2005) studied the effects of different viscosity regularisation models, such as the simple model [Allouche et al. (2000)], the Bercovier and Engleman model [Bercovier & Engleman (1980)] and the Papanastasiou model [Papanastasiou (1987)] on the flow dynamics and found that the latter model performs better than the other two models.

1.3 Immiscible systems

Most of the numerical studies in the above review are for miscible systems, but few computational studies have been carried out on immiscible systems. Numerical simulation of immiscible systems are expensive computationally due to the presence of sharp interfacial dynamics. During the past few decades, lattice Boltzmann method (LBM) has emerged as a promising alternative technique for multiphase flow simulations [Chen & Doolen (1998)]. Based on the class of problem of interest, researchers have been using different LBM approaches for multiphase flows, mainly, the color segregation method [Gunstensen et al. (1991)], method of Shan and Chen [Shan & Chen (1993)], the free energy approach [Swift et al. (1995)] and the method
of He and co-workers [He et al. (1999a,b); Zhang et al. (2000)]. Using the method of Shan & Chen (1993), the displacement flow of two immiscible liquids have been studied by several researchers [Chin et al. (2002); Dong et al. (2010); Grosfils et al. (2004); Kang et al. (2004)]. The Reynolds number considered in these studies are very low, thus they did not observe any interfacial instabilities. Recently, Redapangu et al. (2012a) investigated the displacement flow of two immiscible Newtonian liquids at moderate Reynolds number using the method of Zhang et al. (2000). They investigated the effects of the Atwood number, viscosity ratio, and angle of inclination on the flow dynamics and observed sawtooth-type waves at the interface separating the liquids.

1.4 Buoyancy-driven flows

Sahu & Vanka (2011) studied the buoyancy driven mixing of two immiscible, incompressible, Newtonian fluids having different densities but same dynamic viscosity, in a two dimensional inclined channel. The multiphase LBM algorithm proposed by He and co-workers [He et al. (1999a,b); Zhang et al. (2000)] was used as the numerical method. The code was first validated by simulating Rayleigh-Taylor instability in unstably stratified flows. The effects of various parameters like Reynolds number, tilt angle, Atwood number, surface tension on the front dynamics and inter-penetration of two fluids were investigated. The results were compared with those obtained using a home-made finite volume code and very good agreements were reported. Redapangu et al. (2012b) investigated the effect of viscosity contrast on the flow dynamics in a similar system using the same code developed by Sahu & Vanka (2011). The effect of viscosity ratio was studied in terms of the flow dynamics, average density profiles and front velocities of the inter-penetrating fluids. It was observed that as the viscosity ratio increases the flow becomes more and more coherent and at very high viscosity ratio, two fingers of individual poiseuille flows moving in opposite directions were observed. Transverse inter-penetration and interfacial instabilities were found to be more prominent at lower values of viscosity ratio. Redapangu & Sahu (2013) extended the above study to three-dimension, and studied the lock exchange problem using the three dimensional version of the code developed by Sahu & Vanka (2011) by implementing multiphase lattice Boltzmann algorithm on a graphics processing unit. The authors found that the three dimensional simulation gives more coherent instabilities and longer finger of inter-penetration, as compared to the two dimensional simulation.

1.5 Present study

In spite of the large number of studies carried out on displacement flows, to the best of our knowledge, none of them have examined the pressure-driven displacement flow of immiscible non-Newtonian fluids at higher Reynolds number, which is the subject of the present study. As Frigaard and co-workers were interested in investigating the mud removal in the primary cementing of oil-gas well bore, they considered low Reynolds number in their studies. In the present work, we study the pressure-driven displacement flow of two immiscible liquids of
different densities and viscosities using a multiphase lattice Boltzmann method [Sahu & Vanka (2011); Zhang et al. (2000)]. In order to achieve high computational efficiency, we implemented our LBM algorithm on a graphics processing unit (GPU) [Vanka et al. (2011)]. Our present GPU based double precision LBM solver is 12-times faster than a corresponding CPU based code on a single core. The GPU implementation of the LBM code is discussed next.

1.5.1 GPU implementation

The use of GPU to solve complex computational problem has emerged as a popular method in recent times. This is because of the high performance computing and low power consumption of GPU. Lattice Boltzmann method is easy to implement on a GPU because of its inherent parallelizability. Parallel computing in GPU is achieved by multiple threads, each with an unique thread index. The instructions to GPU are written in a ‘kernel’ which is like a function in C programming. When a ‘kernel’ is executed in a GPU, each of the thread executes the statements written inside the kernel, where each thread points to a different data element. This results in simultaneous updating of all the data elements as compared to the one-by-one updating in ‘for’ loops. The ‘threads’ constitute the ‘block’ and the ‘blocks’ constitute the ‘grid’. The number of threads per block and the number of block per grid has to be explicitly specified by the programmer.

In addition to the architectural improvements, increased memory bandwidth in case of GPU positively affect its performance. Usually, the ‘main’ program is executed in CPU and GPU is utilized by calling the kernels from the main program. So, GPU acts as a co-processor to the CPU. Apart from the conventional programming languages like C/C++ or FORTRAN, GPU is implemented on special programming languages which provide parallel programming platform. We are using CUDA (Compute Unified device Architecture), a parallel programming model developed by Nvidia Corporation. Cuda assumes CPU as the ‘host’ and GPU as the ‘device’. Both the ‘host’ and the ‘device’ maintain their individual memory and CUDA allows data to be transferred from the host to the device and vice versa. However, in order to get maximum speed up, the number of copies from host to device and device to host needs to be minimized. The overall efficiency also depends on the block size and the grid size. More information on this part can be found in Vanka et al. (2011).
CHAPTER 2

Formulation

We consider the pressure-driven displacement of a viscoplastic, incompressible fluid of viscosity $\mu_2$ and density $\rho_2$ (fluid ‘2’) initially filled inside a horizontal two-dimensional channel. A Newtonian fluid (fluid ‘1’) of viscosity $\mu_1$ and density $\rho_1$ is injected from the inlet through an imposed pressure-gradient, as shown in Fig. 2.1. A rectangular coordinate system ($x, y$) is used to model the flow dynamics, where $x$ and $y$ denote the coordinates in the horizontal and the wall-normal directions, respectively. The channel inlet and outlet are located at $x = 0$ and $L$, respectively. The rigid and impermeable walls of the channel are located at $y = 0$ and $H$, respectively. The aspect ratio of the channel, $L/H$, is 48. $g$ is the acceleration due to gravity acting in the negative $y$-direction.

Figure 2.1: Schematic showing the geometry (not to scale) and initial flow configuration. The inlet and outlet are located at $x = 0$ and $x = L$, respectively. The aspect ratio of the channel, $L/H$, is 48. Initially the channel is filled with fluids ‘1’ and ‘2’ from $0 \leq x \leq 5$ and $5 \leq x \leq L$ of the channel, respectively.

2.1 Numerical method

The two-phase lattice Boltzmann method used in the present study is similar to that of He and co-workers [He et al. (1999a,b); Zhang et al. (2000)]. Previously, Sahu & Vanka (2011) modified this approach in order to account for unequal dynamic viscosity of the fluids and studied buoyancy-driven flow in an inclined channel. Recently, Redapangu et al. (2012a) studied pressure-driven displacement flow of Newtonian fluids using the same approach. The methodology is briefly described below.

Two evolution equations for the index distribution function ($f$) and the pressure distribution function ($g$) are given by:

$$
f_{\alpha}(x + e_\alpha \delta t, t + \delta t) - f_{\alpha}(x, t) = -\frac{f_{\alpha}(x, t) - f^eq_{\alpha}(x, t)}{\tau} - \frac{2\tau - 1}{2\tau} \frac{\mathbf{e}_\alpha - \mathbf{u}}{c_s^2} \cdot \nabla \psi(\phi) \Gamma_{\alpha}(\mathbf{u}) \delta t,
$$

$$
g_{\alpha}(x + e_\alpha \delta t, t + \delta t) - g_{\alpha}(x, t) = -\frac{g_{\alpha}(x, t) - g^eq_{\alpha}(x, t)}{\tau}
$$
where
\[ \tau = \frac{1}{2} \left( e_{av} - u \right) \cdot \left[ \Gamma_{\alpha}(u)(F_s + G) - (\Gamma_{\alpha}(u) - \Gamma_{\alpha}(0)) \nabla (p - c_s^2 \rho) \right] \delta t, \]  
(2.2)

and
\[ \Gamma_{\alpha}(u) = t_{\alpha} \left[ 1 + \frac{e_{av} \cdot u}{c_s^2} + \frac{(e_{av} \cdot u)^2}{2c_s^4} - \frac{u^2}{2c_s^2} \right]. \]  
(2.3)

Here \( u = (u, v) \) represents the two-dimensional velocity field; \( u \) and \( v \) denote velocity components in the \( x \) and \( y \) directions, respectively; \( \delta t \) is the time step; \( \tau \) is the single relaxation time using the Bhatnagar-Gross-Krook (BGK) model [Bhatnagar et al. (1954)]. The kinematic viscosity, \( \nu \) is related to the relaxation time as \( \nu = \frac{\tau - 1/2}{2 \tau} \delta t c_s^2 \), where \( c_s^2 = 1/3 \).

### 2.1.1 D2Q9 model

In LBM, we have to choose a discretized velocity model as per our requirement. In literature, the lattice models are commonly designated as \( D_{nQm} \) model, where \( n \) denotes the space dimension and \( m \) denotes the number of possible velocity direction. \( D_{2Q7}, D_{2Q9}, D_{3Q15}, D_{3Q19} \) and \( D_{3Q27} \) are some commonly used models available in the literature. The lattice model restricts the fluid molecules to move in certain specified directions. At each time, the distribution function at one node move to the neighboring node, along which it has the direction of velocity. If two distribution functions arrive at the same point, then they are redistributed as per the collision rules, so as to conserve mass and momentum. The speed of sound in the lattice and the weights in the equilibrium distribution functions are the lattice dependent quantities.

![D2Q9 model](image)

**Figure 2.2:** D2Q9 model

In this present simulation, the evolution equations are simulated with a two-dimensional nine-velocity model (\( D_{2Q9} \)), where

\[ e_{av} = \begin{cases} 0, & \alpha = 0 \\ \cos \left( \frac{\alpha - 1}{2} \pi \right), \sin \left( \frac{\alpha - 1}{2} \pi \right), & \alpha = 1, 2, 3, 4 \\ \sqrt{2} \cos \left( \frac{\alpha - 5}{2} \pi + \frac{\pi}{4} \right), \sin \left( \frac{\alpha - 5}{2} \pi + \frac{\pi}{4} \right), & \alpha = 5, 6, 7, 8. \end{cases} \]  
(2.4)
2.1 Numerical method

The weighing coefficients, $t_\alpha$ are given by:

$$t_\alpha = \begin{cases} 
4/9, & \alpha = 0 \\
1/9, & \alpha = 1, 2, 3, 4 \\
1/36, & \alpha = 5, 6, 7, 8.
\end{cases} \quad (2.5)$$

Here $\alpha$ is the position of the node in the lattice.

2.1.2 Equilibrium distribution functions

The equilibrium distribution functions, $f^{eq}_\alpha$ and $g^{eq}_\alpha$ are given by

$$f^{eq}_\alpha = t_\alpha \left[ 1 + \frac{e_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(e_\alpha \cdot \mathbf{u})^2 - u^2}{2c_s^2} \right] \quad \text{and}$$

$$g^{eq}_\alpha = t_\alpha \left[ p + \rho c_s^2 \left( \frac{e_\alpha \cdot \mathbf{u}}{c_s^2} + \frac{(e_\alpha \cdot \mathbf{u})^2 - u^2}{2c_s^2} \right) \right], \quad (2.7)$$

The index function ($\phi$), pressure ($p$) and velocity field ($\mathbf{u}$) are calculated using:

$$\phi = \sum f_\alpha, \quad (2.8)$$

$$p = \sum g_\alpha - \frac{1}{2} \mathbf{u} \cdot \nabla \psi(\rho) \delta t, \quad (2.9)$$

$$\rho \mathbf{u} c_s^2 = \sum e_\alpha g_\alpha + \frac{c_s^2}{2} (\mathbf{F}_s + \mathbf{G}) \delta t. \quad (2.10)$$

2.1.3 Calculation of variables

The fluid density and kinematic viscosity are calculated from the index function as:

$$\rho(\phi) = \rho_1 + \frac{\phi - \phi_1}{\phi_2 - \phi_1} (\rho_2 - \rho_1), \quad (2.11)$$

$$\nu(\phi) = \nu_1 \exp \left[ \frac{\phi - \phi_1}{\phi_2 - \phi_1} \ln \left( \frac{\nu_2}{\nu_1} \right) \right], \quad (2.12)$$

where $\nu_1$ and $\nu_2$ are the kinematic viscosities of fluid ‘1’ and ‘2’, respectively. $\phi_1$ and $\phi_2$ are minimum and maximum values of the index function; in the present study $\phi_1$ and $\phi_2$ are given values of 0.02381 and 0.2508, respectively [Zhang et al. (2000)].
2.1.4 Carnahan-Starling equation of state

We use the following expression of $\psi(\phi)$ using the Carnahan-Starling fluid equation of state which describes the process of phase separation for non-ideal gases and fluids [Carnahan & Starling (1969); Chang & Alexander (2006); Fakhari & Rahimian (2009, 2010); Premnath & Abraham (2005)]:

$$
\psi(\phi) = c^2 \phi \left[ \frac{1 + \phi + \phi^2 - \phi^3}{(1 - \phi)^3} - 1 \right] - a \phi^2, 
$$

(2.13)

where $a$ determines the strength of molecular interactions. The critical value of Carnahan-Starling equation of state, $a_c = 3.53374$. If $a > a_c$ both the fluids will remain immiscible. Thus $a$ is chosen to be 4 in the present study [Zhang et al. (2000)]. The gradient of $\psi(\phi)$ describe the physical intermolecular interactions for non-ideal gases or dense fluids. This term plays a key role in separating the phases. A fourth order compact scheme is used to discretize $\nabla \psi$ [Lee & Lin (2005)].

2.1.5 Non-Newtonian fluid model

We use the Herschel-Bulkley model in order to describe the flow of the viscoplastic material, which is being displaced by a Newtonian fluid injected at the inlet of the channel. There are three commonly used regularized non-Newtonian fluid models available in the literature [Frigaard & Nouar (2005)], which are given by:

$$
\mu_2 = \mu_0 (\Pi + \epsilon)^{n-1} + \frac{\tau_0}{\Pi + \epsilon}, 
$$

(2.14)

$$
\mu_2 = \mu_0 (\Pi + \epsilon)^{n-1} + \frac{\tau_0}{\sqrt{\Pi^2 + \epsilon^2}}, 
$$

(2.15)

$$
\mu_2 = \mu_0 (\Pi + \epsilon)^{n-1} + \tau_0 \left( \frac{1 - e^{-N\Pi}}{\Pi} \right), 
$$

(2.16)

where $\tau_0$ is the yield shear stress; $\Pi \equiv (2E_{ij}E_{ij})^{1/2}$ represents the second invariant of the strain-rate tensor, $E_{ij} = \frac{1}{2} (\partial u_i/\partial x_j + \partial u_j/\partial x_i)$; $n$ is the power-law flow index of the fluid. $\mu_0$ is the flow consistency index (this is same as the viscosity of fluid 2 when $\tau_0 = 0$ and $n = 1$). $N$ is the stress growth exponent and for $n = 1$ it is equivalent to $\epsilon^{-1}$. We will refer to eqs. (2.14), (2.15) and (2.16) as the simple regularized viscosity model [Allouche et al. (2000)], Bercovier & Engleman (1980) model and Papanastasiou (1987) model, respectively.

2.1.6 Calculation of body and surface forces

The surface tension force ($F_s$) and gravity forces ($G$) are given by

$$
F_s = \kappa \phi \nabla \nabla^2 \phi, \quad \text{and} \quad G = (\rho - \rho_m)g, 
$$

(2.17)
2.2 Boundary conditions

where \( \kappa \) is the magnitude of surface tension and \( \rho_m \equiv (\rho_1 + \rho_2)/2 \). The surface tension, \( \sigma \) can be related to \( \kappa \) as follows Evans (1979):

\[
\sigma = \kappa \int \left( \frac{\partial \phi}{\partial \zeta} \right)^2 d\zeta,
\]

(2.18)

where \( \zeta \) is the direction normal to the interface [Zhang et al. (2000)].

2.2 Boundary conditions

Accurate implementation of boundary conditions is an important issue associated with LBM. In LBM, we have to implement the boundary conditions in terms of the distribution functions. While it is easier to find the macroscopic flow variables from the distribution functions, the reverse is not so easy. Many heuristic approaches were adopted to impose the boundary conditions. The bounce-back scheme was the first of all. It is inspired from LGCA and is easy to implement. However, it is of first order in numerical accuracy. Since the LBE governing equations are second order accurate, the bounce-back scheme degrades the solution near the boundaries. In addition to this, it gives a non-zero slip velocity at the wall, even when we are trying to impose the no-slip boundary condition. To address these issues, improved alternatives like, half-way bounce-back scheme [Zeigler (1993)], hydrodynamic boundary condition [Noble et al. (1995)], extrapolation scheme [Chen et al. (1996)], non-equilibrium bounce back scheme [Zou & He (1997)], hydrodynamic boundary condition along with extrapolation of non-equilibrium values [Guo et al. (2002)], were subsequently proposed.

Zeigler (1993) proposed two alternatives to overcome this problem. First one was to keep the physical wall half-way between the first and second row of nodes and apply usual bounce-back scheme at the first row. However, the author mentioned that, in general, this method does not carry accurate gradient information. For, Couette flow, where velocity gradient is constant, it is completely accurate and for Poiseuille flow, where the gradient is changing, the second order errors still remain. In the second alternative, he proposed to keep the wall coinciding with the first row and use the symmetry to ensure zero normal and zero tangential velocity. The collision operator is applied at both the fluid and wall nodes. Noble et al. (1995) proposed to use the no-slip condition itself to find the missing particle distributions. The most straight-forward hydrodynamic boundary condition is the equilibrium condition at the walls. Streaming components are not used and all the particle distribution functions are set to their equilibrium values. Equilibrium values can be obtained by using velocity and density values at the walls. Chen et al. (1996) introduced the idea of extrapolation scheme in which an imaginary layer of nodes is placed inside the wall and standard finite difference schemes are used to update distribution function at the fictitious nodes. Zou & He (1997) suggested to use the local conservation of mass and momentum to find the missing particle distribution functions at the wall. To eliminate additional unknowns in the equations they proposed to use the bounce-back scheme only for the non-equilibrium part of the distribution function normal to the wall. Guo et al. (2002) extended the extrapolated scheme [Chen et al. (1996)] for a curved boundary. They proposed only to
extrapolate the non-equilibrium part of the interior node and approximate the equilibrium part by using the velocity and density values at the wall nodes.

In this present work, the hydrodynamic boundary conditions based on the ghost-fluid approach are used to simulate the boundaries and equilibrium distribution functions [Sahu & Vanka (2011)]. A Neumann boundary condition for pressure is used at the outlet, while the constant volumetric flow rate condition is imposed at the inlet. In addition, the non-equilibrium distribution functions are extrapolated and added to get the instantaneous distribution functions. Specifically, the boundary conditions are implemented as follows.

**Index function** \( \phi \): We use second-order accurate zero derivative condition by placing the wall boundary condition between lattice points. This implies:

\[
\phi_{1,j} = \phi_{2,j}, \quad j = 1, ny; \quad \phi_{nx,j} = \phi_{nx-1,j}, \quad j = 1, ny, \quad (2.19)
\]

\[
\phi_{i,1} = \phi_{i,2}, \quad i = 1, nx; \quad \phi_{i,ny} = \phi_{i,ny-1}, \quad i = 1, nx, \quad (2.20)
\]

where \( nx \) and \( ny \) are number of lattice points in the x and y directions, respectively.

**Velocities:** Velocities are mirror reflected to impose no slip and no penetration conditions. Thus,

\[
u_{1,j} = 2u_w - u_{2,j}; \quad u_{nx,j} = 2u_w - u_{nx-1,j}; \quad (2.21)
\]

\[
v_{1,j} = 2v_w - v_{2,j}; \quad v_{nx,j} = 2v_w - v_{nx-1,j}; \quad \text{etc.} \quad (2.22)
\]

where \( u_w \) and \( v_w \) are the axial and transverse velocity components of the walls; in the present study \( u_w = v_w = 0 \).

**Index distribution function** \( f \):

\[
f = f^{eq} + f^{neq}, \quad (2.23)
\]

\[
f_{1,j} = f_{1,j}^{eq} + f_{2,j}^{neq}, \quad f_{nx,j} = f_{nx,j}^{eq} + f_{nx-1,j}^{neq}, \quad (2.24)
\]

\[
f_{i,1} = f_{i,1}^{eq} + f_{i,2}^{neq}, \quad f_{i,ny} = f_{i,ny}^{eq} + f_{i,ny-1}^{neq}, \quad (2.25)
\]

**Pressure and pressure function** \( g \): Pressure is extrapolated with zero derivative boundary condition. Thus at walls, we use

\[
p_{1,j} = p_{2,j}; \quad p_{nx,j} = p_{nx-1,j}, \quad (2.26)
\]

\[
p_{1,j} = p_{2,j}; \quad p_{nx,j} = p_{nx-1,j}. \quad (2.27)
\]

This pressure is used to evaluate the equilibrium \( g \) value. However, in the expression for the equilibrium \( g \) function, the velocity at the grid node is taken to be zero instead of the ghost value. The equilibrium value is added to the extrapolated non-equilibrium value to get the final value of \( g \) that is streamed inside.

**Density and \( \psi \):** The density is evaluated from the value of \( \phi \), which is extrapolated with zero derivative condition. The value of \( \psi(\equiv p - \rho RT) \) is evaluated at all the lattice points including
2.3 Dimensionless numbers

The various dimensionless parameters describing the flow characteristics are the Atwood number, $At = (\rho_2 - \rho_1)/(\rho_2 + \rho_1)$, the Reynolds number, $Re = Q\rho_1/\mu_1$, the Bingham number, $Bn = \tau_0 H^2/\mu_1 Q$, the Richardson number, $Ri = gH^3/Q^2$ and the viscosity ratio, $m = \mu_0/\mu_1$. Here, $Q$ is the total flow rate per unit length in the spanwise direction. The dimensionless time is defined as $t = H^2/Q$. To accelerate the computational efficiency, the algorithm is implemented on a Graphics Processing Unit (GPU). Our GPU based multiphase lattice Boltzmann solver using the double-precision variable provides a speed-up factor of 12 as compared to a corresponding CPU based solver [Redapangu & Sahu (2013)].
CHAPTER 3

Results and discussion

In this chapter, the results obtained from the LBM simulations are presented.

3.1 Grid convergence test

We begin presenting our results by conducting a grid convergence test. In Fig. 3.1(a), (b) and (c), the spatio-temporal evolution of the contours of the index function, $\phi$ are shown for grids $3168 \times 66$, $4704 \times 98$ and $6240 \times 130$, respectively, for $Re = 100$, $At = 0.2$, $Ri = 0.1$, $m = 2$, $\kappa = 0$, $Bn = 10$ and $n = 1.1$. The simple regularized viscosity model is used to generate this plot. The parameter values used in generating this figure correspond to a situation where a highly viscous, denser non-Newtonian fluid (fluid ‘2’) is displaced by a lighter, Newtonian fluid of lower viscosity (fluid ‘1’). In this case, we would expect the flow to be destabilized because of the viscosity contrast and via a Rayleigh-Taylor (RT) instability. It can be seen that due to the imposed pressure-gradient a ‘finger’ of the less viscous lighter fluid penetrates into the bulk of the more viscous, denser fluid. The ‘finger’ is symmetrical at early times, but becomes asymmetrical at later times due to the gravity force acting in the vertically downward direction. The instabilities of sawtooth-like shape appear at the interface separating the fluids. The interfacial waves resulting from the instabilities at the downstream portion of the channel (obtained using $6240 \times 130$ grid at $t = 50$) are shown as the inset at the bottom of Fig. 3.1. The flow dynamics obtained using the different grids look qualitatively similar with some minor quantitative variations magnifying themselves upon mesh-refinement.
Figure 3.1: Contours of the index function, $\phi$ for different mesh densities: (a) $3168 \times 66$, (b) $4704 \times 98$, (c) $6240 \times 130$. The rest of the parameters are $Re = 100$, $At = 0.2$, $Ri = 0.1$, $m = 2$, $\kappa = 0$, $Bn = 10$ and $n = 1.1$. The inset at the bottom represents the enlarged view of the contours at $t = 30$ obtained using $6240 \times 130$ grid.
3.1 Grid convergence test

Figure 3.2: (a) Temporal variation of volume fraction of the displaced fluid ($M_t/M_0$), (b) the average residual thickness of the bottom layer, $\bar{h}$, obtained using different mesh densities. The rest of the parameters are $Re = 100$, $At = 0.2$, $Ri = 0.1$, $m = 2$, $\kappa = 0$, $Bn = 10$ and $n = 1.1$. The dotted line in panel (a) represents the analytical solution of the plug-flow displacement given by $M_t/M_0 = 1 - tH/L$.

In Fig. 3.2(a) and (b), we plot the temporal variation of the dimensionless volume of fluid ‘2’, $M_t/M_0$, and the average residual thickness of the bottom layer, $\bar{h}$ for the parameter values the same as those used to generate Fig. 3.1. Here, $M_t = \int_0^L \int_0^H \frac{\phi - \phi_1}{\phi_2 - \phi_1} dxdy$, $M_0$ denotes the volume of fluid ‘2’ initially occupying the channel ($M_0 = \frac{\phi - \phi_1}{\phi_2 - \phi_1} LH$), and $\bar{h} = \frac{1}{x_l - x_t} \int_{x_l}^{x_t} \int_0^{H/2} \frac{\phi - \phi_1}{\phi_2 - \phi_1} dxdy$, where $x_l$ and $x_t$ are the position of the leading and trailing edges of the finger, respectively. It can be seen in Fig. 3.2(a) that $M_t/M_0$ undergoes an almost linear decrease at the earlier stages ($t < 32$) of the flow due the displacement of fluid ‘2’ by fluid ‘1’. It can be observed that slope of $M_t/M_0$ versus time plot is steeper than that of the plug flow line, given by $M_t/M_0 = 1 - tH/L$ (shown by the dotted line in Fig. 3.2(a)). At approximately $t = 32$ for this set of parameters a transition to another linear regime occurs. The slope of the $M_t/M_0$ versus time plot in this regime is much smaller than the previous one, which signifies a slower displacement process. This is due to the increase in the removal time of the residual layer which remains adjacent to the walls after the ‘finger’ has exited the simulation domain. However, for high Bingham number cases the results in the later stage (once the finger exited the simulation domain) becomes doubtful; thus we do not present the results at the later stages for higher Bingham number. However in this paper, we mainly concentrate on the flow dynamics at the early stages, i.e before the finger crossed the simulation domain. It can be seen in Fig. 3.2(b) that the height of the residual bottom layer remains almost constant till $t < 32$, then it decreases linearly for this set of parameter values. The thickness of this residual layer, and the removal time, was also previously studied by Frigaard and co-workers [Allouche et al. (2000); Wielage-Burchard & Frigaard (2011)] for low Reynolds number flows. Inspection of Fig. 3.2 also reveals that the difference in the results obtained using $4704 \times 98$ and $6240 \times 130$ are very small. Thus we use $6240 \times 130$ grid for generating all the rest of the results presented in this work.
3.2 Effects of viscosity regularization parameter, $\epsilon$

Next, we investigate the effects of viscosity regularization parameter ($\epsilon$) in the simple viscosity regularized model (given by Eq. 2.14) on the flow dynamics by plotting the spatio-temporal evolution of the $\phi$ contours for different values of $\epsilon$. The rest of the parameter values are $Re = 100$, $Ri = 1$, $At = 0.2$, $m = 2$, $\kappa = 0.0075$, $Bn = 30$ and $n = 1.1$. As discussed by Frigaard & Nouar (2005), the discontinuous Bingham model can be regularized by adding a small numerical parameter $\epsilon$ is added to the second invariant of the strain-rate tensor in order to avoid the singularity in the low shear region. It can be seen in Fig. 3.3 that the flow dynamics looks qualitatively similar for $10^{-6} \leq \epsilon \leq 10^{-12}$. The lowest value for $\epsilon$, although in principle it is the most accurate, increases the stiffness of the system of partial differential equations and thus we have used $\epsilon = 10^{-9}$ to generate the rest of the results in this paper. Inspection of Fig. 3.3 also reveals that the sawtooth shape interfacial instabilities which was observed in Fig. 3.1 did not appear in this case. On the other hand, we have observed a few drops of the non-Newtonian fluid in the middle of the channel. Also as $Ri = 1$ in this case, the flow becomes more asymmetrical as compared to that in Fig. 3.1 ($Ri = 0.1$).

![Figure 3.3](image)

**Figure 3.3:** The effects of viscosity regularization parameter ($\epsilon$) on the spatio-temporal evolution of the $\phi$ contours obtained using the simple model: (a) $\epsilon = 10^{-6}$, (b) $\epsilon = 10^{-9}$ and (c) $\epsilon = 10^{-12}$. The rest of the parameter values are $Re = 100$, $Ri = 1$, $At = 0.2$, $m = 2$, $\kappa = 0.0075$, $Bn = 30$ and $n = 1.1$. 
3.3 Effects of viscosity regularized models

Then, we investigate the effects of various viscosity regularized models (given by Eqs. (2.14)-(2.16)) proposed in literature (see for instance Ref. [Frigaard & Nouar (2005)]) on the flow dynamics. In Fig. 3.4(a), (b) and (c), we present the spatio-temporal contours of the index function obtained using the simple model, Bercovier and Engleman’s model and Papanastasiou’s model, respectively for the parameter values $Re = 100$, $Ri = 0.5$, $At = 0.2$, $m = 2$, $\kappa = 0.0075$, $Bn = 30$ and $n = 1.1$. We also plot spatio-temporal evolution of the unyielded domains (shown in black) obtained using the simple model, Bercovier and Engleman’s model and Papanastasiou’s model for the parameter values same as those used in Fig. 3.4 in Fig. 3.5(a), (b) and (c), respectively. The unyielded domain is the region where shear stress, $\tau \leq \tau_0$. It can be seen that the black region in the downstream (just after the ‘finger’) is the unyielded region which opposes the motion of the ‘finger’ of fluid ‘1’ into the bulk of fluid ‘2’. Close inspection of Fig. 3.5 and the enlarged view of the region marked by rectangles, shown at the bottom of each panels, reveals that the thin region just above the interface separating the fluids and the drops of fluid ‘2’ which appear inside the finger are also surrounded by unyielded material. This effect will be discussed below. It can be observed that the thickness of the residual layer, the small scale structures and location of the yield surface obtained using all these models match very well for the set of parameter values considered. Thus we use the simple regularized viscosity model in our study. However, Frigaard & Nouar (2005) showed that for strain rate close to zero (i.e when the material is almost stationary) the results obtained from Papanastasiou’s model is closer to the theoretical prediction.
Figure 3.4: Spatio-temporal evolution of $\phi$ contours obtained using the (a) simple, (b) Bercovier and Engleman’s, and (c) Papanastasiou’s model. The rest of the parameter values are $Re = 100$, $Ri = 0.5$, $At = 0.2$, $m = 2$, $\kappa = 0.0075$, $Bn = 30$ and $n = 1.1$. 
Figure 3.5: Spatio-temporal evolution of the unyielded domains obtained, shown in black, using (a) simple model, (b) Bercovier and Engleman’s model and (c) Papanastasiou’s model. The rest of the parameter values are the same as those used to generate Fig. 3.4. The insets at the bottom represent the corresponding enlarged view of the region shown by rectangles.
3.4 Effects of $Bn$

Next, we investigate the effects of $Bn$ on the flow dynamics. The contours of the index function, $\phi$ at $t = 20$ and $t = 30$ are shown for three values of Bingham number in Fig. 3.6. The rest of the parameter values are $Re = 100$, $At = 0.2$, $Ri = 1$, $\kappa = 0.0075$, $m = 2$ and $n = 1$. We set the value of the flow index, $n$ to be 1 in order to isolate the effects of $Bn$ on the flow dynamics. The results shown in Fig. 3.6(a) are associated with the case when fluid ‘2’ is also Newtonian. It can be seen in Fig. 3.6(a) that as the finger of fluid ‘1’ penetrates inside the channel, the upper elongated region of the finger becomes unstable, and a sawtooth shape wave is clearly visible at the later time. Close inspection of the contours at $t = 20$ reveals that this wave originates at early times ($t \approx 20$). When the fluid ‘2’ is non-Newtonian it can be seen in panels (b), (c) and (d) of Fig. 3.6 that the width of the finger increases with increasing $Bn$. This is due to the presence of the unyielded region at the front of the finger (shown in Fig. 3.7 for $Bn = 50$). We observed that the shear stress in this region decreases with increasing $Bn$, which in turn decreases the velocity of the tip of the finger (this is evident in Fig. 3.6). However, for $Bn = 0$ it can be seen that the velocity of the finger tip is slightly lower than that for $Bn = 20$. An explanation for this is as follows: in the Newtonian case, there are no unyielded regions, but for any finite $Bn$ we observed that the residual layers become unyielded (shown as an inset at the bottom of Fig. 3.7). This creates a three-layer configuration, where the viscosity of the fluid in the near wall region increases as compared to that of the Newtonian fluid displacement. This increases the fluid velocity in the core region in case of non-Newtonian fluid with low $Bn$, but as the $Bn$ increases the unyielded region at the front of the finger becomes an important factor, which decreases the velocity of the finger tip. The presence of the unyielded material at the residual leads to the suppression of the interfacial instability at higher $Bn$. 
3.4 Effects of $Bn$

![Figure 3.6](image)

**Figure 3.6:** Contours of the index function, $\phi$ for (a) $Bn = 0$, (b) $Bn = 20$, (c) $Bn = 50$ and (d) $Bn = 100$ at $t = 20$ and $t = 30$. The rest of the parameters are $Re = 100$, $At = 0.2$, $Ri = 1$, $\kappa = 0.0075$, $m = 2$ and $n = 1$.

![Figure 3.7](image)

**Figure 3.7:** Unyielded domains, shown in black, for $Bn = 50$ at $t = 20$ and $t = 30$. The rest of the parameters are values are the same as those used in Fig. 3.6.
Figure 3.8: (a) Temporal variation of volume fraction of the displaced fluid \( \left( \frac{M_t}{M_0} \right) \), (b) the rate of displacement, \( \left( \frac{M_t}{M_0} \right)' \), and (c) the average residual thickness of the bottom layer, \( \bar{h} \), for different values of \( Bn \). Here \('\) represents the derivative with respect to time. The rest of the parameters values are the same as those used in Fig. 3.6.

In Fig. 3.8(a), (b) and (c), we plot temporal variation of volume fraction of the displaced fluid \( \left( \frac{M_t}{M_0} \right) \) at early stages, the displacement rate of ‘fluid 2’, given by \( \left( \frac{M_t}{M_0} \right)' \), where prime represents the differentiation with respect to time, and the average residual thickness of the bottom layer, \( \bar{h} \), respectively for different values of \( Bn \). It can be seen in Fig. 3.8(a) and (b) that the effects of \( Bn \) is non-monotonic. The displacement rate increases with increasing the value of \( Bn \) upto \( Bn \approx 30 \), but, further increase in \( Bn \) decreases the displacement rate. This may be due to the formation of three-layer structure discussed above. It can be seen in Fig. 3.8(b) that increasing the value of \( Bn \) increased the average residual thickness of the bottom layer. The thickness of the residual layer at the bottom is more than that at the top. The viscosity of this material increases with increasing the Bingham number and becomes unyielded (as shown in Fig. 3.7). Thus this residual material becomes increasingly difficult to be removed for higher value of \( Bn \).
3.5 Effects of $n$

Finally, we investigate the effects of the flow index, $n$. In Fig. 3.9, the contours of the index function, $\phi$ and the unyielded domains (shown in black) are plotted at $t = 20$ and $t = 30$ for different values of $n$. The rest of the parameters are $Re = 100$, $At = 0.2$, $Ri = 1$, $\kappa = 0.0075$, $m = 2$ and $Bn = 30$. Here decreasing the value of $n$ reflects an increase in the shear-thinning tendency of the non-Newtonian fluid. It can be seen that for $n = 0.7$ (i.e. for shear thinning fluid) the interfacial instability becomes vigorous. In this case, there is a competition between the effects created by the Bingham number with that of the shear thinning. For $n = 0.7$ the unyielded material is absent in the region in front of the finger for the set of parameter values considered. Thus the finger penetrates freely inside the channel. For $n = 1.3$ the effects of Bingham number and the flow index reinforce one another, i.e. to decrease the shear stress in the flow region. The rate of displacement, $(M/M_0)'$, and the average residual thickness of the bottom layer, $\bar{h}$, for different values of $n$ are shown in Fig. 3.10. It can be observed in Fig. 3.10(a) that the disappearance of the unyielded material due to the shear thinning behaviour of the fluid (decreasing the value of $n$) makes it easier for the fluid to penetrate inside the channel, thus leading to faster displacement. In Fig. 3.10(b), it can be seen that the average residual thickness of the bottom layer, $\bar{h}$ increases almost linearly with time and decreases with increasing the value of $n$. Thus increasing the value of $n$ increases the unyielded region in the downstream of the channel, which in turn decreases the velocity of the finger tip. As expected, we observed (not shown) that the instabilities associated with different values of $n$ for $Bn = 0$ are more vigorous than those shown in Fig. 3.9 (for $Bn = 30$).
Figure 3.9: Contours of the index function, $\phi$ (top), and unyielded surface (bottom) for (a) $n = 0.7$, (b) $n = 1$ and (c) $n = 1.3$ at $t = 20$ and $t = 30$. The rest of the parameters are $Re = 100$, $At = 0.2$, $Ri = 1$, $\kappa = 0.0075$, $m = 2$ and $Bn = 30$.

Figure 3.10: (a) The rate of displacement, $(M_t/M_0)'$, and (b) the average residual thickness of the bottom layer, $\bar{h}$, for different values of $n$. Here $(')$ represents the the derivative with respect to time. The rest of the parameters values are the same as those used in Fig. 3.9.
CHAPTER 4

Conclusions

The pressure-driven displacement flow of a non-Newtonian fluid by a Newtonian fluid in a two-dimensional channel is investigated via a multiphase lattice Boltzmann method using the Carnahan-Starling equation of state. This method was originally proposed by He and co-workers [He et al. (1999a,b); Zhang et al. (2000)] and recently used by many researchers [Fakhari & Rahimian (2009); Sahu & Vanka (2011)]. This method uses two distribution functions in order to evaluate the flow variables, hydrodynamic pressure and the index function. The index function is used to distinguish both the fluids. We used three models for the non-Newtonian fluid, namely, the simple model, the Bercovier & Engleman (1980) model and Papanastasiou (1987) model. We found that for the parameter values considered in this study all the models give nearly the same results. The effects of Bingham number (which characterises the behaviour of the yield-stress of the fluid) and the flow index (which reflects the shear-thinning tendency of the fluid) are studied. We observed that increasing Bingham number and increasing the flow index increases the unyielded region of the fluid in the downstream of the channel and the residual layer. This in turn decreases the interfacial instabilities and the speed of the propagating finger.

In future, we are planning to extend this work to understand the flow dynamics in three dimensional geometries, such as square and rectangular ducts, and circular pipe.
APPENDIX I

Navier-Stokes equation from the Boltzmann equation

It is well known that hydrodynamic equations can be obtained from the continuous Boltzmann equation [Wagner (2008)].

A Maxwell-Boltzmann equilibrium distribution function and some important identities

Maxwell-Boltzmann equilibrium distribution function is given by

\[ f^0(v) = \frac{n}{(2\pi\theta)^{3/2}} e^{-\frac{(v-u)^2}{2\theta}}. \]  \hspace{1cm} (I.1)

In this section we are showing the proof of the following important identities which will be used in the subsequent derivations.

\[ \int_{-\infty}^{\infty} f^0 = n, \] \hspace{1cm} (I.2)

\[ \int_{-\infty}^{\infty} f^0(v_{\alpha} - u_{\alpha}) = 0, \] \hspace{1cm} (I.3)

\[ \int_{-\infty}^{\infty} f^0(v_{\alpha} - u_{\alpha})(v_{\beta} - u_{\beta}) = n\theta \delta_{\alpha\beta}, \] \hspace{1cm} (I.4)

\[ \int_{-\infty}^{\infty} f^0(v_{\alpha} - u_{\alpha})(v_{\beta} - u_{\beta})(v_{\gamma} - u_{\gamma}) = 0, \] \hspace{1cm} (I.5)

\[ \int_{-\infty}^{\infty} f^0(v_{\alpha} - u_{\alpha})(v_{\beta} - u_{\beta})(v - u)^2 = 5n\theta^2 \delta_{\alpha\beta}. \] \hspace{1cm} (I.6)
A.1 Proof of Eq. (I.2)

Left hand side of Eq. (I.2) is given by
\[
\int_{-\infty}^{\infty} f^0 dv = \int_{-\infty}^{\infty} \frac{n}{(2\pi\theta)^{3/2}} e^{-(v-u)^2/2\theta} dv
= \frac{n}{(2\pi\theta)^{3/2}} \int_{-\infty}^{\infty} e^{-(v_1-u_1)^2/2\theta} dv_1 \int_{-\infty}^{\infty} e^{-(v_2-u_2)^2/2\theta} dv_2 \int_{-\infty}^{\infty} e^{-(v_3-u_3)^2/2\theta} dv_3
= \frac{n}{(2\pi\theta)^{3/2}} I^3,
\]
where
\[
I = \int_{-\infty}^{\infty} e^{-(v_1-u_1)^2/2\theta} dv_1.
\]
Let \( t = v_1 - u_1 \Rightarrow dt = dv_1 \)
So,
\[
I = \int_{-\infty}^{\infty} e^{-t^2/2\theta} dt = \sqrt{2\pi\theta}.
\]
So, Eq. (I.7) can be written as
\[
\int_{-\infty}^{\infty} f^0 dv = \frac{n}{(2\pi\theta)^{3/2}} I^3
= \frac{n}{(2\pi\theta)^{3/2}} \left((2\pi\theta)^{1/2}\right)^3
= n.
\]

A.2 Proof of Eq. (I.3)

Left hand side of Eq. (I.3) is given by
\[
\int_{-\infty}^{\infty} f^0(v_\alpha - u_\alpha) dv = \int_{-\infty}^{\infty} \frac{n}{(2\pi\theta)^{3/2}} e^{-(v-u)^2/2\theta} (v_\alpha - u_\alpha) dv
= \frac{n}{(2\pi\theta)^{3/2}} \int_{-\infty}^{\infty} e^{-(v_1-u_1)^2/2\theta} (v_\alpha - u_\alpha) dv_1 \int_{-\infty}^{\infty} e^{-(v_2-u_2)^2/2\theta} dv_2 \int_{-\infty}^{\infty} e^{-(v_3-u_3)^2/2\theta} dv_3
= \frac{n}{(2\pi\theta)^{3/2}} I_1 \times I_2 \times I_3,
\]
where \( \alpha \) can take values 1, 2, 3.
For \( \alpha = 1 \),
\[
I_1 = \int_{-\infty}^{\infty} e^{-(v_1-u_1)^2/2\theta} (v_1 - u_1) dv_1.
\]
Let $t = (v_1 - u_1)^2 \implies dt = 2(v_1 - u_1)dv_1$

So,

$$I_1 = \int_{-\infty}^{\infty} e^{-t/2\theta} dt = 0.$$  

Similarly, for $\alpha = 2$, it can be shown that $I_2 = 0$ (keeping \(v_2 - u_2\) in $I_2$ term).

and for $\alpha = 3$ it can be shown that $I_3 = 0$ (keeping \(v_3 - u_3\) in $I_3$ term).

So, for any values of $\alpha$ we have, $I_1 \times I_2 \times I_3 = 0$.

So, LHS :

$$\int_{-\infty}^{\infty} f^0(v_\alpha - u_\alpha) dv = \frac{n}{(2\pi \theta)^{3/2}} \times 0 = 0.$$  

A.3 Proof of Eq. (I.4)

Left hand side of Eq. (I.4) is given by

$$\int_{-\infty}^{\infty} f^0(v_\alpha - u_\alpha)(v_\beta - u_\beta) dv = \int_{-\infty}^{\infty} \frac{n}{(2\pi \theta)^{3/2}} e^{-(v-u)^2/2\theta} (v_\alpha - u_\alpha)(v_\beta - u_\beta) dv$$

$$= \frac{n}{(2\pi \theta)^{3/2}} \int_{-\infty}^{\infty} e^{-(v_1-u_1)^2/2\theta}(v_\alpha - u_\alpha)(v_\beta - u_\beta) dv_1 \int_{-\infty}^{\infty} e^{-(v_2-u_2)^2/2\theta} dv_2 \int_{-\infty}^{\infty} e^{-(v_3-u_3)^2/2\theta} dv_3$$

$$= \frac{n}{(2\pi \theta)^{3/2}} I_1 \times I_2 \times I_3,$$  

(I.8)

where $\alpha$ and $\beta$ both can take values 1, 2, 3.

For $\alpha = 1$ and $\beta = 1$,

$$I_1 = \int_{-\infty}^{\infty} e^{-(v_1-u_1)^2/2\theta}(v_1 - u_1)^2 dv_1.$$  

Let $t = v_1 - u_1 \implies dt = dv_1$

So,

$$I_1 = \int_{-\infty}^{\infty} t^2 e^{-t/2\theta} dt = \frac{\sqrt{\pi}}{2}(2\theta)^{3/2},$$

$$\left( \int_{-\infty}^{\infty} x^2 e^{-ax^2} dx = \frac{\sqrt{\pi}}{2} a^{-3/2} \right)$$

$$I_2 = \sqrt{2\pi \theta},$$

$$I_3 = \sqrt{2\pi \theta}.$$  

Similarly for $\alpha = 2$ and $\beta = 2$, (including $(v_2 - u_2)^2$ in $I_2$ term)

$$I_1 = \sqrt{2\pi \theta},$$
\[ I_2 = \frac{\sqrt{\pi}}{2} (2\theta)^{\frac{3}{2}}, \]
\[ I_3 = \sqrt{2\pi}\theta. \]

and for \(\alpha = 3\) and \(\beta = 3\), (including \((v_3 - u_3)^2\) in \(I_3\) term)
\[ I_1 = \sqrt{2\pi}\theta, \]
\[ I_2 = \sqrt{2\pi}\theta, \]
\[ I_3 = \frac{\sqrt{\pi}}{2} (2\theta)^{\frac{3}{2}}. \]

So, for any \(\alpha = \beta\), we can say that
\[ I_1 \times I_2 \times I_3 = \sqrt{2\pi}\theta \times \sqrt{2\pi}\theta \times \frac{\sqrt{\pi}}{2} (2\theta)^{\frac{3}{2}} \]
\[ \Rightarrow I_1 \times I_2 \times I_3 = \theta \times (2\pi\theta)^{\frac{3}{2}} \] (I.9)

For \(\alpha = 1\) and \(\beta = 2\),
\[ I_1 = \int_{-\infty}^{\infty} e^{-\frac{(v_1 - u_1)^2}{2\theta}} (v_2 - u_2)(v_1 - u_1)dv_1 \]
\[ = (v_2 - u_2) \int_{-\infty}^{\infty} e^{-\frac{(v_1 - u_1)^2}{2\theta}} (v_1 - u_1)dv_1 \]
\[ = 0 \] (I.10)

Similarly, it can be said that for any \(\alpha \neq \beta\), at least one of the integral will be zero. So,
\[ I_1 \times I_2 \times I_3 = 0 \]

From Eq.(I.9) and Eq.(I.10) we can say that
\[ I_1 \times I_2 \times I_3 = \theta \times (2\pi\theta)^{\frac{3}{2}} \delta_{\alpha\beta}. \]

where \(\delta_{\alpha\beta}\) = Kronecker delta.

So, LHS of Eq.(I.4)
\[ \int_{-\infty}^{\infty} f_0(v_\alpha - u_\alpha)(v_\beta - u_\beta)dv \]
\[ = \frac{n}{(2\pi\theta)^{\frac{3}{2}}} \times \theta \times (2\pi\theta)^{\frac{3}{2}} \delta_{\alpha\beta} \]
\[ = n\theta \delta_{\alpha\beta}. \]
A.4 Proof of Eq. (I.5)

Left hand side of Eq.(I.5) is given as

\[ \int_{-\infty}^{\infty} f_0 (v_\alpha - u_\alpha)(v_\beta - u_\beta)(v_\gamma - u_\gamma) dv \]

\[ = \frac{n}{(2\pi\theta)^{3/2}} \int_{-\infty}^{\infty} e^{-(v-u)^2/2\theta} (v_\alpha - u_\alpha)(v_\beta - u_\beta)(v_\gamma - u_\gamma) dv \]

\[ = \frac{n}{(2\pi\theta)^{3/2}} \left[ \int_{-\infty}^{\infty} e^{-(v_1-u_1)^2/2\theta} dv_1 \int_{-\infty}^{\infty} e^{-(v_2-u_2)^2/2\theta} dv_2 \int_{-\infty}^{\infty} e^{-(v_3-u_3)^2/2\theta} dv_3 \right] \]

\[ = \frac{n}{(2\pi\theta)^{3/2}} I_1 \times I_2 \times I_3, \]

For \( \alpha = 1, \beta = 1 \) and and \( \gamma = 1 \), we have

\[ I_1 = \int_{-\infty}^{\infty} (v_1 - u_1)^3 e^{-(v_1-u_1)^2/2\theta} dv_1. \]

Let \( t = v_1 - u_1 \implies dt = dv_1 \)

So,

\[ I_1 = \int_{-\infty}^{\infty} t^3 e^{-t^2/2\theta} dt = 0. \]

For any set of values of \( \alpha, \beta, \) and \( \gamma \) we can group together the term in \( I_1, I_2 \) and \( I_3 \) in such a way that at least one of them will be zero. So, for any set of values of \( \alpha, \beta, \) and \( \gamma \),

\[ I_1 \times I_2 \times I_3 = 0. \]

So, LHS of Eq.(I.5)

\[ \int_{-\infty}^{\infty} f_0 (v_\alpha - u_\alpha)(v_\beta - u_\beta)(v_\gamma - u_\gamma) dv = 0. \]

A.5 Proof of Eq. (I.6)

Left hand side of Eq.(I.6) is given as

\[ \int_{-\infty}^{\infty} f_0 (v_\alpha - u_\alpha)(v_\beta - u_\beta)(v - u)^2 dv \]
By making the above substitution, we can write the above integral as

\[ \frac{n}{(2\pi\theta)^{3/2}} \int_{-\infty}^{\infty} e^{-(v-u)^2/2\theta} (v_\alpha - u_\alpha)(v_\beta - u_\beta)(v - u)^2 \, dv \]

\[ = \frac{n}{(2\pi\theta)^{3/2}} \int_{-\infty}^{\infty} e^{-(v_1 - u_1)^2/2\theta} e^{-(v_2 - u_2)^2/2\theta} e^{-(v_3 - u_3)^2/2\theta} (v_\alpha - u_\alpha)(v_\beta - u_\beta) [(v_1 - u_1)^2 + (v_2 - u_2)^2 + (v_3 - u_3)^2] \, dv, \]

(I.11)

For \( \alpha = 1 \) and \( \beta = 1 \), the above integral becomes

\[ \frac{n}{(2\pi\theta)^{3/2}} \int_{-\infty}^{\infty} e^{-(v_1 - u_1)^2/2\theta} e^{-(v_2 - u_2)^2/2\theta} e^{-(v_3 - u_3)^2/2\theta} (v_1 - u_1)^2 [(v_1 - u_1)^2 + (v_2 - u_2)^2 + (v_3 - u_3)^2] \, dv \]

Let \( v_1 - u_1 = x, v_2 - u_2 = y, v_3 - u_3 = z \)

By making the above substitution, we can write the above integral as

\[ \frac{n}{(2\pi\theta)^{3/2}} \int_{-\infty}^{\infty} e^{-x^2/2\theta} e^{-y^2/2\theta} e^{-z^2/2\theta} x^2(x^2 + y^2 + z^2) \, dx \, dy \, dz \]

\[ = \frac{n}{(2\pi\theta)^{3/2}} \left[ \left( \int_{-\infty}^{\infty} x^4 e^{-x^2/2\theta} \, dx \right) \left( \int_{-\infty}^{\infty} e^{-y^2/2\theta} \, dy \right) \left( \int_{-\infty}^{\infty} e^{-z^2/2\theta} \, dz \right) \right. \]

\[ + \left( \int_{-\infty}^{\infty} x^2 e^{-x^2/2\theta} \, dx \right) \left( \int_{-\infty}^{\infty} y^2 e^{-y^2/2\theta} \, dy \right) \left( \int_{-\infty}^{\infty} e^{-z^2/2\theta} \, dz \right) \]

\[ + \left( \int_{-\infty}^{\infty} x^2 e^{-x^2/2\theta} \, dx \right) \left( \int_{-\infty}^{\infty} e^{-y^2/2\theta} \, dy \right) \left( \int_{-\infty}^{\infty} z^2 e^{-z^2/2\theta} \, dz \right) \]

(I.12)

\[ = \frac{n}{(2\pi\theta)^{3/2}} \left[ \left( \sqrt{\pi}3/4(2\theta)^{5/2} \times \sqrt{2\theta\pi} \times \sqrt{2\theta\pi} \right) \right. \]

\[ + \left( \frac{\sqrt{\pi}}{2} (2\theta)^{3/2} \times \frac{\sqrt{\pi}}{2} (2\theta)^{3/2} \times \sqrt{2\theta\pi} \right) \]

\[ + \left( \frac{\sqrt{\pi}}{2} (2\theta)^{3/2} \times \sqrt{2\theta\pi} \times \frac{\sqrt{\pi}}{2} (2\theta)^{3/2} \right) \]

(I.13)

\[ = \frac{n}{(2\pi\theta)^{3/2}} \left[ \left( 2\pi\theta \times \sqrt{\pi}3/4(2\theta)^{5/2} \right) + \left( 2 \times (2\theta)^{3/2} \times \sqrt{2\theta\pi} \right) \right. \]

\[ + \left. \left( \frac{\sqrt{\pi}}{2} (2\theta)^{3/2} \times \sqrt{2\theta\pi} \times \frac{\sqrt{\pi}}{2} (2\theta)^{3/2} \right) \right] \]

\[ = \frac{n}{(2\pi\theta)^{3/2}} \times (2\theta)^{7/2} \times \left( \frac{3}{4} \frac{\pi}{\theta} \times \frac{2}{4} \frac{\pi}{\theta} \right) = n(2\theta)^2 \times 5/4 = 5n\theta^2. \]

(I.14)

We can obtain the same result for \( \alpha = 2; \beta = 2 \) and \( \alpha = 3; \beta = 3 \), by grouping together the terms in appropriate integrals.

So, for any \( \alpha = \beta \), LHS of Eq.(1.6) = \( 5n\theta^2 \).

But for any \( \alpha \neq \beta \), for example \( \alpha = 1, \beta = 2 \)
LHS of Eq. (I.6)

\[= \frac{n}{(2\pi\theta)^{3/2}} \int_{-\infty}^{\infty} e^{-\frac{(v_1-u_1)^2}{2\theta}} e^{-\frac{(v_2-u_2)^2}{2\theta}} e^{-\frac{(v_3-u_3)^2}{2\theta}} \left[ (v_1 - u_1)^2 + (v_2 - u_2)^2 + (v_3 - u_3)^2 \right] (v_1 - u_1)(v_2 - u_2)\]

Let \(v_1 - u_1 = x, v_2 - u_2 = y, v_3 - u_3 = z\)

So,

\[= \frac{n}{(2\pi\theta)^{3/2}} \left[ \int_{-\infty}^{\infty} (x^2 + y^2 + z^2)xy \left( e^{-\frac{x^2}{2\theta}} \times e^{-\frac{y^2}{2\theta}} \times e^{-\frac{z^2}{2\theta}} \right) \right]\]

\[= \frac{n}{(2\pi\theta)^{3/2}} \left[ \left( \int_{-\infty}^{\infty} x^3 e^{-\frac{x^2}{2\theta}} dx \int_{-\infty}^{\infty} ye^{-\frac{y^2}{2\theta}} dy \int_{-\infty}^{\infty} e^{-\frac{z^2}{2\theta}} dz \right) \right.

\[+ \left( \int_{-\infty}^{\infty} xe^{-\frac{x^2}{2\theta}} dx \int_{-\infty}^{\infty} y^3 e^{-\frac{y^2}{2\theta}} dy \int_{-\infty}^{\infty} e^{-\frac{z^2}{2\theta}} dz \right) \]

\[+ \left( \int_{-\infty}^{\infty} xe^{-\frac{x^2}{2\theta}} dx \int_{-\infty}^{\infty} ye^{-\frac{y^2}{2\theta}} dy \int_{-\infty}^{\infty} z e^{-\frac{z^2}{2\theta}} dz \right) \]

\[= \frac{n}{(2\pi\theta)^{3/2}} (0 + 0 + 0) = 0 \quad (I.15)\]

So, for any \(\alpha \neq \beta\), LHS of Eq. (I.6) = 0.

Thus, we can say that

\[\int_{-\infty}^{\infty} f^0(v_\alpha - u_\alpha)(v_\beta - u_\beta)(v - u)^2 = 5n\theta^2\delta_{\alpha\beta}.\]

where \(\delta_{\alpha\beta}\) is Kronecker delta.

### B Moments of Maxwell-Boltzmann equilibrium distribution function

#### B.1 Zeroth moment of equilibrium distribution function

Zeroth moment of equilibrium distribution function is given by Eq. (I.2) which we have proved in the previous section.

#### B.2 First moment of equilibrium distribution function

First velocity moment of equilibrium distribution function is

\[\int_{-\infty}^{\infty} f^0 v_\alpha = nu_\alpha.\]
To prove this we start from Eq. (I.3) (which we have proved in the previous section) i.e.

\[ \int_{-\infty}^{\infty} f^0(v_\alpha - u_\alpha) = 0 \]

\[ \Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha - \int_{-\infty}^{\infty} f^0 u_\alpha = 0 \]

\[ \Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha = u_\alpha \int_{-\infty}^{\infty} f^0 \]

\[ \Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha = nu_\alpha \] (I.16)

**B.3 Second moment of equilibrium distribution function**

Second velocity moment of equilibrium distribution function is

\[ \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta = nu_\alpha u_\beta + n\theta \delta_{\alpha\beta}. \]

To prove this we start from Eq. (I.4) (which we have proved in the previous section) i.e.

\[ \int_{-\infty}^{\infty} f^0 (v_\alpha - u_\alpha)(v_\beta - u_\beta) = n\theta \delta_{\alpha\beta} \]

\[ \Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta - \int_{-\infty}^{\infty} f^0 v_\alpha u_\beta - \int_{-\infty}^{\infty} f^0 u_\alpha v_\beta + \int_{-\infty}^{\infty} f^0 u_\alpha u_\beta = n\theta \delta_{\alpha\beta} \]

\[ \Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta - \int_{-\infty}^{\infty} f^0 v_\alpha u_\beta - \int_{-\infty}^{\infty} f^0 u_\alpha v_\beta + \int_{-\infty}^{\infty} f^0 u_\alpha u_\beta = n\theta \delta_{\alpha\beta} \]

\[ \Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta = nu_\alpha u_\beta + n\theta \delta_{\alpha\beta} \] (I.17)

**B.4 Third moment of equilibrium distribution function**

Third velocity moment of equilibrium distribution function is

\[ \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta v_\gamma = n\theta(u_\alpha \delta_{\beta\gamma} + u_\beta \delta_{\alpha\gamma} + u_\gamma \delta_{\alpha\beta}) + nu_\alpha u_\beta u_\gamma. \]
To prove this we start from Eq. (I.5) (which we have proved in the previous section) i.e.

\[
\int_{-\infty}^{\infty} f^0 (v_\alpha - u_\alpha)(v_\beta - u_\beta)(v_\gamma - u_\gamma) = 0
\]

\[
\Rightarrow \int_{-\infty}^{\infty} f^0 (v_\alpha v_\beta - v_\alpha u_\beta - u_\alpha v_\beta + u_\alpha u_\beta)(v_\gamma - u_\gamma) = 0
\]

\[
\Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta v_\gamma - \int_{-\infty}^{\infty} f^0 v_\alpha u_\beta v_\gamma - \int_{-\infty}^{\infty} f^0 u_\alpha v_\beta v_\gamma + \int_{-\infty}^{\infty} f^0 u_\alpha u_\beta v_\gamma
\]

\[
- \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta u_\gamma + \int_{-\infty}^{\infty} f^0 v_\alpha u_\beta u_\gamma + \int_{-\infty}^{\infty} f^0 u_\alpha v_\beta u_\gamma - \int_{-\infty}^{\infty} f^0 u_\alpha u_\beta u_\gamma = 0
\]

\[
\Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta v_\gamma - u_\beta \int_{-\infty}^{\infty} f^0 v_\alpha v_\gamma - u_\alpha \int_{-\infty}^{\infty} f^0 v_\beta v_\gamma + u_\alpha u_\beta \int_{-\infty}^{\infty} f^0 v_\gamma
\]

\[
- u_\gamma \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta + u_\beta u_\gamma \int_{-\infty}^{\infty} f^0 v_\alpha + u_\alpha u_\gamma \int_{-\infty}^{\infty} f^0 v_\beta - u_\alpha u_\beta u_\gamma \int_{-\infty}^{\infty} f^0 = 0
\]

\[
\Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta v_\gamma - u_\beta (nu_\alpha u_\gamma + n\theta \delta_{\alpha \gamma}) - u_\alpha (nu_\beta u_\gamma + n\theta \delta_{\beta \gamma}) + u_\alpha u_\beta (nu_\gamma) - u_\gamma (nu_\alpha u_\beta + n\theta \delta_{\alpha \beta}) + u_\alpha u_\gamma (nu_\beta) + u_\beta u_\gamma (nu_\alpha) - nu_\alpha u_\beta u_\gamma = 0
\]

\[
\Rightarrow \int_{-\infty}^{\infty} f^0 v_\alpha v_\beta = nu_\alpha u_\beta u_\gamma + n\theta (u_\alpha \delta_{\beta \gamma} + u_\beta \delta_{\alpha \gamma} + u_\gamma \delta_{\alpha \beta})
\] (I.18)

C Conservation of mass

Boltzmann equation with BGK approximation for collision operator can be written as

\[
\partial_t f + v_\alpha \partial_v f + F \partial_v f = \frac{1}{\tau} (f^0 - f).
\] (I.19)

Integrating, we get

\[
\int \partial_t f \, dv + \int v_\alpha \partial_v f \, dv + \int F \partial_v f \, dv = \int \frac{1}{\tau} (f^0 - f) \, dv
\]

\[
\Rightarrow \partial_t \int f \, dv + \partial_v \int v_\alpha f \, dv + \partial_v \int F f \, dv = \int \frac{1}{\tau} (f^0 - f) \, dv
\]

\[
\Rightarrow \partial_t n + \partial_\alpha (nu_\alpha) + F \partial_v n = \frac{1}{\tau} (n - n)
\]

\[
\Rightarrow \partial_t n + \partial_\alpha (nu_\alpha) = 0
\]

(I.20)
D Conservation of momentum

From Eq. (I.19), we can write

\[ f = f^0 - \tau (\partial_t f + v_\alpha \partial_\alpha f + F_\beta \partial_\beta f). \] (I.21)

Eq. (I.19) can be re-written as

\[ \partial_t f + v_\beta \partial_\beta f + F_\beta \partial_\beta f = \frac{1}{\tau} (f^0 - f). \]

Multiplying “\( v_\alpha \)” on both sides of the above equation and integrating, we get

\[ \int v_\alpha \partial_t f \, dv + \int v_\alpha v_\beta \partial_\beta f \, dv + \int F_\beta v_\alpha \partial_\beta f \, dv = \int \frac{1}{\tau} (f^0 v_\alpha - f v_\alpha) \, dv \]

\[ \Rightarrow \partial_t \int v_\alpha f \, dv + \partial_\beta \int v_\alpha v_\beta f \, dv + F_\beta \int v_\alpha \partial_\beta f \, dv = \frac{1}{\tau} \int (f^0 v_\alpha - f v_\alpha) \, dv \]

\[ \Rightarrow \partial_t \int v_\alpha f \, dv + \partial_\beta \int v_\alpha v_\beta f \, dv + F_\beta \int v_\alpha \partial_\beta f \, dv = \frac{1}{\tau} (nu_\alpha - nu_\alpha) \]

\[ \Rightarrow \partial_t \int v_\alpha f \, dv + \partial_\beta \int v_\alpha v_\beta f \, dv + F_\beta \int v_\alpha \partial_\beta f \, dv = 0 \] (I.22)

Now, we simplify each term of Eq. (I.22) one by one.

Third term of left hand side of Eq. (I.22) is

\[ F_\beta \int v_\alpha \partial_\beta f \, dv = F_\beta \left[ v_\alpha \int \partial_\beta f \, dv - \int \left( \int \partial_\beta f \, dv \right) \, dv \right] \]

\[ = F_\beta \left[ v_\alpha \int f \, dv - \int \left( \int f \, dv \right) \, dv \right] \]

\[ = F_\beta (v_\alpha \partial_\beta n - \int f \, dv) \]

\[ = F_\beta (0 - n) \]

\[ = -nF_\alpha \] (I.23)

Substituting Eq. (I.23) in Eq. (I.22), we get

\[ \partial_t \int v_\alpha f \, dv + \partial_\beta \int v_\alpha v_\beta f \, dv - nF_\alpha = 0 \]

\[ \Rightarrow \partial_t (nu_\alpha) + \partial_\beta \int v_\alpha v_\beta f \, dv - nF_\alpha = 0 \] (I.24)
Eq. (I.21) can be re-written as
\[ f = f^0 - \tau (\partial_i f + v_\gamma \partial_\gamma f + F_\gamma \partial_\gamma f). \]

multiplying “\(v_\alpha v_\beta\)” with all the terms of the above equation and integrating, we get
\[ \int f v_\alpha v_\beta \, dv = \int f^0 v_\alpha v_\beta \, dv \]
\[ \Rightarrow \int f v_\alpha v_\beta \, dv = n u_\alpha u_\beta + n \theta \delta_{\alpha\beta} \]  
(I.26)

Substituting Eq. (I.26) in Eq. (I.24), we get
\[ \partial_i (n u_\alpha) + \partial_\beta (nu_\alpha u_\beta + n \theta \delta_{\alpha\beta}) - n F_\alpha = 0 \]
\[ \Rightarrow \partial_i (n u_\alpha) + \partial_\beta (nu_\alpha u_\beta) = n F_\alpha - \partial_\alpha (n \theta) \]  
(I.27)

where Kronecker delta, \(\delta_{\alpha\beta}\), is given as
\[ \delta_{\alpha\beta} = \begin{cases} 1, & \alpha = \beta \\ 0, & \alpha \neq \beta \end{cases} \]  
(I.28)

So, we can write Eq. (I.27) as
\[ \partial_i (n u_\alpha) + \partial_\beta (nu_\alpha u_\beta) = n F_\alpha - \partial_\alpha (n \theta) \]  
(I.29)

The bracketed term of left hand side of Eq. (I.29) is zero by equation of continuity(Eq. (I.20)).
So, Eq. (I.29) can be written as
\[ \partial_i u_\alpha + n \partial_i u_\alpha = F_\alpha - \frac{1}{n} \partial_\alpha (n \theta). \]  
(I.31)

We will use Eqs. (I.30) and (I.31) when we will derive Eq. (I.23) up to second order in derivative and then we will substitute that in Eq. (I.24). That will give us the Navier Stokes equation. So, we have to evaluate three more terms of Eq. (I.25).
Force term in Eq. (I.25) is

\[ F \gamma \int v_\alpha v_\beta \partial_v f \ dv = F \gamma \left[ v_\alpha v_\beta \left( \int f \ dv \right) - \int (v_\alpha v_\beta) \left( \int \partial_v f \ dv \right) \right] \]

\[ = F \gamma \left[ v_\alpha v_\beta \partial_v n - \int (v_\beta + v_\alpha) f \ dv \right] \]

\[ = F \gamma (-nu_\beta - nu_\alpha) \]

\[ = -nF_\alpha u_\beta - nF_\beta u_\alpha \] (I.32)

Substituting Eq. (I.32) in Eq. (I.25), we get

\[ \int f v_\alpha v_\beta \ dv = \int f^0 v_\alpha v_\beta \ dv - \tau \left[ \partial_t \int f^0 v_\alpha v_\beta \ dv + \partial_\gamma \int f^0 v_\alpha v_\beta v_\gamma \ dv - nF_\alpha u_\beta - nF_\beta u_\alpha \right] \] (I.33)

While obtaining Eq. (I.33) from Eq. (I.25), we have also made the following approximation

\[ \partial_t \int f v_\alpha v_\beta \ dv \approx \partial_t \int f^0 v_\alpha v_\beta \ dv, \]

\[ \partial_\gamma \int f v_\alpha v_\beta v_\gamma \ dv \approx \partial_\gamma \int f^0 v_\alpha v_\beta v_\gamma \ dv. \]

The time derivative term of Eq. (I.33) can be simplify as

\[ \partial_t \left( \int f^0 v_\alpha v_\beta \ dv \right) = \partial_t(nu_\alpha u_\beta + n\theta \delta_{\alpha\beta}) \]

\[ = u_\beta \partial_t (nu_\alpha) + nu_\alpha \partial_t u_\beta + \theta \delta_{\alpha\beta} \partial_t n + n\partial_t \theta \delta_{\alpha\beta} \] (I.34)

From Eq. (I.29), we can say that

\[ \partial_t (nu_\alpha) = nF_\alpha - \partial_\gamma (n\theta) - \partial_\gamma (nu_\alpha u_\gamma) \] (I.35)

From Eq. I.31, we can say that

\[ \partial_\gamma u_\beta = F_\beta - \frac{1}{n} \partial_\beta (n\theta) - u_\gamma \partial_\gamma u_\beta \] (I.36)

From equation of continuity(Eq. I.20), we can say that

\[ \partial_t n = -\partial_\gamma (nu_\gamma) \] (I.37)

and we use the relation

\[ \partial_\gamma \theta = -u_\gamma \partial_\gamma \theta - \frac{2}{3} \partial_\gamma (\theta u_\gamma) \] (I.38)

We have used the above relation directly but this can also be derived from by multiplying \((v - u)^2\) with Eq. (I.22). Substituting Eqs. (I.35), (I.36), (I.37) and (I.38) in Eq. (I.34), we
The space derivative term in Eq. (I.33) can be simplified as

\[
\partial_t \left( \int f^0 \nu v_{\beta} \, dv \right) = u_\beta \left[ n F_\alpha - \partial_\alpha (n\theta) - \partial_\gamma (nu_\alpha u_\gamma) \right] + nu_\alpha \left[ F_\beta - \frac{1}{n} \partial_\beta (n\theta) - u_\gamma \partial_\gamma u_\beta \right] + n \theta \delta_{\alpha \beta} (-\partial_\gamma (nu_\gamma)) + n \delta_{\alpha \beta} \left[ -u_\gamma \partial_\gamma \theta - \frac{2}{3} \partial_\gamma (\theta u_\gamma) \right]
\]

The space derivative term in Eq. (I.33) can be simplified as

\[
\partial_\gamma \left( \int f^0 \nu v_\beta v_\gamma \, dv \right) = \partial_\gamma \left[ n \theta (u_\alpha \delta_\beta\gamma + u_\beta \delta_\alpha\gamma + u_\gamma \delta_\alpha\beta) + nu_\alpha u_\beta u_\gamma \right]
\]

Adding Eqs. (I.39) and (I.40), we get

\[
\partial_t \left( \int f^0 \nu v_\beta \, dv \right) + \partial_\gamma \left( \int f^0 \nu v_\beta v_\gamma \, dv \right) = -\partial_\gamma (nu_\alpha u_\beta u_\gamma) - u_\alpha \partial_\beta (n\theta) - u_\beta \partial_\alpha (n\theta) + n (F_\alpha u_\beta + F_\beta u_\alpha) - \frac{2}{3} n \delta_{\alpha \beta} \partial_\gamma (\theta u_\gamma)
\]

Substituting Eq. (I.41) in Eq. (I.33), we get

\[
\partial_t \left( \int f v_\alpha v_\beta \, dv \right) = nu_\alpha u_\beta + n \theta \delta_{\alpha \beta}
\]

\[
-\tau \left[ n \theta (\partial_\beta u_\alpha + \partial_\alpha u_\beta) + n (F_\alpha u_\beta + F_\beta u_\alpha) - \frac{2}{3} n \delta_{\alpha \beta} \partial_\gamma (u_\gamma \theta) - n F_\alpha u_\beta - n F_\beta u_\alpha \right]
\]

\[
\Rightarrow \int f v_\alpha v_\beta \, dv = nu_\alpha u_\beta + n \theta \delta_{\alpha \beta} - n \theta \tau \left( \partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{3} \delta_{\alpha \beta} \partial_\gamma (u_\gamma) \right)
\]

\[
\Rightarrow \int f v_\alpha v_\beta \, dv = nu_\alpha u_\beta + n \theta \delta_{\alpha \beta} - \eta \left( \partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{3} \delta_{\alpha \beta} \partial_\gamma (u_\gamma) \right)
\]

where \( \eta = n \theta \tau \).

Now, substituting Eq. (I.42) in Eq. (I.25), we get

\[
\partial_t (nu_\alpha) + \partial_\beta \left( nu_\alpha u_\beta + n \theta \delta_{\alpha \beta} - \eta \left( \partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{3} \delta_{\alpha \beta} \partial_\gamma (u_\gamma) \right) \right) - n F_\alpha = 0
\]

\[
\Rightarrow \partial_t (nu_\alpha) + \partial_\beta (nu_\alpha u_\beta) + \partial_\beta (n\theta) \delta_{\alpha \beta} = n F_\alpha + \partial_\beta \left[ \eta \left( \partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{3} \delta_{\alpha \beta} \partial_\gamma (u_\gamma) \right) \right]
\]
For $\alpha = \beta$, $\delta_{\alpha\beta} = 1$.
So, Eq. (I.43) can be written as

$$u_\alpha \partial_t n + u_\alpha \partial_\beta(n u_\beta) + n u_\beta \partial_\beta u_\alpha = -\partial_\alpha(n \theta) + n F_\alpha + \partial_\beta \left[ \eta \left( \partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma(u_\gamma) \right) \right]$$

$$\Rightarrow u_\alpha \left( \partial_t n + \partial_\beta(n u_\beta) \right) + n \partial_\alpha(u_\alpha) + n u_\beta \partial_\beta u_\alpha = -\partial_\alpha(n \theta) + n F_\alpha + \partial_\beta \left[ \eta \left( \partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma(u_\gamma) \right) \right]$$

(I.44)

Using equation of continuity i.e Eq. (I.20) in the above equation, we get

$$n \partial_\alpha(u_\alpha) + n u_\beta \partial_\beta u_\alpha = -\partial_\alpha(n \theta) + n F_\alpha + \partial_\beta \left[ \eta \left( \partial_\beta u_\alpha + \partial_\alpha u_\beta - \frac{2}{3} \delta_{\alpha\beta} \partial_\gamma(u_\gamma) \right) \right].$$

(I.45)

Eq. (I.45) is the compressible Navier stokes equation in tensor notation.

He & Luo (1997a, b) gave a much needed theoretical foundation to the lattice Boltzmann method by deriving the lattice Boltzmann equation from the Boltzmann equation. Navier-Stokes equation can also be derived from the lattice Boltzmann equation by following the Chapman-Enskog multi-scale expansion. A detail derivation of Navier-Stokes equation from lattice Boltzmann equation was also given by Dr. Erlend M. Viggen in his doctoral thesis [Viggen (2009)].
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