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Lattice Boltzmann modeling for mass transport equations in porous media

Borja Servan Camas
Louisiana State University and Agricultural and Mechanical College

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LATTICE BOLTZMANN MODELING FOR MASS TRANSPORT EQUATIONS IN POROUS MEDIA

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Civil and Environmental Engineering

by

Borja Serván Camas
Ingeniero Naval, Universidad Politécnica de Madrid, 2002
(Naval Engineer, Polytechnic University of Madrid, 2002)
M. S. in Civil Engineering, Louisiana State University, 2007
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To my family,
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It has been three years since I started my graduate studies under the advice of Dr. Frank T-C. Tsai. Along this period of time, many people have made many types of contributions to the success in completing this long journey.

I want to acknowledge the support of my family, those old friends that always kept in touch, and the new ones that I made during my stay at LSU and made life more joyful.

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ABSTRACT

The aim of this dissertation is to extend the lattice Boltzmann method (LBM) to cope with parameter heterogeneity and anisotropy in mass transport equations in porous media, as well as investigating the stability and accuracy.

Although the LBM is a well known and effective numerical method to solve fluid flows, LBM has not been extensively applied to mass transport equations in porous medium flow yet, and only a few works can be found on improving LBM to cope with mass transport equations other than the diffusion and advection-diffusion equations. One of the reasons why LBM has not been extensively used is because it is not clearly understood how LBM solve mass transport equations.

We first focus on investigating what type of partial differential equation (PDE) the LBM recovers. The recovery procedure is carried out in detail up to third order accuracy and including the effect of forcing terms. Once the recovered PDE is known, LBM can be tailored to solve targeted mass transport equations. In order to improve the accuracy of LBM, the analysis is based on the lattice Boltzmann equation with a two-relaxation-time collision operator. Regarding the stability of LBM, the von Neumann stability analysis is used and linear stability boundaries are found under different scenarios.

By an appropriate selection of the equilibrium distribution functions (EDF) and forcing terms, LBM is able to cope with parameter heterogeneity and anisotropy in mass transport equations in porous media. The relaxation times offer some degrees of freedom that allows LBM to improve the accuracy without decreasing computational efficiency.

For validation purposes LBM has been implemented to simulate saltwater intrusion in the Henry problem and modified versions, and the results are in good agreement with available analytical solutions and numerical solutions obtained by other methods.
CHAPTER 1. INTRODUCTION

Transport in porous media has become an important area of research focusing on aspects of the transport of extensive quantities, and is presented in the context of environmental, chemical, agricultural, petroleum, mechanical and civil engineering. The scope of transport in porous media reaches, among others, the simulation of groundwater flow, multiphase flows, movement of oil and gas in petroleum reservoirs, saltwater intrusion, and spreading of contaminants, radioactive pollutants, viruses, etc. The development of simulation tools allows us to better understand transport processes in porous media, which may be very complicated to observe directly or might be happening too slowly or too fast. Moreover, the complexity of the geometry of a porous medium at pore scale results in the need to identify structures at different length scales involved in the transport processes as well as the interaction among those scales. Then successful predictions will depend on the reliability of the modeling process.

The modeling process can usually be split into two steps: first, it is necessary to identify and understand transport processes at pore scale before we can describe their manifestation at the macroscopic scale; and second, developing a mathematical model based on the knowledge gathered from the first step. The understanding of the transport processes at pore scale can be achieved by direct observation of the phenomena or via studying the models of simpler phenomena constituting the transport process. Then once the underlying physics is understood, it is time to give shape to the mathematical model. This model is usually a set of governing equations describing the spatial distribution and evolution in time of the extensive quantities under study.

Care must be taken when developing the mathematical model since the success of the modeling process will greatly depend on obtaining the right governing equations. Commonly, one is not interested in the microscale details of solutes and fluid distributions and it is usually
not feasible computationally to resolve a model at such small scales. Instead, one is interested in the lumped effects of such heterogeneities. Then, in order to succeed in this stage, we need to identify the level of detail required, which will provide us with a sense of the length and time scales we need to accurately resolve. Then, the right mathematical model will accurately represent the scales of our interest while including upscaling approaches to represent the smaller scales in a simple manner.

The governing equations for these processes are obtained via imposing mass conservation in the representative elementary volume (REV). On one side, REV is an upscaling approach to represent, in average, porous media properties such that porosity, avoiding then the necessity of modeling and solving the transport problem at pore scale. On the other side, REV has to be small enough in comparison with the length scale of our problems so that we can consider the porous media as a continuum. Then the governing equations will become a set of partial differential equations.

1.1 Traditional Numerical Methods

1.1.1 Numerical Methods for the Groundwater Flow Equation

The finite difference method (FDM) is the numerical method that is probably used the most in groundwater flow modeling because the FDM is very well understood and does not require a deep mathematical background. We find the first application of the FDM to groundwater flow in Remson et al. (1965). Since then, many works have been done in developing the FDM for solving the groundwater flow equation. For instance, MODFLOW (Harbaugh et al. 2000) is a three-dimensional finite-difference groundwater model that was first published in 1984 and is still being developed. In fact, MODFLOW-2005 Version 1.5.00 was recently released in April 2008.
Another well known numerical method is the finite element method (FEM), which is based on solving the weak or variational form of the problem. An implementation of the FEM to groundwater flows can be found in FEMWATER (Lin et al. 1997), and an introduction to FEM as well as to FDM for the groundwater equation can be found in Segol (1994), Yeh (1999) and Batu (2006).

1.1.2 Numerical Methods for the Transport Equation

Intensive research has been done in the past few decades to numerically solve the advection-dispersion equation. This is because there is a fundamental difficulty resulting from the fact that advection and dispersion promote mass transport very differently. Mathematically, the advection is represented in the transport equation by the hyperbolic terms, while the dispersion is represented by the parabolic terms.

As for the groundwater flow equation, the FDM is the most used method for the transport equation. In advection dominated cases, numerical schemes for the advection terms are likely either to show numerical oscillations, like central finite difference schemes, or to introduce too much numerical diffusion, like upwind finite difference schemes. Hence, more sophisticated schemes have been developed incorporating high order corrections and limiters. For instance, QUICKEST (Ekebjærg and Justesen 1991) is an explicit finite difference scheme that successfully eliminates the numerical wiggling caused by central difference schemes for the advection term, while minimizing the numerical dumping caused by the upwind scheme.

The FEM has also been extensively applied to solve the transport equation in the last few decades (Grove 1977), and more recently, a mixed hybrid finite element and discontinuous finite element methods were developed to increase numerical stability for solving transport problems (Ackerer et al. 1999; Bues and Oltean 2000).
A different approach from Eulerian methods such as FDM or FEM is given by Lagrangian methods such as the method of the characteristics (MOC) (Pinder and Cooper 1970). MOC has the advantage of solving the hyperbolic terms (advective terms) of the transport equations via streaming the concentration values along the characteristics. Then by means of interpolation, the values of concentration are calculated at the points of discretization so that the partial derivatives of the parabolic terms can be estimated, for example, using a finite difference scheme.

Another Lagrangian method is the particle tracking method (Yeh 1999). As indicated by its name, the particle tracking method is based on tracking the movement of individual particles, and the movement associated to each particle is based on the local values of the advective flow and dispersion coefficient. The particle tracking method does not suffer from numerical oscillations or numerical damping. However, the main problem associated with this method is that the number of particles required to obtain accurate solutions can be simply too large to be computed.

1.2 Lattice Boltzmann Method for Transport Equations in Porous Media

The lattice Boltzmann method (LBM) was first introduced as a numerical method to solve fluid flows (Higuera and Jimenez 1989) by mimicking the behavior of microscopic particles on a mesoscopic scale. Hence LBM falls into the category of mesoscopic methods. Although LBM has been intensely studied in fluid dynamics, LBM in the heterogeneous porous medium flow is still under development. When applying LBM to flow in porous media, one can either model the flow dynamics in the pore scale with complex pore geometry using the standard LBM or in the REV scale where average hydraulic properties are considered. Inamuro et al. (1999) carried out direct Navier-Stokes simulations in a three dimensional porous structure. The porous structure consists of a box containing a few spheres representing the grains in a porous
medium. As a result, LBM was effective to study microscopic properties of the flow through porous media. Guo and Zhao (2002) developed a LBM to solve incompressible flow in porous media modeling the Navier-Stokes equation in the REV, in which the main idea is to include the porosity into the equilibrium distribution functions and add a forcing term accounting for the drag forces of the medium. LBM has been also applied to solve other equations, such as reaction-diffusion and contaminant transport equations. Dawson et al. (1993) introduced the pure diffusion equation with a reaction term that can be easily modeled by introducing an extra term in the collision equation and keeping an easy formulation for the equilibrium distribution functions. Deng et al. (2001) combined the LBM with techniques coming from finite volume methods (FVM) in order to include extra terms that allow solving even the pure advection equation with minimum dispersion or instability.

LBM has been extensively used to solve the diffusion and advection-diffusion equation since (Flekkøy 1993), and many approaches and assumptions used to recover the advection-diffusion equation using LBM are different. This leads to various ways of using LBM parameters to represent the diffusion coefficient. The most popular recovery approach is using equilibrium distribution functions (EDFs) depending linearly on the macroscopic velocity with the assumption of no rapid time variations (Dawson et al. 1993; Chen et al. 1995; Stockman 1999). Also, Inamuro et al. (2002) justified the use of EDFs depending linearly on the macroscopic velocity by an asymptotic analysis and under the assumption of moderately varying solutions.

A step to improve on using LBM for mass transport equations is found in Ginzburgh (2005), where the LBM was extended to solve the anisotropic advection-dispersion equation. Ginzburgh (2005) discussed the second order correction via introducing quadratic terms in velocity into the EDFs. Besides, the anisotropic dispersion tensor was recovered by two different ways: extending the work of Zhang et al. (2002a) using multi-relaxation technique; and by
modifying the isotropic and anisotropic parts of the EDFs. Moreover, the Chapman-Enskog expansion was used to recover the macroscopic equations up to second order accuracy. Furthermore, the dispersion method was used to carry out third order analysis on the advection terms, and to carry out fourth and sixth order analysis on diffusion terms. Ginzburg (2006) extended the previous work and applied the anisotropic LBM to solve Richard’s equation for variably saturated porous medium flow, where the main focus is on ensuring interlayer continuity of Darcy’s law with heterogeneous and anisotropic hydraulic conductivity. Ginzburg (2007) presented LBM and analytical solutions for steady-state saturated flows in heterogeneous and anisotropic aquifers, as well as some stability aspects of the anisotropic LB schemes.

1.3 LBM

While most popular methods used to solve mass transport equations and fluid flows, such as FDM and FEM, have been intensively developed for the past five decades, LBM has only been around for almost two decades. Despite of the youth of LBM, this numerical method has awakened interest among researchers to model fluid flows in particular and transport problems in general. Hence the number of works based on LBM has greatly increased in the last decade and LBM has been applied in many different areas. The reason why LBM has awakened such an interest is because LBM has some desirable features such as easy implementation and suitability for parallel computing.

1.3.1 LBM vs. Traditional Numerical Methods

Although the LBM is raising popularity among numerical methods, there is still some distrust on whether LBM performs better than others numerical methods such as FDM and FEM. Therefore, in this section some works carried out to compare LBM with FDM will be pointed out.
The standard LBM, based on solving the lattice Boltzmann equation (LBE) with a single relaxation collision operator (LBGK), is the simplest LBM scheme. In the specific case where the relaxation time is equal to unity, the LBM scheme can be rewritten as a finite difference method. van der Sman (2006) showed that in particular, if the LBM is intended to solve the advection-diffusion equation and the equilibrium state of the LBM is constrained to fulfill the zero, first and second moment of the Maxwell-Boltzmann distribution, the LBM scheme becomes a Lax–Wendroff finite difference scheme. This equivalency is due to the homology of constructing the finite difference stencils via Taylor expansion and the construction of the equilibrium in the LBM via the Maxwell-Boltzmann constraints.

While choosing appropriately the equilibrium can provide similar accuracy than Lax-Wendroff finite difference schemes, LBM offers the advantage of having some extra degrees of freedom that, without increasing the computational effort, can improve the accuracy of the scheme. In Chapter 2 and Chapter 3 will be shown that a wise choice of relaxation times can eliminate oscillations in sharp gradients caused by third order numerical dispersion terms. Moreover in Chapter 5 will be shown that developing new equilibrums not restricted to the Maxwell-Boltzmann constraints can recover more complex equations without a large increase of computational cost.

Manwart et al. (2002) carried out some comparisons between the FDM and standard LBM to simulate the permeability in three-dimensional porous media by solving the Stokes equation. Manwart found that similar performance was obtained. However, a standard implementation of the LBM was used, and probably much better performance could be achieved if the latest development in LBM had been incorporated.

Geller et al. (2006) compared a standard version of LBM to the FEM based code FEATFLOW and the FVM based code CFX. For a time dependent test of incompressible flow,
LBM results were similar in accuracy at comparable or lower expenses in terms of CPU time. Besides, for flows with small but finite Mach number, the LBM shows a substantial advantage in computational effort. This advantage is due to the fact that LBM does not need to solve a costly Poisson equation for the pressure in each time step since it has an equation of state for the pressure built in and therefore, incompressible flows can be simulated by limiting the Mach number. On the other hand, the LBM was less efficient for steady-state problems, which is expected since LBM is an explicit time-marching method that solves steady-states as the asymptotic solution in time.

However, care must be taken when making statements such as one numerical method is better than other. Accurate and quantitative comparisons between numerical methods are complicated since different methods have different underlying approaches (Manwart et al. 2002; Geller et al. 2006).

1.3.2 LBM for Parallel Computing

The current trend to increase computational capacity is based on clustering CPUs altogether rather than on improving the CPU performance. Hence, in order to decrease the computational time required for computation, numerical algorithms have to be developed such that they can be efficiently parallelized. An efficient parallelization requires keeping low the communication overheads caused by the exchange of information among different CPUs.

Complex implicit schemes, based on other FDM, FEM, FVM and others numerical methods, were intensively developed in order to minimize the computational cost and speed up the CPU time. However, implicit schemes often require iterative calculations to solve global systems of equations involving the values of the variables all over the computational domain. Hence communication overheads can easily decrease the efficiency of the parallelization and
make even impossible to carry out simulations in large number of CPUs due to poor parallel scalability.

The main advantage of LBM over other numerical methods is that LBM solves complex PDEs by explicitly solving a system of first order linear differential equations. LBM does not involve the resolution of any global system of equations and only information from neighboring nodes is needed (locality) for evolving variables. Therefore, the explicit nature along with the locality property makes the LBM have almost no communication overheads between CPUs and therefore ideal for parallel computing. Moreover, the time step is relatively inexpensive since it involves simple arithmetic calculations.

Noble et al. (1996) compared the accuracy and performance of LBM and FDM for steady and viscous flow. The LBM showed good accuracy results when compared to those obtained by the FDM. Besides, Noble et al. (1996) showed that overall LBM is well suited for parallel computation since operations involved in the collision process, streaming process and boundary conditions are local. This conclusion was based on the scalability results obtained on the CM-5 parallel computer at the National Center for Supercomputing Applications (NCSA), where up to 512 processors were used in the simulations.

1.4 Motivation of this Dissertation

The numerical simulating of large systems leads to the necessity of largely increasing the computational capability available. Nowadays, the main trend to increment this computational capability is based on clustering CPUs to operate in parallel rather than on increasing CPUs processing speeds. Hence the suitability of a numerical scheme to be parallelized is becoming an important feature to be considered. In this framework LBM offers a great capability to be parallelized based on its explicit nature and locality, which results in high scalability performance.
On one hand LBM is still under development and the reason is because LBM is barely two decades old, which makes it a relatively new numerical method in comparison with traditional methods such as FDM, FEM and FVM. First developed to model fluid flows, LBM has been mainly implemented for this purpose. On the other hand, LBM is gaining attention to model transport problems in many areas. Since LBM is still in disadvantage with respect to its competitors regarding solving complex problems, more research has to be put on developing the theoretical basis and implementation techniques to make LBM capable of coping with complicated problems.

The main purpose of this dissertation is to extend the LBM to make it capable of coping with heterogeneous and anisotropic mass transport problems in porous media, as well as to investigate the theoretical basis of the method in order to gain knowledge regarding accuracy and stability.

1.5 Outline

This dissertation is organized as follows: Chapter 2 introduces LBM and recovers the general expression of the macroscopic PDE solved by LBM; Chapter 3 shows the basis of LBM by solving the advection-diffusion equation; Chapter 4 contains an analysis on how to correct numerical dispersion introduced by third order terms; Chapter 5 extends LBM to cope with mass transport equations containing heterogeneity and anisotropy; Chapter 6 studies analytically the non-negativity of the equilibrium distribution functions of LBM; Chapter 7 analyzes the linear stability of LBM and its relationship with the non-negativity analysis of the equilibrium; Chapter 8 implements LBM to saltwater intrusion problems in coastal aquifers for validation purposes; Chapter 9 contains the main conclusions of this dissertation.
CHAPTER 2. LBM FOR MASS TRANSPORT EQUATIONS

2.1 Origin of LBM

The LBM was first developed to solve the hydrodynamic equations mimicking the kinetic theory of gases. Based on the kinetic theory, in the microscale particles are moving and colliding randomly, and the distribution of particles velocity is continuously relaxed to an equilibrium state given by the Maxwell-Boltzmann distribution, which depends on the temperature $T$ and the universal constant of gases $R$.

In the original Boltzmann equation $f$ represents the probability of one single particle moving with speed $c$ at a specific time. Therefore, $f$ is a probability density function (PDF) for the random variable $c$. Although this PDF is neither constant in time nor uniform in space, we know that is always close to the equilibrium distribution, whose mean value corresponds to the local value of the macroscopic velocity $u$ and variance is proportional to the local absolute temperature. The distance between $f$ and the Maxwell-Boltzmann equilibrium $f^{eq}$ is $f - f^{eq} = O(\varepsilon)$, where $\varepsilon$ is the Knudsen number, which represents the ratio between the characteristic length of the microscale (mean free path between collisions) and the characteristic length of the macroscale.

The LBM mimics the Boltzmann equation in a simplified way at mesoscale level. To do so, first the random variable $c$ is discretized in such a way that only few speeds are considered. Second, instead of considering particles moving along the lattices directions and colliding at the nodes like in the LGA, averaged values of particles moving along a lattice structure are considered (Higuera and Jimenez 1989). Then the discrete Boltzmann equation for describing dynamics of local particle distribution functions in a discrete velocity field is

$$\frac{\partial f_i}{\partial t} + c_i \cdot \nabla f_i = \Omega_i + \Omega_F \quad (1)$$
where \( f_i(x,t) \) are the particle distribution function moving along \( i \) direction at time \( t \), at location \( x \); \( c_i \) is the particle velocity along \( i \) direction; \( \Omega \) is the collision operator and depends on all the particle distribution functions converging at a same node; and \( \Omega_f \) is a forcing term.

One of the main advantages of the LBM is that is capable of solving complex non-linear PDEs by solving the system of first order linear PDEs given by Eq. (1). For instance, solving Eq. (1) and imposing conservation of mass and momentum in the collisions operator, the incompressible Navier-Stokes equations can be recovered at the macroscopic level (Chen and Doolen 1998).

In order to solve Eq. (1) we need to specify how to discretize space and time. This discretization is made by discretizing space in lattices (Figure 2.1) and time in time steps, and allowing the particles to move only from one lattice node to another one in each time step.

Figure 2.1: D2Q5 and D2Q9 lattices. D stands for the number of dimensions and Q stands for the number of lattice velocities.
The discrete velocity fields used in this study include D1Q3 (one dimension and three lattice speeds), D2Q5 lattice (two dimensions and five lattice speeds) and D2Q9 lattice (two dimensions and nine lattice speeds), all of them including a particle distribution function with zero velocity for resting particles. Each direction given by \( \mathbf{e}_i \) (Figure 2.1) represents a characteristic direction for Eq. (1) and for the corresponding particle distribution function and in each time step, the particle distribution functions arrive at neighboring nodes at the same time through the prescribed connections.

The LBE is obtained by integrating Eq. (1) in time along the \( i \) direction. This yields to:

\[
\frac{\partial f_i}{\partial t}(x + c_i \Delta t, t + \Delta t) = f_i(x, t) + \Delta t \Omega_i + \Delta t F_i
\]

where \( \Delta t \) is the time step, and \( F_i \) represents the forcing term. The next step in developing the LBM is to specify how the collision process is carried out. The collision process has to relax the particle distribution functions to a prescribed equilibrium state that depends on the macroscopic variables (in this work, concentration and velocity). The Bhatnagar-Gross-Krook (BGK) model (Bhatnagar et al. 1954) has been used as a collision operator due to its simplicity while keeping the essence of the collision process. The BGK operator consists of relaxing the particle distribution to the equilibrium proportionally to the deviation from the equilibrium:

\[
\Delta t \Omega_i = -\frac{1}{\tau}(f_i(x,t) - f_i^{eq}(x,t))
\]

where \( f_i^{eq} \) is the EDF for particles moving with lattice speed \( \mathbf{e}_i \); and \( \tau \) is called the single relaxation time and is a numerical parameter that relates to the viscosity in fluid flows and to the dispersion coefficients when solving advection-dispersion type equations. Moreover, the relaxation time plays an essential role in the stability and accuracy of the LBM. Inserting Eq. (3) into Eq. (2), the lattice Boltzmann equation with BGK collision operator (LBGK) reads
\[ f_i(x + c_i\Delta t, t + \Delta t) = f_i(x, t) - \frac{1}{\tau_s}(f_i(x, t) - f_i^{eq}(x, t)) + \frac{1}{\tau_a}(f_i^{as}(x, t) - f_i^{aeq}(x, t)) + F_i(x, t)\Delta t \] (4)

The LBM is classified within the mesoscopic methods because LBM simulates macroscopic transport processes based on microscopic models and mesoscopic kinetic equations (Chen and Doolen 1998).

### 2.2 From the Discrete Boltzmann Equation to the LTRT Model

Although the BGK is the collision operator most extensively used, other collision operators such as the two relaxation times (TRT) have been introduced to improve the performance of the LBM. The lattice Boltzmann equation with TRT collision operator (LTRT) is equivalent to two BGK operators, each one relaxing the symmetric and anti-symmetric parts of the particle distribution functions respectively. Then, the LTRT reads as follows

\[ f_i(x + c_i\Delta t, t + \Delta t) = f_i(x, t) - \frac{1}{\tau_s}(f_i^{as}(x, t) - f_i^{aeq}(x, t)) + \frac{1}{\tau_a}(f_i^{as}(x, t) - f_i^{aeq}(x, t)) + F_i(x, t)\Delta t \] (5)

where the superscripts \( s \) and \( a \) stand for symmetric and anti-symmetric parts. The symmetric and anti-symmetric parts of \( f_i \) and \( f_i^{eq} \) are obtained as follows

\[ f_i^{as} = \frac{f_i + \bar{f}_i}{2}; \quad f_i^{aeq} = \frac{f_i - \bar{f}_i}{2} \]
\[ f_i^{as} = \frac{f_i^{eq} + \bar{f}_i^{eq}}{2}; \quad f_i^{aeq} = \frac{f_i^{eq} - \bar{f}_i^{eq}}{2} \] (6)

where the over bar means particles moving in opposite direction to the \( i \) direction (\( \bar{c}_i = -c_i \)).

The LTRT model, despite of being more sophisticated than the LBGK, it does not significantly increases the computational effort to compute Eq. (5) over the LBGK (Ginzburg 2005). Besides, the memory demand is the same for the LTRT and LBGK. It can be easily seen that the LTRT becomes the LBGK models when \( \tau_a = \tau_s \).
Evolution of particle distribution functions using Eq.(5) can be split in two steps: the collision step and the streaming step. In the collision step, the collision operation takes place immediately when \( f_i(x,t) \) arrives at the node. According to TRT collision operator the changes of \( f_i(x,t) \) due to collision are denoted by \( \Delta f_i(x,t) = -\tau_x^{-1}(f'^i_i(x,t) - f^{\text{seq}}_i(x,t)) - \tau_a^{-1}(f'^a_i(x,t) - f^{\text{aeq}}_i(x,t)) \). Therefore, the new particle distribution functions after collision are the summation of \( f_i \), \( \Delta f_i(x,t) \), and \( F_i(x,t)\Delta t \)

\[
f'^i_i(x,t) = f_i(x,t) + \Delta f_i(x,t) + F_i(x,t)\Delta t
\] (7)

Once the particle distribution functions after collision have been obtained, they are streamed to the neighboring nodes with velocity \( c_i \) (Figure 2.2), which is expressed in the following equation

\[
f_i(x + c_i\Delta t, t + \Delta t) = f'^i_i(x,t)
\] (8)

and it is obvious that Eq. (5) is obtained by combining Eq. (7) and (8).

---

**STREAMING STEP**

\[
f'_i(x+c_i\Delta t,t+\Delta t)=f'_i(x,t)
\]

\[
f'_i(x,t)\quad f'_i(x+c_i\Delta t,t+\Delta t)
\]

**COLLISION STEP**

\[
f'_i(x,t)=f_i(x,t)-1/\tau_s(f^s_i(x,t)-f^{\text{seq}}_i(x,t))-1/\tau_a(f^a_i(x,t)-f^{\text{aeq}}_i(x,t))+F_i\Delta t
\]

\[
f_i(x,t)\quad f'_i(x,t)
\]

**Figure 2.2:** Collision and streaming steps.
2.3 LBM for Mass Transport

Although the LBM was first developed to solve hydrodynamics equations, we focus in this work to solve transport equations such as diffusion and advection-dispersion type equations. When using the LBM to solve hydrodynamics equations, two constraints are imposed to the particle distributions: conservation of mass and momentum in the collision operator. These two constraints are expressed as follows:

\[
\sum_i f_i(x, t) = \sum_i f_i^{eq}(x, t) = \rho(x, t)
\]

\[
\sum_i f_i(x, t) c_{ia} = \sum_i f_i^{eq}(x, t) c_{ia} = \rho(x, t) u_\alpha(x, t)
\]

(9)

where \(\rho\) represents the density of the fluid and \(u_\alpha\) is the macroscopic velocity. The density is obtained in each time step by \(\rho = \sum_i f_i\), and the flow field is obtained afterwards by \(u_\alpha = \sum_i f_i c_{ia} / \rho\). On the other hand, when solving mass transport problems, the conservation of momentum is not necessary since the flow field is given beforehand, and only \(\sum_i f_i = \sum_i f_i^{eq}\) is imposed.

2.4 Equilibrium Distribution Functions

In the previous sections, the LBM has been introduced as a set of first order partial linear differential equations (with \(f_i\) as independent variables) that are solved simultaneously by alternating collision and streaming steps with the only constraint of \(\sum_i f_i = \sum_i f_i^{eq}\). Now the reader may ask: how can the LBM solve different types of equations? What is to be chosen by the practitioner to guarantee that the former technique solves a specific PDE? The answer is: the equilibrium and the forcing terms.
The EDFs are the key for making the LBM suitable to solve a specific partial PDE. Specifically the moments of the EDFs and forcing terms in the kinetic space are what determine the macroscopic PDE recovered by the LBM, and they are giving by:

\[
M_0(x,t) = \sum_i f_{i}^{eq} (x,t) = \sum_i f_{i}^{eq} (x,t) \\
M_{1a}(x,t) = \sum_i f_{i}^{eq} (x,t)c_{i\alpha} = \sum_i f_{i}^{eq} (x,t)c_{i\alpha} \\
M_{2ab}(x,t) = \sum_i f_{i}^{eq} (x,t)c_{i\alpha}c_{i\beta} = \sum_i f_{i}^{eq} (x,t)c_{i\alpha}c_{i\beta} \\
M_{3abc}(x,t) = \sum_i f_{i}^{eq} (x,t)c_{i\alpha}c_{i\beta}c_{i\gamma} = \sum_i f_{i}^{eq} (x,t)c_{i\alpha}c_{i\beta}c_{i\gamma}
\] (10)

The EDFs can be expressed as

\[
f_{i}^{eq} (x,t) = M_0(x,t)g_{i}^{eq}(x,t)
\] (11)

where \(g_{i}^{eq}\) is a dimensionless EDF, and represents how the conserve variable is distributed along each direction. In following sections, it is shown that the dimensionless EDFs depend on local dimensionless numbers such as the Courant number and the lattice Peclet number.

2.5 Recovery of Macroscopic PDE

In this section we show what PDE is recovered by the LTRT model when only conservation of \(\sum_i f_i = \sum_i f_i^{eq}\) is imposed. To obtain the macroscopic differential equation, \(f_i(x + c_i \Delta t, t + \Delta t)\) is expanded around \((x,t)\) using Taylor series expansion:

\[
f_i(x + c_i \Delta t, t + \Delta t) = f_i(x) + \sum_{n=1}^{\infty} \frac{\Delta t^n}{n!} \left( \frac{\partial}{\partial t} + c_i \frac{\partial}{\partial x} \right)^n f_i(x)
\] (12)

The recovery procedure is based on a multi-scale analysis, in which time and space derivatives are expanded as follows:

\[
\frac{\partial}{\partial t} = \epsilon \frac{\partial}{\partial t_1} + \epsilon^2 \frac{\partial}{\partial t_2} + \epsilon^3 \frac{\partial}{\partial t_3}
\] (13)
\[ \frac{\partial}{\partial \alpha} = \varepsilon \frac{\partial}{\partial \alpha_i} \]  

(14)

where \( \varepsilon \) is the Knudsen number (Chen and Doolen 1998). Particle distribution functions \( f_i(x, t) \), \( f_i^x(x, t) \) and \( f_i^a(x, t) \) are perturbed around the equilibrium distribution functions \( f_i^{eq}(x, t) \), \( f_i^{seq}(x, t) \) and \( f_i^{aeq}(x, t) \), respectively:

\[
f_i = f_i^{eq} + \sum_{k=1}^{\infty} \left[ \varepsilon^k f_i^{(k)} \right] 
\]

\[
f_i^x = f_i^{seq} + \sum_{k=1}^{\infty} \left[ \varepsilon^k f_i^{x(k)} \right] 
\]

\[
f_i^a = f_i^{aeq} + \sum_{k=1}^{\infty} \left[ \varepsilon^k f_i^{a(k)} \right] 
\]

where \( f_i^{(k)} \), \( f_i^{x(k)} \) and \( f_i^{a(k)} \) are the perturbation terms. The forcing term is also expanded as

\[
F_i = \sum_{k=1}^{\infty} \left[ \varepsilon^k F_i^{(k)} \right] 
\]

(15)

Introducing Eqs.(12)-(15) into Eq.(5), we obtain

\[
\sum_{n=1}^{\infty} \left[ \frac{\Delta n}{n!} \left\{ \varepsilon \frac{\partial}{\partial t} + \varepsilon^2 \frac{\partial}{\partial t_2} + \varepsilon^3 \frac{\partial}{\partial t_3} + \varepsilon c_{ia} \frac{\partial}{\partial \alpha_i} \right\}^n \left( f_i^{eq} + \sum_{k=1}^{\infty} \left[ \varepsilon^k f_i^{(k)} \right] \right) \right] 
\]

\[
= \sum_{k=1}^{\infty} \left[ \varepsilon^k \left( -\frac{1}{\tau_s} f_i^{x(k)} - \frac{1}{\tau_a} f_i^{a(k)} + \Delta t F_i^{(k)} \right) \right] 
\]

(17)

Grouping terms of same order leads to

\[
O(\varepsilon): \Delta t \left\{ \frac{\partial}{\partial t_1} + c_{ia} \frac{\partial}{\partial \alpha_i} \right\} f_i^{eq} = -\frac{1}{\tau_s} f_i^{x(1)} - \frac{1}{\tau_a} f_i^{a(1)} + \Delta t F_i^{(1)} 
\]

(18)

\[
O(\varepsilon^2): \Delta t \left\{ \frac{\partial}{\partial t_2} f_i^{eq} + \left\{ \frac{\partial}{\partial t_1} + c_{ia} \frac{\partial}{\partial \alpha_i} \right\} f_i^{(1)} \right\} + \frac{\Delta t}{2} \left( \frac{\partial}{\partial t_1} + c_{ia} \frac{\partial}{\partial \alpha_i} \right)^2 f_i^{eq} 
\]

\[
= -\frac{1}{\tau_s} f_i^{x(2)} - \frac{1}{\tau_a} f_i^{a(2)} + \Delta t F_i^{(2)} 
\]

(19)
Let the n\textsuperscript{th} moments of \( f_i^{eq} \), \( f_i^{(k)} \) and \( F^{(k)} \) in the particle velocity field be

\[
M_{n\alpha\beta\gamma} = \sum_i f_i^{eq} c_{i\alpha} c_{i\beta} \cdots c_{i\gamma} \\
M_{n\alpha\beta\gamma}^{(k)} = \sum_i f_i^{(k)} c_{i\alpha} c_{i\beta} \cdots c_{i\gamma} \\
M_{n\alpha\beta\gamma}^{F(k)} = \sum_i F_i^{(k)} c_{i\alpha} c_{i\beta} \cdots c_{i\gamma}
\]

Therefore, \( \sum_i \text{Eq. (18)} \) derives the first order equation:

\[
O(\varepsilon): \quad \frac{\partial M_0}{\partial t_1} + \frac{\partial M_{1a}}{\partial \alpha_1} = M_0^{F(1)}
\]

\( \sum_i \text{Eq. (19)} \) derives the second order equation:

\[
O(\varepsilon^2): \quad \frac{\partial M_0}{\partial t_2} + \frac{\partial M_{1a}}{\partial t_1} + \frac{\partial M_{1a}}{\partial \alpha_1} + \frac{\Delta t}{2} \left( \frac{\partial^2 M_0}{\partial t_1^2} + 2 \frac{\partial^2 M_{1a}}{\partial t_1 \partial \alpha_1} + \frac{\partial^2 M_{2\alpha\beta}}{\partial \alpha_1 \partial \beta_1} \right) = M_0^{F(2)}
\]

where \( M_0^{(1)} = 0 \) since \( \sum_i f_i = \sum_i f_i^{eq} \), which implies \( M_0^{(k)} = 0 \) \( \forall k \geq 1 \). \( \sum c_{i\alpha} \text{Eq. (18)} \) derives

\[
M_{1a}^{(1)}:
\]

\[
M_{1a}^{(1)} = -\Delta t \tau_a \left( \frac{\partial M_{1a}}{\partial t_1} + \frac{\partial M_{2\alpha\beta}}{\partial \beta_1} \right) + \Delta t \tau_a M_0^{F(1)}
\]

Inserting Eq. (22) and Eq. (24) into Eq. (23):

\[
O(\varepsilon^2):
\]

\[
\frac{\partial M_0}{\partial t_2} = \Delta t \left[ \tau_a - \frac{1}{2} \left( \frac{\partial^2 M_{1a}}{\partial t_1 \partial \alpha_1} + \frac{\partial^2 M_{2\alpha\beta}}{\partial \alpha_1 \partial \beta_1} \right) - \Delta t \frac{\partial M_0^{F(1)}}{\partial t_1} - \Delta t \tau_a \frac{\partial M_{1a}^{F(1)}}{\partial \alpha_1} + M_0^{F(2)} \right]
\]
\[ \sum_i \text{Eq. (20)} \text{ derives the third order equation:} \]

\[
O(e^3): \frac{\partial M_{0}}{\partial t_3} + \frac{\partial M_{1}^{(1)}}{\partial t_2} + \left( \frac{\partial M_{0}^{(2)}}{\partial t_1} + \frac{\partial M_{1}^{(2)}}{\partial \alpha_1} \right) + \Delta t \frac{\partial}{\partial t_2} \left( \frac{\partial M_{0}}{\partial t_1} + \frac{\partial M_{1}^{(1)}}{\partial \alpha_1} \right) \\
+ \frac{\Delta t}{2} \left( \frac{\partial^2 M_{0}}{\partial t_1 \partial \alpha_2} + \frac{\partial^2 M_{1}^{(1)}}{\partial \alpha_1 \partial \alpha_2} \right) + \frac{\Delta t}{2} \left( \frac{\partial^2 M_{0}^{(1)}}{\partial \alpha_1 \partial \alpha_2} + \frac{\partial^2 M_{1}^{(2)}}{\partial t_1 \partial \alpha_2} \right) \\
+ \frac{\Delta t^2}{6} \left( \frac{\partial^3 M_{0}}{\partial t_1^3} + \frac{3 \partial^3 M_{1}^{(1)}}{\partial t_1 \partial \alpha_1 \partial \alpha_2} + \frac{3 \partial^3 M_{2 \alpha \beta}}{\partial t_1 \partial \alpha_1 \partial \beta_1} + \frac{\partial^3 M_{3 \alpha \beta \gamma}}{\partial \alpha_1 \partial \beta_1 \partial \gamma_1} \right) = M_0^{F(3)} \tag{26} \\
\]

\[ M_{2 \alpha \beta}^{(1)} \text{ is derived from } \sum_i c_{\alpha \beta} \text{ Eq. (18):} \]

\[
M_{2 \alpha \beta}^{(1)} = -\Delta t \tau_s \left( \frac{\partial M_{2 \alpha \beta}}{\partial t_1} + \frac{\partial M_{3 \alpha \beta \gamma}}{\partial \gamma_1} \right) + \Delta t \tau_s M_{2 \alpha \beta}^{F(1)} \tag{27} \\
\]

\[ M_{1 \alpha}^{(2)} \text{ is obtained by } \sum_i c_{\alpha} \text{ Eq. (19):} \]

\[
M_{1 \alpha}^{(2)} = -\tau_a \Delta t \frac{\partial M_{1 \alpha}}{\partial t_2} - \Delta t \left( \frac{\partial M_{1 \alpha}}{\partial t_1} + \frac{\partial M_{2 \alpha \beta}}{\partial \beta_1} \right) \\
- \tau_a \frac{\Delta t^2}{2} \left( \frac{\partial^2 M_{1 \alpha}}{\partial t_1^2} + \frac{3 \partial^2 M_{2 \alpha \beta}}{\partial t_1 \partial \beta_1} + \frac{3 \partial^2 M_{3 \alpha \beta \gamma}}{\partial t_1 \partial \beta_1 \partial \gamma_1} \right) + \Delta t \tau_a M_{1 \alpha}^{F(2)} \tag{28} \\
\]

Inserting Eqs. (24) and (27) into Eq. (28):

\[
M_{1 \alpha}^{(2)} = -\tau_a \Delta t \frac{\partial M_{1 \alpha}}{\partial t_2} + \Delta t \tau_s \left( \tau_s - \frac{1}{2} \right) \left( \frac{\partial^2 M_{3 \alpha \beta}}{\partial t_1^2} + \frac{\partial^2 M_{2 \alpha \beta}}{\partial \beta_1^2} \right) \\
+ \Delta t \tau_s \left( \tau_s - \frac{1}{2} \right) \left( \frac{\partial^2 M_{3 \alpha \beta \gamma}}{\partial t_1 \partial \beta_1 \partial \gamma_1} + \Delta t \tau_s M_{1 \alpha}^{F(2)} - \Delta t \tau_s \frac{\partial M_{1 \alpha}^{(1)}}{\partial t_2} - \Delta t \tau_s \frac{\partial M_{1 \alpha}^{(1)}}{\partial \beta_1} \right) \tag{29} \\
\]

Inserting \( M_0^{(4)} = 0 \), Eqs. (22) and (25) into Eq. (26):

\[
O(e^3): \frac{\partial M_{0}}{\partial t_3} + \frac{\partial M_{1}^{(2)}}{\partial t_2} + \Delta t \left( \frac{\partial^2 M_{1}^{(2)}}{\partial t_1 \partial \alpha_1} + \frac{\partial^2 M_{1}^{(1)}}{\partial \alpha_1 \partial \beta_1} \right) + \Delta t \left( \frac{\partial^2 M_{0}^{(2)}}{\partial \alpha_1 \partial \beta_1} + \frac{\partial^2 M_{1}^{(1)}}{\partial t_1 \partial \beta_1} \right) \\
+ \frac{\Delta t^2}{6} \left( 2 \frac{\partial^3 M_{1 \alpha}}{\partial t_1^2 \partial \alpha_1} + 3 \frac{\partial^3 M_{2 \alpha \beta}}{\partial t_1 \partial \alpha_1 \partial \beta_1} + \frac{\partial^3 M_{3 \alpha \beta \gamma}}{\partial \alpha_1 \partial \beta_1 \partial \gamma_1} \right) = M_0^{F(3)} - \frac{\Delta t \partial M_{0}^{(4)}}{2 \partial t_2} - \frac{\Delta t^2 \partial^2 M_{0}^{(1)}}{6 \partial t_1^2} \tag{30} \\
\]
Inserting Eqs. (24), (27) and (29) into Eq.(30):

\[
O(\varepsilon^3): \quad \frac{\partial M_0}{\partial t_3} = \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial^2 M_{1\alpha}}{\partial t_3 \partial \alpha_1} - \Delta t^2 h_1(\tau_a) \left( \frac{\partial^3 M_{1\alpha}}{\partial t_3 \partial \alpha_1} + \frac{\partial^3 M_{2\alpha\beta}}{\partial t_3 \partial \alpha_1 \partial \beta_1} \right) \\
- \Delta t^2 h_2(\tau_a, \tau_s) \left( \frac{\partial^3 M_{2\alpha\beta}}{\partial t \partial \alpha_1 \partial \beta_1} + \frac{\partial^3 M_{3\alpha\beta\gamma}}{\partial \alpha_1 \partial \beta_1 \partial \gamma_1} \right) + M_{0}^{F(3)} - \frac{\Delta t}{2} \frac{\partial M_{0}^{F(2)}}{\partial t_1} - \frac{\Delta t}{2} \frac{\partial M_{0}^{F(1)}}{\partial t_2} \\
- \Delta \tau_a \frac{\partial M_{1\alpha}^{F(2)}}{\partial \alpha_1} + \Delta \tau_a \left( \frac{1}{12} \partial^2 M_{0}^{F(1)} \right) + \Delta \tau_a \left( \frac{\tau_a - 1}{2} \right) \frac{\partial^2 M_{1\alpha}^{F(1)}}{\partial t \partial \alpha_1} + \Delta \tau_a \left( \frac{\tau_a - 1}{2} \right) \frac{\partial^2 M_{2\alpha\beta}^{F(1)}}{\partial \alpha_1 \partial \beta_1}
\]

where

\[
h_1(\tau_a) = (\tau_a - 1/2)^2 - 1/6 \tag{32}
\]

\[
h_2(\tau_a, \tau_s) = (\tau_a - 1/2)(\tau_s - 1/2) - 1/12 \tag{33}
\]

The macroscopic PDE recovered is obtained via $\varepsilon x$ Eq.(22) + $\varepsilon^2$ Eq.(25) + $\varepsilon^3$ xEq.(31), using $\partial \alpha_1 = \partial \alpha$ and $\partial \beta_1 = \partial \beta$, and neglecting forth and fifth terms in $\varepsilon$:

\[
\frac{\partial M_0}{\partial t} + \frac{\partial M_{1\alpha}}{\partial \alpha} = \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial^2 M_{2\alpha\beta}}{\partial \alpha \partial \beta} + \Delta t \left( \tau_s - \frac{1}{2} \right) \frac{\partial^3 M_{1\alpha}}{\partial t \partial \alpha} \\
- \Delta t^2 h_1(\tau_a) \left( \frac{\partial^3 M_{1\alpha}}{\partial t^2 \partial \alpha} + \frac{\partial^3 M_{2\alpha\beta}}{\partial t \partial \alpha \partial \beta} \right) - \Delta t^2 h_2(\tau_a, \tau_s) \left( \frac{\partial^3 M_{2\alpha\beta}}{\partial t \partial \alpha \partial \beta} + \frac{\partial^3 M_{3\alpha\beta\gamma}}{\partial \alpha \partial \beta \partial \gamma} \right) \\
+ M_{0}^{F} - \frac{\Delta t}{2} \frac{\partial M_{0}^{F}}{\partial t} - \Delta \tau_a \frac{\partial M_{1\alpha}^{F}}{\partial \alpha} + \Delta \tau_a \left( \frac{1}{12} \partial^2 M_{0}^{F} \right) + \Delta \tau_a \left( \tau_a - \frac{1}{2} \right) \frac{\partial^2 M_{1\alpha}^{F}}{\partial t \partial \alpha} + \Delta \tau_a \left( \frac{\tau_a - 1}{2} \right) \frac{\partial^2 M_{2\alpha\beta}^{F}}{\partial \alpha \partial \beta}
\]

2.6 Summary

In this chapter, the LBM has been introduced from its origin to solve fluid flows based on the kinetic theory of gases and extended for applications to mass transport problems in general. Then, the standard BGK and the more sophisticated TRT collision operator has been introduced.

The equilibrium and the forcing terms have been shown to be the key to recover a specific PDE. Finally, general expressions of the macroscopic PDE recovered up to third order in $\varepsilon$ have been obtained by means of multi-scale analysis, showing the dependency of this PDE on the kinetic moments of the equilibrium.
3.1 Recovery of the Diffusion Equation

This section shows how LBM can be used to solve the diffusion equation. Although this might be the simplest case, it is very valuable in order to understand how the recovery of the macroscopic PDE is carried out. The diffusion equation can be expressed as

\[
\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial \alpha \partial \alpha}
\]  

(35)

where we assume that \( C \) is concentration of some conservative substance (or simply an extensive variable); \( D \) is the diffusion coefficient; \( \alpha \) represents the Cartesian variables and repeated indexes means summation. In order to solve the diffusion equation with the LBM, we need to carefully select appropriate EDFs. We use

\[
f_{i}^{eq} = C \omega_i \frac{c^2}{c_x^2} \quad i > 0
\]

\[
f_{0}^{eq} = C - \sum_{i>0} f_{i}^{eq}
\]

(36)

where \( c = \Delta x / \Delta t \) is called the lattice speed; \( c_s \) is a numerical parameter; and \( \omega_i \) are weighting factors that depend on the lattice to be used:

\[
\begin{align*}
D1Q3: & \quad \omega_i = 1/2 \quad i = 1, 2 \\
D2Q5: & \quad \omega_i = 1/2 \quad i = 1, 2, 3, 4 \\
D2Q9: & \quad \omega_i = \begin{cases} 
1/3 & i = 1, 2, 3, 4 \\
1/9 & i = 5, 6, 7, 8 
\end{cases}
\end{align*}
\]  

(37)

The parameter \( c_s \) is known as the speed of sound because it represents a numerical speed of sound when using LBM to solve fluid flows. However, it does not represent any speed of sound when solving mass transport problems.
The EDFs in Eq. (36) recover the following moments

\[ M_0 = C \]
\[ M_{1\alpha} = 0 \]
\[ M_{2\alpha\beta} = \delta_{\alpha\beta}c_s^2 \]  

(38)

Introducing Eq. (38) into Eqs. (22) and (25) we get

\[ O(\varepsilon) : \frac{\partial C}{\partial t_i} = 0 \]  

(39)

\[ O(\varepsilon^2) : \frac{\partial C}{\partial t_2} = \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial^2 C}{\partial \alpha_i^2} \]  

(40)

\[ O(\varepsilon^3) : \frac{\partial C}{\partial t_3} = -\Delta t^2 \left[ h_1(\tau_a) + h_2(\tau_a, \tau_s) \right] \frac{\partial^3 C}{\partial t_i \partial \alpha_i} \]  

(41)

Using a constant and uniform value for \( c_s^2 \)

\[ O(\varepsilon^2) : \frac{\partial C}{\partial t_2} = \Delta t \left( \tau_a - \frac{1}{2} \right) c_s^2 \frac{\partial^2 C}{\partial \alpha_i^2} \]  

(42)

\[ O(\varepsilon^3) : \frac{\partial C}{\partial t_3} = -\Delta t^2 c_s^2 \left[ \left( \tau_a - \frac{1}{2} \right)^2 + \left( \tau_a - \frac{1}{2} \right) \left( \tau_s - \frac{1}{2} \right) - \frac{1}{4} \right] \frac{\partial^3 C}{\partial t_i \partial \alpha_i} \]  

(43)

In order to obtain the macroscopic PDE solved by the LBM, we need to combine the equations obtained by the multi-scale analysis as follows: \( \varepsilon \) x Eq. (39) + \( \varepsilon^2 \) x Eq. (42) + \( \varepsilon^3 \) x Eq. (43)

\[ \left( \varepsilon \frac{\partial}{\partial t_1} + \varepsilon^2 \frac{\partial}{\partial t_2} + \varepsilon^3 \frac{\partial}{\partial t_3} \right) C = \Delta t \left( \tau_a - \frac{1}{2} \right) c_s^2 \varepsilon^2 \frac{\partial^2 C}{\partial \alpha_i^2} - \Delta t^2 c_s^2 \left[ \left( \tau_a - \frac{1}{2} \right)^2 + \left( \tau_a - \frac{1}{2} \right) \left( \tau_s - \frac{1}{2} \right) - \frac{1}{4} \right] \frac{\partial^3 C}{\partial t_i \partial \alpha_i} \]  

(44)

and considering the multi-scale expansion up to third order in time \( \partial_t = \varepsilon \partial_{t_1} + \varepsilon^2 \partial_{t_2} + \varepsilon^3 \partial_{t_3} \); and first order in space \( \partial_\alpha = \varepsilon \partial_{\alpha_i} \)
\[ \frac{\partial C}{\partial t} = \Delta t \left( r_s - \frac{1}{2} \right) c_s^2 \frac{\partial^2 C}{\partial \alpha_i^2} - \Delta t^2 c_s^2 \left[ \left( r_s - \frac{1}{2} \right)^2 + \left( r_s - \frac{1}{2} \right) \left( r_s - \frac{1}{2} \right) - \frac{1}{4} \right] \frac{\partial^3 C}{\partial t \partial \alpha^2} + O(\varepsilon^4) \] (45)

Finally, selecting the time step, anti-symmetric relaxation time and speed of sound such that
\[ D = c_s^2 \Delta t \left( r_s - \frac{1}{2} \right) \] (46)
the macroscopic equation recovered up to third order in \( \varepsilon \) is
\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial \alpha_i^2} - \Delta t D \left( r_s - \frac{1}{2} \right)^{-1} \left[ \left( r_s - \frac{1}{2} \right)^2 + \left( r_s - \frac{1}{2} \right) \left( r_s - \frac{1}{2} \right) - \frac{1}{4} \right] \frac{\partial^3 C}{\partial t \partial \alpha^2} \] (47)

Choosing the relaxation times such that \( (r_s - 1/2)^2 + (r_s - 1/2) (r_s - 1/2) - 1/4 = 0 \), the diffusion equation is recovered up to third order in \( \varepsilon \). For the special case where the BGK model is used (\( r_s = r_s = r \)), the aforementioned condition becomes: \( 2 (r - 1/2)^2 - 1/4 = 0 \). And the resulting relaxation time for obtaining third order accuracy is: \( r = 0.5 + 8^{-1/2} \approx 0.8536 \).

3.2 Advection-Diffusion Equation

Proceeding as in section 3.2 the advection-diffusion equation can be recovered by an appropriate selection of EDFs. In this section the multi-scale expansion is considered only up to second order in time: \( \partial_i = \omega \partial_{i_1} + \varepsilon^2 \partial_{i_2} \). Third order analysis on the advection-diffusion equation is carried out in Chapter 4.

3.2.1 Recovery with Linear EDFs

When the LBM was first used to solve the advection-diffusion equation in Flekkøy (1993), the EDFs used were linearly dependent on the macroscopic velocity. The linear EDFs are as follows
\[ f_i^{eq} = C \omega_i \left( \frac{c_s^2}{c_i^2} + \frac{u \cdot c_i}{c^2} \right), \quad i > 0; \quad f_0^{eq} = C - \sum_{i>0} f_i^{eq} \] (48)
with weighting factors depending on the lattice to be used.

\[ D1Q3: \omega_i = \frac{1}{2} \quad i = 1, 2 \]
\[ D2Q5: \omega_i = \frac{1}{2} \quad i = 1, 2, 3, 4 \]
\[ D2Q9: \omega_i = \begin{cases} 
\frac{1}{3} & i = 1, 2, 3, 4 \\
\frac{1}{9} & i = 5, 6, 7, 8 
\end{cases} \quad (49) \]

The EDFs in Eq. (36) recover the following moments

\[ M_0 = C \]
\[ M_{i\alpha} = C \mu_\alpha \]
\[ M_{i\alpha j\beta} = \delta_{\alpha j} C c_s^2 \]

Introducing Eq. (38) into Eqs. (22) and (25)

\[ O(\varepsilon): \quad \frac{\partial C}{\partial t} + \frac{\partial C u_\alpha}{\partial \alpha_i} = 0 \quad (51) \]
\[ O(\varepsilon^2): \quad \frac{\partial C}{\partial t^2} = \Delta t \left( \tau - \frac{1}{2} \right) \frac{\partial^2 C c_s^2}{\partial \alpha_i^2} + \Delta t \left( \tau - \frac{1}{2} \right) \frac{\partial^3 C u_\alpha}{\partial t \partial \alpha_i} \quad (52) \]

Using Eq. (46) in Eq. (52) and combining \( \varepsilon \times \text{Eq. (51)} + \varepsilon^2 \times \text{Eq. (52)} \)

\[ \frac{\partial C}{\partial t} + \frac{\partial C u_\alpha}{\partial \alpha} = D \frac{\partial^2 C}{\partial \alpha^2} + \frac{D}{c_s^2} \frac{\partial}{\partial \alpha} \left( \varepsilon \frac{\partial C u_\alpha}{\partial t} \right) \quad (53) \]

Eq. (53) is the advection-diffusion equation plus a second order numerical diffusion term. The term \( \partial_i C u_\alpha \) can be split as \( C \partial_i u_\alpha + u_\alpha \partial_i C \). Then, using Eq. (51) it becomes

\[ \partial_i C u_\alpha = C \partial_i u_\alpha + u_\alpha \partial_i C \]. Finally Eq. (53) becomes

\[ \frac{\partial C}{\partial t} + \frac{\partial C u_\alpha}{\partial \alpha} = D \frac{\partial^2 C}{\partial \alpha^2} + \frac{D}{c_s^2} \frac{\partial}{\partial \alpha} \left( C \frac{\varepsilon}{c_s^2} \frac{\partial u_\alpha}{\partial t} + u_\alpha \frac{\partial C u_\beta}{\partial \beta} \right) \quad (54) \]

Assuming that there are no rapid time variations of flow \( \partial_i u_\alpha \approx 0 \) and incompressible flow \( \partial_\beta u_\beta = 0 \) (Flekkøy 1993), Eq. (54) becomes
\[
\frac{\partial C}{\partial t} + \frac{\partial C u_\alpha}{\partial \alpha} = D \frac{\partial}{\partial \alpha} \left( \frac{\delta_{\alpha\beta} + \frac{u_\alpha u_\beta}{c_s^2}}{\frac{\partial}{\partial \beta}} \frac{\partial C}{\partial \beta} \right) \tag{55}
\]

Eq. (55) becomes the advection-diffusion equation if \( u_\alpha u_\beta / c_s^2 \ll 1 \) (Flekkøy 1993). On the other hand, the speed ratio \( \Omega = c / c_s \) has to be higher than one since LBM is an explicit scheme and therefore nothing can propagate faster than the lattice speed to obtain stable solutions. Therefore, the condition \( u_\alpha u_\beta / c_s^2 \ll 1 \) implies that the Courant number has to be such that \( Cr^2 = u \cdot u / c^2 \ll 1 \), which imposed a big constraint for the applicability of the LBM.

### 3.2.2 Recovery with Quadratic EDFs

Ginzburg (2005) investigated how the second order numerical diffusion can be corrected by including quadratic terms of \( u \) in the EDFs. The quadratic EDFs are as follows

\[
f_{i}^{eq} = C \omega \left( \frac{c_s^2}{c^2} + \frac{\mathbf{u} \cdot \mathbf{c}}{c^2} + \frac{3}{2} \left( \frac{\mathbf{u} \cdot \mathbf{e}}{c^4} - \frac{1}{2} \frac{u \cdot u}{c^2} \right) \right), \quad i > 0
\]

\[
f_{0}^{eq} = C - \sum_{i=0} f_{i}^{eq}
\]

\[D1Q3: \omega_{i} = 1/2 \quad i = 1, 2\]

\[D2Q9: \omega_{i} = \begin{cases} 1/3 & i = 1, 2, 3, 4 \\ 1/9 & i = 5, 6, 7, 8 \end{cases} \tag{57}\]

The zero, first and second moments of the EDFs are

\[
M_0 = C
\]

\[
M_{1\alpha} = Cu_\alpha
\]

\[
M_{2\alpha\beta} = C \delta_{\alpha\beta} c_s^2 + Cu_\alpha u_\beta
\]

Introducing Eqs. (58) into Eqs. (22) and (25), and using \( D = c_s^2 AT (\tau_a - 1/2) \), the differential equation up to the first two orders in \( \varepsilon \) are

\[
O(\varepsilon): \quad \frac{\partial C}{\partial t} + \frac{\partial C u_\alpha}{\partial \alpha} = 0 \tag{59}
\]
\[ O(\varepsilon^2) : \frac{\partial C}{\partial t_2} = D \frac{\partial^2 C}{\partial \alpha_1^2} + \Delta t \left( \tau_\alpha - \frac{1}{2} \right) \frac{\partial}{\partial \alpha_1} \left[ \frac{\partial C u_\alpha}{\partial t_1} + \frac{\partial C u_{\alpha\beta}}{\partial \beta_1} \right] \] (60)

where the term \( \partial_\alpha (C u_\alpha) + \partial_\beta (C u_{\alpha\beta}) \) can be split as

\[ \frac{\partial C u_\alpha}{\partial t_1} + \frac{\partial C u_{\alpha\beta}}{\partial \beta_1} = u_\alpha \left( \frac{\partial C}{\partial t_1} + \frac{\partial C u_\beta}{\partial \beta_1} \right) + C \left( \frac{\partial u_\alpha}{\partial t_1} + u_\beta \frac{\partial u_\alpha}{\partial \beta_1} \right) \] (61)

In this work we assume that we are coping with Darcian flows (flows in porous media with Reynolds number based on the grain diameter of \( O(1) \)); therefore \( \partial_\alpha u_\alpha + u_\beta \partial_\beta u_\alpha \approx 0 \). Then, considering the first order equation (Eq. (59)), Eq. (61) becomes

\[ \frac{\partial C u_\alpha}{\partial t_1} + \frac{\partial C u_{\alpha\beta}}{\partial \beta_1} \approx 0 \] (62)

And Eq. (60) is further changed to

\[ O(\varepsilon^2) : \frac{\partial C}{\partial t_2} = D \frac{\partial^2 C}{\partial \alpha_1^2} \] (63)

Applying \( \varepsilon \times \text{Eq. (59)} + \varepsilon^2 \times \text{Eq. (63)} \), the macroscopic differential equation recovered is

\[ \left( \varepsilon \frac{\partial}{\partial t_1} + \varepsilon^2 \frac{\partial}{\partial t_2} \right) C + \varepsilon \frac{\partial C u_\alpha}{\partial t_1} = D \varepsilon^2 \frac{\partial^2 C}{\partial \alpha_1^2} \] (64)

and Eq. (64) recovers the advection-diffusion equation after the multi-scale expansion. Notice that in order to correct the second order diffusion, the second moment of the EDFs has to be \( M_{u_{\alpha\beta}} = C \delta_{u_{\alpha\beta}} c_\alpha^2 + C u_{\alpha\beta} \), which implies \( M_{2xy} = C u_x u_y \). In two dimensional cases, this condition cannot be achieved by all lattices. For instance, the \( D2Q5 \) lattice has \( M_{2xy} = 0 \). Hence than quadratic EDFs on \( D2Q5 \) lattices does not correct the second order numerical diffusion.

### 3.2.3 Recovery with Linear EDFs and Second Order Correction

Linear EDFs can recover the advection-diffusion equation on either \( D1Q3 \), \( D2Q5 \) or \( D2Q9 \) lattices, but only for small values of the Courant number. On the other hand, although
quadratic EDFs have no such a limitation in the Courant number, they require in the 2D case increasing the number of lattice directions from D2Q5 to D2Q9 in order to be capable of correcting the second order numerical diffusion. Hence, in this section new EDFs are proposed to achieve second order accuracy without the limitation of \( Cr^2 \ll 1 \) on a D2Q5.

The PDE recovered by the LBM when using linear EDFs is given in Eq. (53). Reordering terms we get

\[
\frac{\partial C}{\partial t} + \frac{\partial C u_a}{\partial \alpha} - \varepsilon \frac{\partial}{\partial \alpha_i} \left( \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial C u_a}{\partial \tau_i} \right) = D \frac{\partial^3 C}{\partial \alpha^2} \tag{65}
\]

Introducing \( \varepsilon \partial_t = \partial_t - \varepsilon^2 \partial_{t^2} \) and neglecting third order terms in \( \varepsilon \)

\[
\frac{\partial C}{\partial t} + \frac{\partial C u_a}{\partial \alpha} = D \frac{\partial^3 C}{\partial \alpha^2} + \varepsilon \frac{\partial}{\partial \alpha_i} \left( \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial C u_a}{\partial t} \right) \tag{66}
\]

In order to correct the numerical error, we introduce the following forcing term

\[
F_0 = 0 \tag{67}
\]

\[
F_i = \frac{1}{2 \tau_a} \left( \tau_a - \frac{1}{2} \right) \left[ C u \cdot c_i \right] - \left[ C u \cdot c_i \right]^{t - \Delta t} \frac{1}{c^2}; \quad i = 1, 2, 3, 4
\]

Using Taylor series expansion for \( C u \)

\[
F_0 = 0 \tag{68}
\]

\[
F_i = \frac{1}{2 \Delta t \tau_a} \left( \tau_a - \frac{1}{2} \right) \frac{1}{c^2} \left( \Delta t \frac{\partial C u \cdot c_i}{\partial t} - \frac{\Delta t^2}{2} \frac{\partial^2 C u \cdot c_i}{\partial t^2} + \ldots \right); \quad i = 1, 2, 3, 4
\]

Introducing \( \varepsilon \partial_t = \varepsilon \partial_t + \varepsilon^2 \partial_{t^2} \) into Eq. (68) we obtain

\[
F_0^{(i)} = 0 \tag{69}
\]

\[
F_i^{(i)} = \frac{1}{2 \tau_a} \left( \tau_a - \frac{1}{2} \right) \frac{1}{c^2} \frac{\partial C u \cdot c_i}{\partial \tau_i}; \quad i = 1, 2, 3, 4
\]

\[
F_i^{(2)} = \frac{1}{2 \tau_a} \left( \tau_a - \frac{1}{2} \right) \frac{1}{c^2} \left( \frac{\partial C u \cdot c_i}{\partial \tau_i} - \frac{\Delta t}{2} \frac{\partial^2 C u \cdot c_i}{\partial \tau_i^2} \right); \quad i = 1, 2, 3, 4
\]
And the moments of the forcing terms are

\[ M_{a}^{F(k)} = 0; \quad k \geq 1 \]
\[ M_{1a}^{F(1)} = \frac{1}{\tau_{a}} \left( \frac{1}{2} \right) \partial_{t} \partial_{t_{1}} C_{u_{a}}; \quad i = 1, 2, 3, 4 \]
\[ M_{1a}^{F(2)} = \frac{1}{\tau_{a}} \left( \frac{1}{2} \right) \left( \frac{\partial C_{u_{a}}}{\partial t_{2}} - \frac{\Delta t}{\partial t_{1}^{2}} \right); \quad i = 1, 2, 3, 4 \]
\[ M_{2a}^{F(4)} = 0; \quad i = 1, 2, 3, 4 \]  

(70)

Inserting Eq. (50) and Eq. (70) into Eqs. (22) and (25):

\[ O(\varepsilon): \quad \frac{\partial C}{\partial t_{1}} + \frac{\partial C_{u_{a}}}{\partial \alpha_{i}} = 0 \]  

(71)

\[ O(\varepsilon^{2}): \quad \frac{\partial C}{\partial t_{2}} = D \frac{\partial^{2} C}{\partial \alpha_{i}^{2}} \]  

(72)

summing up \( \varepsilon \) x Eq. (71) + \( \varepsilon^{2} \) x Eq. (72), the advection-diffusion equation is recovered up to second order. The main advantage of using the second order correction via forcing term is that the advection-diffusion equation can be recovered up to second order on a D2Q5 lattice, while using quadratic EDFs require the D2Q9 lattice. Moreover, the forcing terms only depend on the local values of \( C \) at the present and previous time steps, keeping the LBM features of simplicity, locality and explicit scheme.

3.3 Dimensionless EDFs

In section 2.4, the dimensionless EDFs were introduced in Eq. (11). When solving the diffusion equation or the advection-diffusion equation, the dimensionless EDFs are

\[ f_{i}^{eq}(x, t) = C(x, t) g_{i}^{eq}(x, t) \]  

(73)

3.3.1 Dimensionless EDFs for the Diffusion Equation

The EDFs for the diffusion equation were given in Eq. (36). Applying Eq. (73) we obtain
\[ g_i^{eq} = \omega_i \Omega^{-2} \quad i > 0 \]
\[ g_0^{eq} = 1 - \sum_{i>0} g_i^{eq} \]  

(74)

where we have introduced the speed ratio \( \Omega = c / c_s \).

### 3.3.2 Dimensionless EDFs for the Advection-Diffusion Equation

Before writing down the dimensionless EDFs for the advection-diffusion equation, let’s introduce the lattice Peclet number and the local Courant number as

\[ Pe_{\Delta x} = \frac{|u| \Delta x}{D} \]  

(75)

\[ Cr = \frac{|u| \Delta t}{\Delta x} \]  

(76)

respectively. Both dimensionless variables are local since they depend on the local value of the velocity \( |u| \). Inserting \( D = c_s^2 \Delta t (\tau_a - 1/2) \) in Eq. (75) and \( c = \Delta x / \Delta t \), the following relationship appears

\[ \Omega^2 = \frac{Pe_{\Delta x}(\tau_a - 1/2)}{Cr} = \frac{Pe^*_x}{Cr} \]  

(77)

where \( Pe^*_x = Pe_{\Delta x}(\tau_a - 1/2) \) is the scaled Peclet number. The dimensionless symmetric and anti-symmetric EDFs for the advection-diffusion equation as functions of \( Pe^*_x \) and \( Cr \) become:

**Linear EDFs**

\[ g_i^{seq} = \omega_i \frac{Cr}{Pe^*_x} \quad , i > 0; \quad g_0^{seq} = 1 - \sum_{i>0} g_i^{seq} \]

\[ g_i^{aeq} = \omega_i Cr (\mathbf{e}_i \cdot \mathbf{e}_a) \quad , i > 0; \quad g_0^{aeq} = 0 \]

D1Q3: \( \omega_1 = \omega_2 = 1/2; \quad D2Q5: \quad \omega_1 = \omega_2 = \omega_3 = \omega_4 = 1/2 \)
Quadratic EDFs

\[ g_{i}^{\text{seq}} = \omega_{i} \left( \frac{Cr}{Pe_{\lambda}} + Cr^2 \left( \frac{3}{2} (\mathbf{e}_{i} \cdot \mathbf{e}_{u})^2 - \frac{1}{2} \right) \right), \quad i > 0; \quad g_{0}^{\text{seq}} = 1 - \sum_{i=1}^{N} g_{i}^{\text{seq}} \]

\[ g_{i}^{\text{seq}} = \omega_{i} Cr (\mathbf{e}_{i} \cdot \mathbf{e}_{u}), \quad i > 0; \quad g_{0}^{\text{seq}} = 0 \]

D1Q3: \[ \omega_{1} = \omega_{2} = 1/2 \]

D2Q9: \[ \begin{cases} \omega_{1} = \omega_{2} = \omega_{3} = \omega_{4} = 1/3 \\ \omega_{5} = \omega_{6} = \omega_{7} = \omega_{8} = 1/12 \end{cases} \]

where \( \mathbf{e}_{u} = \mathbf{u} / |\mathbf{u}| \) and \( \mathbf{e}_{i} = \mathbf{e}_{i} / c \). Notice that dimensionless EDFs only depend on the dimensionless parameters \( Pe_{\lambda}^{*}, Cr \) and the relative direction of the flow respect to the lattice orientation \( (\mathbf{e}_{i} \cdot \mathbf{e}_{u}) \) (Figure 3.1). In order to identify the direction of the flow, we define \( \theta \) as the angle between \( \mathbf{u} \) and \( \mathbf{c}_{i} \) clockwise; therefore, \( \mathbf{e}_{i} \cdot \mathbf{u} = c |\mathbf{u}| \cos \theta \).

3.4 Numerical Examples

3.4.1 One-Dimensional Transport with Gaussian Initial Condition

This section conducts numerical experiments to demonstrate the suitability of LBM to solve transport problems. We consider the transport of a conservative substance in uniform flow with initial condition given by a Gaussian distribution. The governing equation for uniform flow is:

\[ \frac{\partial C}{\partial t} + U \frac{\partial C}{\partial x} = D \frac{\partial^2 C}{\partial x^2} \]  

where \( C \) is the concentration of a substance, \( U \) is the velocity of the flow in the \( x \) direction, and \( D \) is the diffusion coefficient. We consider that the domain is infinite and the following initial condition

\[ C(x, t = 0) = \frac{1}{\sqrt{10 \pi}} \exp \left( -\frac{x^2}{10} \right) \]
Figure 3.1: Macroscopic velocity $\mathbf{u}$ and lattice speeds $c_i$ in D2Q9.

The exact solution of Eq. (80) with initial condition Eq. (81) is

$$C(x,t) = \frac{1}{\sqrt{\pi (4Dt + 10)}} \exp \left( -\frac{(x-Ut)^2}{4Dt + 10} \right)$$

We use a lattice size $\Delta x = 1$ and time step $\Delta t = 1$ for all the simulations. The case studies test different values of $Pe_{\Delta x}$, $Cr$ and relaxation times. We use the LBGK model with single relaxation time $\tau = \tau_x = \tau_y$. Then, the velocity $U$ and diffusion coefficient $D$ are obtained from the following relationships

$$U = \frac{Cr \Delta x}{\Delta t}$$

$$D = \frac{U \Delta x}{Pe_{\Delta x}} = \frac{Cr \Delta x^2}{Pe_{\Delta x} \Delta t}$$

The initialization of the particle distribution functions is as follows

$$f_i(x,t = 0) = f_i^{eq}(x,t = 0) = C(x,t = 0)g_i^{eq}$$

where the dimensionless EDFs are given by Eq. (78) and Eq. (79).
In each time step, we calculate the deviation of the LBM solution from the analytical solution at each node, i.e., \( \varepsilon_j = |C_a(x_j, t) - C_a(x_j, t)| \). Then, the total error at time \( t \) is obtained by summing the nodal errors all over the computational domain, \( \varepsilon_t = \sum_j \varepsilon_j \). The computational domain is large enough to ensure that the concentrations at the extremes are very close to zero so that no significant error is introduced from the edges of the computational domain.

Figure 3.2 compares the total errors and solutions after 1000 time steps using linear and quadratic EDFs for \( Pe_{\lambda} = 10 \) and \( Cr = 0.15 \). Quadratic EDFs produce more accurate solutions and have much less numerical dispersion than linear EDFs. Moreover, when using linear EDFs the numerical dispersion increases as \( \tau \) increases.

### 3.4.2 Two-Dimensional Transport with Gaussian Initial Condition

We conduct a two-dimensional mass transport problem to verify the performance of quadratic EDFs against the linear EDFs with second order correction. The following Gaussian initial condition is considered:

\[
C(x, y, t = 0) = \frac{1}{10\pi} e^{-\left(-\frac{x^2 + y^2}{10}\right)}
\]  

(86)

The exact solution to this problem is

\[
C(x, t) = \frac{1}{\pi(4Dt + 10)} e^{-\left(-\frac{(x-Ut)^2 + (y-Vt)^2}{4Dt + 10}\right)}
\]  

(87)

where \( U \) and \( V \) are velocity components along \( x \) and \( y \) directions. We initialize the particle distribution functions as follows

\[
f_i(x, y, t = 0) = f_i^{eq}(x, y, t = 0) = C(x, y, t = 0)\left(g_i^{eq} + g_i^{eq}\right)
\]  

(88)

where the dimensionless EDFs are given by Eq. (78) and Eq. (79).
We used a square lattice with $\Delta x = \Delta y = 1$ and time step $\Delta t = 1$. Once the lattice Peclet number, Courant number, and flow direction $\theta$ are given in the case, the velocity $\mathbf{u} = (U, V)$ is obtained from $|\mathbf{u}| = Cr\Delta x / \Delta t$, where $U = |\mathbf{u}| \cos \theta$ and $V = |\mathbf{u}| \sin \theta$. The diffusion coefficient $D$ is obtained by $D = |\mathbf{u}| \Delta x / Pe_{\Delta x}$.

Figure 3.3 shows the LBGK numerical results for $Pe_{\Delta x} = 40$, $Cr = 0.1$, $\theta = \pi / 8$ and $\tau_a = \tau_s = 0.789$ using linear EDFs on D2Q5, linear EDFs with second order correction on D2Q5, and quadratic EDFs on D2Q9. Solutions using D2Q9 with quadratic EDFs and D2Q5 with linear EDFs and second order correction match the analytical solution while linear EDFs do not. Based on Figure 3.3(b), using linear EDFs is unstable while using quadratic EDFs or linear EDFs with second order correction is stable. Moreover, the evolutions of errors using quadratic EDFs and linear EDFs with second order correction present similar accuracy.

### 3.5 Summary

In this chapter has been shown how to use LBM to solve the diffusion equation and the second order advection-diffusion equation. For the specific case of the advection-diffusion equation, linear and quadratic EDFs are compared, and a new second order corrections based on a forcing term has been proposed.

This chapter has also introduced dimensionless formulation for the EDFs. This dimensionless formulation reduced the number of variables involved in LBM and is being used in following chapters to facilitate studying the non-negativity of EDFs as well as the stability of LBM.
Figure 3.2: Comparison between linear (figures (a) and (c)) and quadratic (figures (b) and (d)) EDFs for 1D transport problem. $Pe_{\Delta t} = 10$ and $Cr = 0.15$. Figures (a) and (b): evolution of errors. Figures (c) and (d): normalized concentration distribution after one thousand time steps. LBM solutions (dash lines); exact solution (solid lines).
Figure 3.3: 2D Transport problem: $Pe_{Ax} = 40$, $Cr = 0.1$, $\theta = \pi / 8$ and $\tau_a = \tau_s = 0.789$. 
CHAPTER 4. THIRD ORDER ANALYSIS FOR ADVECTION-DIFFUSION EQUATION

4.1 Introduction

In the previous chapter, the LBM has been investigated to recover the advection-diffusion equation up to second order in $\varepsilon$. Different EDFs capable of correcting second order numerical diffusion have been studied. This section is intended to improve the accuracy of the LBM over second order accuracy by looking at third order terms.

Third order terms are known to introduce numerical dispersion, which causes oscillations (wiggling) in the numerical solutions. This numerical oscillations are more likely to happen in cases where the Peclet number is high (diffusion is not strong enough to smooth out numerical oscillations) and near high gradients of concentrations. Hence this section focuses in cases with high Peclet number.

4.2 Third Order Analysis

4.2.1 Quadratic EDFs on D2Q9

Third order terms are recovered in general form by Eq.(31), depending on the zero, first, second and third moments of the EDFs. The zero, first and second moments of quadratic EDFs are given in Eq.(58), and the third moment is given by

$$M_{3\alpha\beta} = C\frac{c^2}{3}\left(\delta_{\beta\gamma}u_{\alpha} + \delta_{\alpha\gamma}u_{\beta} + \delta_{\alpha\beta}u_{\gamma}\right)$$  (89)

Introducing these moments into Eq. (31)

$$O(\varepsilon^3): \frac{\partial C}{\partial t_3} = \Delta t\left(\tau_{\alpha} - \frac{1}{2}\frac{\partial^2 C_{u\alpha}}{\partial t_2 \partial \alpha_i} - \Delta t^2 h_1(\tau_a)\left(\frac{\partial^2 C_{u\alpha}}{\partial t_2 \partial \alpha_i} + \frac{\partial C_{u\alpha} u_{\beta}}{\partial \beta_i} + \frac{\partial^3 C_{\gamma}^2}{\partial t_i \partial \alpha_i} \right)\right)$$

$$- \Delta t^2 h_2(\tau_{\alpha} , \tau_s)\left(\frac{\partial^3 C_{\gamma}^2}{\partial t_i \partial \alpha_i} + \frac{\partial^3 C_{u\alpha} u_{\beta}}{\partial \beta_i} + \frac{c^2}{3} \frac{\partial^3 C_{\gamma}}{\partial \alpha_i \partial \beta_i^2}\right)$$  (90)

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Considering that \( \partial_t (Cu) + \partial_{\alpha}(Cu_u) \approx 0 \) (Eq.(62)), Eq. (90) becomes

\[
O(\varepsilon^3): \quad \frac{\partial C}{\partial t} = \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial}{\partial \alpha} \left( u_a \frac{\partial C}{\partial t} + C \frac{\partial u_a}{\partial t} \right) - \Delta t^2 h_2(\tau_a) \frac{\partial^3 C}{\partial t \partial \alpha^3} + \frac{\partial^3 C}{\partial t \partial \alpha \partial \beta} \left( \frac{3}{2} \frac{\partial^3 C}{\partial \beta \partial \gamma} \right) \quad (91)
\]

Notice that \( \tau_s \) is not involved in the recovery of the advection-diffusion equation up to second order, but \( \tau_s \) appears in Eq. (91). Therefore, we can consider \( \tau_s \) as a free parameter that we can select such that \( h_2(\tau_a, \tau_s) = 0 \) to reduce third order terms. This selection results in decreasing the numerical dispersion of the LBM as it is shown in the numerical examples later on. However, it is not possible to cancel out all terms in the right hand side of Eq. (91) in a general case.

Assuming uniform and steady flow, and using \( \partial_t C = -\partial_{\alpha}(Cu) \) (Eq.(59)) and \( \partial_t C = D \partial_{\alpha}^2 C \) (Eq. (63)), Eq. (91) become

\[
O(\varepsilon^3): \quad \frac{\partial C}{\partial t} = \Delta t^2 h_3(\tau_a) c_s^3 u_a \frac{\partial^3 C}{\partial \alpha \partial \beta} - \Delta t^2 h_2(\tau_a, \tau_s) \left( \frac{3}{2} - c_s^2 \right) u_a \frac{\partial^3 C}{\partial \alpha \partial \beta} - u_a u_{\beta} u_{\gamma} \frac{\partial^3 C}{\partial \alpha \partial \beta \partial \gamma} \quad (92)
\]

with \( h_3(\tau_a) = 2 \left( \tau_a - 1/2 \right) - 1/12 \). The macroscopic equation is derived by \( \varepsilon \times \text{Eq.} \ (59) + \varepsilon^2 \times \text{Eq.(63)} + \varepsilon^3 \times \text{Eq.(92)}: \)

\[
\frac{\partial C}{\partial t} + u_a \frac{\partial C}{\partial \alpha} = D \frac{\partial^2 C}{\partial \alpha^2} + \Delta t^2 h_3(\tau_a) c_s^3 u_a \frac{\partial^3 C}{\partial \alpha \partial \beta} - \Delta t^2 h_2(\tau_a, \tau_s) \left( \frac{3}{2} - c_s^2 \right) u_a \frac{\partial^3 C}{\partial \alpha \partial \beta} - u_a u_{\beta} u_{\gamma} \frac{\partial^3 C}{\partial \alpha \partial \beta \partial \gamma} \quad (93)
\]
where the last two terms at the right hand side of Eq. (93) are third-order error terms, responsible for numerical dispersion. To carry out a third-order correction, we can select \( \tau_a \) and \( \tau_s \) such that \( h_2(\tau_a, \tau_s) = 0 \) and \( h_3(\tau_a) = 0 \). This leads to

\[
\tau_a = \tau_s = 0.5 + 12^{-1/2}
\]

(94)

For this specific case the LTRT becomes the LBGK model with a single relaxation time \( \tau = \tau_a = \tau_s = 0.789 \). It is recommended to select \( \tau_s \) such that \( h_2(\tau_a, \tau_s) = 0 \), and then select \( \tau_a \) based on, for example, stability considerations. Therefore we can at least partially reduce the third-order error while keeping stability as a main requirement. By doing this, we have \( \tau_s = \frac{1}{2} + \left[12(\tau_a - 1/2)\right]^{-1} \), and the macroscopic equation becomes

\[
\frac{\partial C}{\partial t} + u_a \frac{\partial C}{\partial \alpha} = D \frac{\partial^2 C}{\partial \alpha^2} + \Delta t \frac{2(\tau_0 - 1/2)^2 - 1/6}{(\tau_0 - 1/2)} Du_a \frac{\partial^3 C}{\partial \alpha \partial \beta^2}
\]

(95)

As seen in Eq.(95), one should avoid using a \( \tau_a \) value very close to 0.5 because that would magnify the numerical dispersion. For the specific case of the LBGK model is considered \( (\tau = \tau_a = \tau_s) \), equation (93) becomes

\[
\frac{\partial C}{\partial t} + u_a \frac{\partial C}{\partial \alpha} = D \frac{\partial^2 C}{\partial \alpha^2} + \Delta t \left[ \left(\tau - 1/2\right)^2 - 1/12 \right] \left[ 3c_s^2 - \frac{c^2}{3} \right] u_a \frac{\partial^3 C}{\partial \alpha \partial \beta \partial \gamma} + u_a u_\beta u_\gamma \frac{\partial^3 C}{\partial \alpha \partial \beta \partial \gamma}
\]

(96)

For the LBGK model, the third-order error terms are proportional to \( (\tau - 1/2)^2 - 1/12 \). Hence the numerical dispersion increases as \( \tau \) increases over 0.789.

### 4.2.2 Linear EDFs with Second Order Correction on D2Q5 Lattice

In this section the third order analysis is carried out in linear EDFs with second order corrections on a D2Q5 lattice. The zero, first and second moments of the linear EDFs are given in Eq. (50), and the third moment is
\[ M_{3\alpha \beta \gamma} = C \delta_{\alpha \gamma} \delta_{\beta \alpha} c^2 u_a \] \hspace{1cm} (97)

Introducing these moments and Eq. (70) into Eq. (31) leads to

\[
O(\varepsilon^3): \frac{\partial C}{\partial t_3} = \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial^3 C u_a}{\partial t_2 \partial \alpha_1} - \Delta t^2 h_2(\tau_a) \left( \frac{\partial^3 C u_a}{\partial t^2_2 \partial \alpha_1} + \frac{\partial^3 C c^2}{\partial t_2 \partial \alpha_1 \partial \beta_1} \right)
- \Delta t^2 h_2(\tau_a, \tau_s) \left( \frac{\partial^3 C c^2}{\partial t_2 \partial \alpha_1 \partial \beta_1} + c^2 \frac{\partial^3 C u_a}{\partial \alpha_1 \partial \beta_1 \partial \gamma_1} \right)
- \Delta t^2 \frac{\partial}{\partial \alpha_1} \left( \frac{1}{\tau_a} \left( \tau_a - \frac{1}{2} \right) \left( \frac{\partial C u_a}{\partial t_2} - \frac{\Delta t}{2} \frac{\partial^2 C u_a}{\partial t^2_2} \right) \right) + \Delta t^2 \tau_a \left( \tau_a - \frac{1}{2} \right) \frac{\partial^2}{\partial \alpha_1} \left( \frac{1}{\tau_a} \left( \tau_a - \frac{1}{2} \right) \frac{\partial C u_a}{\partial t_1} \right)
\] \hspace{1cm} (98)

Reordering terms, Eq. (98) becomes

\[
O(\varepsilon^3): \frac{\partial C}{\partial t_3} = -\Delta t^2 \left( h_1(\tau_a) + h_2(\tau_a, \tau_s) \right) \frac{\partial^3 C c^2}{\partial t_2 \partial \alpha_1 \partial \beta_1}
- \Delta t^2 \left( h_1(\tau_a) + \tau_a \left( \tau_a - \frac{1}{2} \right) \frac{\partial^3 C u_a}{\partial t_2 \partial \alpha_1} - \Delta t^2 h_2(\tau_a, \tau_s) c^2 \frac{\partial^3 C u_a}{\partial \alpha_1 \partial \beta_1 \partial \gamma_1} \right) \hspace{1cm} (99)
\]

Selecting \( \tau_s \) such that \( h_2(\tau_a, \tau_s) = 0 \) in order to partially reduce third order errors, Eq. (99) becomes

\[
O(\varepsilon^3): \frac{\partial C}{\partial t_3} = -\Delta t^2 h_1(\tau_a) \frac{\partial^3 C c^2}{\partial t_2 \partial \alpha_1 \partial \beta_1} - \Delta t^2 \left( h_1(\tau_a) + \tau_a \left( \tau_a - \frac{1}{2} \right) \right) \frac{\partial^3 C u_a}{\partial t_2 \partial \alpha_1} \hspace{1cm} (100)
\]

### 4.2.3 Special Case: Steady State

In the specific case of solving steady state solutions for the advection-diffusion equation, the macroscopic equations recovered are obtained by eliminating the temporal derivatives in Eqs. (22), (25) and (31):

\[
O(\varepsilon): \frac{\partial M_{1\alpha \gamma}}{\partial \alpha_1} = 0 \hspace{1cm} (101)
\]

\[
O(\varepsilon^2): 0 = \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial^2 M_{2\alpha \beta \gamma}}{\partial \alpha_1 \partial \beta_1} \hspace{1cm} (102)
\]
\[ O(\varepsilon^3): \quad 0 = -\Delta t^2 h_2(\tau_a, \tau_s) \frac{\partial^3 M_{\alpha\beta\gamma}}{\partial \alpha_i \partial \beta_i \partial \gamma_1} \] (103)

Using linear EDFs, \( D = c_3^2 \Delta t (\tau_a - 1/2) \), selecting \( \tau_s \) such that \( h_2(\tau_a, \tau_s) = 0 \), and introducing \( \partial \alpha_i = \partial_a \), the steady state ADE is recovered up to third order in \( \varepsilon \).

4.3 Numerical Examples

4.3.1 One-Dimensional Transport with Pulse Initial Condition

It is known that numerical oscillations occur due to high gradients of concentration when Peclet number is high. This numerical example will demonstrate the reduction of numerical dispersion obtained using LTRT and compare the results against the LBGK.

We carry out simulations of mass transport in constant and uniform flow with the pulse initial concentration:

\[
C(x, t = 0) = \begin{cases} 
0 & \text{if } x \notin \left[50, 100\right] \\
1 & \text{if } x \in \left[50, 100\right]
\end{cases}
\] (104)

The initial condition has an infinite gradient at \( x=50 \) and \( x=100 \). The LBM with quadratic EDFs is used to compute numerical solutions with \( Pe_{\Delta x} = 25 \) and \( Cr = 0.2 \). We used lattice size \( \Delta x = 1 \) and flow velocity \( U = 1 \). The time step is determined by \( \Delta t = Cr \Delta x / U \), and the diffusion coefficient is determined by \( D = U \Delta x / Pe_{\Delta x} \). The particle distribution functions are initialized using Eq. (85) and \( g_{i}^{eq} \) and \( g_{i}^{a} \) are given by Eq. (79).

Figure 4.1(a) and (c) show the concentration distributions at \( t = 750 \Delta t \) for the LBGK model. From the third-order analysis result in Eq.(96), we confirm that numerical dispersion in the LBGK model decreases as the relaxation time approaches to the optimum value \( \tau = \tau_a = \tau_s = 0.789 \). At the same time, the numerical dispersion increases as \( \tau_a \) increases over 0.789 because third order errors are proportional to \( (\tau_a - 1/2)^2 - 1/12 \).
Figure 4.1: 1D Transport problem: $Pe_{Ax} = 25$, $Cr = 0.2$. (a) and (c): LBGK, $\tau_s = \tau_a$; (b) and (d): LTRT with $\tau_s = 0.5 + \left[12(\tau_a - 1/2)\right]^{-1}$. Figures (c) and (d) are zoomed in views of (a) and (b) respectively.
For the same problem, as shown in Figure 4.1(b) and (d), the LTRT outperforms the LBGK because the LTRT is able to select the symmetric relaxation times based on 
\[ \tau_s = 0.5 + \left[12\left(\tau_a - 1/2\right)\right]^{-1} \]
to significantly reduce the numerical dispersion. The LTRT results show no oscillations in Figure 4.1(d), except for \( \tau_a = 0.51 \). The third-order analysis results (Eq.(95)) has shown that the numerical dispersion would be magnified when \( \tau_a \) is very close to 0.5.

4.3.2 Two-Dimensional Transport with Gaussian Initial Condition

This case considers the mass transport of a conservative solute in a two-dimensional infinite domain as described in section 3.4.2, and the problem set up was described in the aforementioned section. In the first case study, we compare the performance of the LBGK versus the LTRT using quadratic EDFS. The dimensionless EDFs are \( g_i^{eq} \) and \( g_i^{aeq} \) are calculated using Eq.(79).

Figure 4.2(a) and (b) show stable iso-concentration solutions using LBGK and LTRT, respectively, for quadratic EDFs with \( Pe_{\Delta x} = 40 \), \( Cr = 0.2 \) and \( \theta = \pi / 8 \) at \( t = 1000\Delta t \). Again, the LTRT outperforms the LBGK. LTRT results agree very well with the analytical solution using different \( \tau_a \) values. However, LBGK results show strong numerical dispersion.

Based on Figure 4.2(c), the LBGK model is stable for \( \tau_a = 0.51, 0.8, 0.9, \) and 1.0 and unstable for \( \tau_a = 0.6 \) and 0.7. Based on Figure 4.2(d), the LTRT is stable for \( \tau_a = 0.8, 0.9, \) and 1.0 and unstable for \( \tau_a = 0.51, 0.6, \) and 0.7.

4.4 Summary

This chapter has shown how to analyze third order terms recovered by LBM. A third order correction is possible with no increase of computational cost through a wise choice of the
relaxation times. One and two dimensional case studies have been carried out to verify the theoretical findings, and good agreement between the LBM numerical results and the theoretical expectations have been found.

Figure 4.2: 2D Transport problem: $Pe_{\text{ax}} = 40$, $Cr = 0.2$, $\theta = \pi / 8$. (a) and (c): LBGK, $\tau_s = \tau_a$; (b) and (d): LTRT with $\tau_s = 0.5 + [12(\tau_a - 1/2)]^{-1}$.
CHAPTER 5. LBM FOR MASS TRANSPORT EQUATIONS IN POROUS MEDIA

5.1 LBM for Anisotropic Advection-Dispersion Equation in Porous Media

The anisotropic advection-dispersion equation (AADE) in porous media is given by

\[
\frac{\partial (nC)}{\partial t} + \sum_{\alpha} \frac{\partial (n u_{\alpha} C)}{\partial \alpha} = \sum_{\alpha \beta} \left( n D_{\alpha\beta} \frac{\partial C}{\partial \beta} \right) + SS
\]  

(105)

where \( u = q / n \) is the average pore velocity and \( q \) the specific discharge; and \( D_{\alpha\beta} \) are the component of the dispersion tensor. The porosity \( n \) is considered non-uniform \( n = n(x) \) and the dispersion tensor is assumed to depend on the velocity as follows (Bear 1972)

\[
D_{\alpha\beta} = \delta_{\alpha\beta} \kappa + (\kappa_L - \kappa_T) \frac{u_{\alpha} u_{\beta}}{|u|} + D_m
\]  

(106)

where \( \kappa_L \) and \( \kappa_T \) are the longitudinal and transversal dispersivities; and \( D_m \) is the molecular diffusion.

5.1.1 EDFs for the AADE

In order to recover Eq.(105), we introduce the following EDFs and forcing terms to be used on a D2Q9 lattice:

\[
f_i^{eq} = C \omega_i \left( \frac{c_{Si}^2}{c^2} + \frac{c_i \cdot q}{c^2} + 3 \left( \frac{c_i \cdot q}{nc^2} \right)^2 - \frac{1}{2} \frac{q \cdot q}{nc^2} \right)
\]  

(107)

where \( c_{Si}^2 \) are multidirectional square speeds of sound (MSSS), which are introduced to recover the anisotropic nature of the dispersion tensor. The MSSS are calculated as follows
\[ c_{S1}^2 = c_{S3}^2 = \frac{3c_{Sxx}^2 - c_{Sxx}c_{Sy}c_{Syy}}{2} \]
\[ c_{S2}^2 = c_{S4}^2 = \frac{3c_{Syy}^2 - c_{Sxx}c_{Sy}c_{Syy}}{2} \]
\[ c_{S5}^2 = c_{S7}^2 = 3c_{Syy}^2 + c_{Sxx}c_{Sy}c_{Syy} \]
\[ c_{S6}^2 = c_{S8}^2 = -3c_{Syy}^2 + c_{Sxx}c_{Sy}c_{Syy} \]

Where

\[ c_{S\alpha\beta}^2 = \frac{nD_{\alpha\beta}}{\Delta t(\tau_a - 1/2)} \]  \hspace{1cm} (109)

The zero, first and second moments of the EDFs are

\[ M_0 = nC \]
\[ M_{1\alpha} = Cq_\alpha \]  \hspace{1cm} (110)
\[ M_{2\alpha\beta} = C \frac{nD_{\alpha\beta}}{\Delta t(\tau_a - 1/2)} + C \frac{q_\alpha q_\beta}{n} \]

Introducing Eq. (110) into Eqs. (22) and (25), and assuming Darcian flow in porous media \( \partial \mu_\alpha + \mathbf{u}_\beta \partial \mu_\alpha \approx 0 \), the macroscopic equation recovered is

\[ \frac{\partial nC}{\partial t} + \frac{\partial Cq_\alpha}{\partial \alpha} \left[ \frac{\Delta t(\tau_a - 1/2) \partial}{\partial \alpha} \left( C \frac{\partial nD}{\partial \alpha} \right) \right] = \frac{\partial^2 \left( nD_{\alpha\beta}C \right)}{\partial \alpha \partial \beta} \]  \hspace{1cm} (111)

The third term of the left hand side in Eq. (111) disappears in steady state problems. For transient problems, the term \( \Delta t(\tau_a - 1/2) \partial, (C \frac{\partial nD}{\partial \alpha}) \sim O(CqL^{-1}\Delta t^{-1}) \), where \( T_C \) is the characteristic time for changes in concentration and \( L \) is the characteristic length for spatial variations of the flow. Then, the error term will vanish respect to the advection term if \( (\kappa L^{-1})(\Delta t T_C^{-1}) \ll 1 \). Considering cases where the dispersivity is smaller than \( L \) and the time step is small enough \( (\Delta t \ll T_C) \), then Eq. (111) becomes

\[ \frac{\partial nC}{\partial t} + \frac{\partial Cq_\alpha}{\partial \alpha} = \frac{\partial^2 \left( nD_{\alpha\beta}C \right)}{\partial \alpha \partial \beta} \]  \hspace{1cm} (112)
Eq. (112) recovers the AADE without sinks/sources only if the porosity and flow are uniform, and so is the dispersion tensor. However, if the flow is not uniform, neither is the dispersion tensor. Then Eq. (112) is not the AADE.

5.1.2 Forcing Terms

Eq. (112) can be written as follows

\[
\frac{\partial nC}{\partial t} + \frac{\partial Cq_{\alpha}}{\partial \alpha} = \frac{\partial}{\partial \alpha} \left( nD_{\alpha\beta} \frac{\partial C}{\partial \beta} \right) + \frac{\partial}{\partial \alpha} \left( C \frac{\partial nD_{\alpha\beta}}{\partial \beta} \right) \tag{113}
\]

The second term of the right hand side represents a numerical error term introduced by spatial variations of the porosity and the dispersion tensor. The aim of this section is to introduce forcing terms to introduce the effect of sink/sources as well as to cancel out the effect of this error term. We will consider two families of forcing terms, and the LTRT model reads:

\[
f_i(x + c_{\Delta t}, t + \Delta t) = f_i(x, t) - \frac{1}{\tau_s} (f_i^s(x, t) - f_i^{seq}(x, t)) - \frac{1}{\tau_{a}} (f_i^{a}(x, t) - f_i^{a_{eq}}(x, t)) + SS_i(x, t)\Delta t + F_i(x, t)\Delta t \tag{114}
\]

Sinks/Sources

The term \( SS \) in Eq. (105) can be recovered by introducing the following forcing term

\[
SS_i(x, t) = 0; \quad i > 0
\]

\[
SS_0(x, t) = SS(x, t) + \left( \frac{SS(x, t) - SS(x, t - \Delta t)}{2} \right) \tag{115}
\]

Using Taylor series expansion in Eq. (115), one obtains

\[
SS_i = 0; \quad i > 0
\]

\[
SS_0 = SS + \frac{\Delta t}{2} \frac{\partial SS}{\partial t} - \frac{\Delta t^2}{4} \frac{\partial^2 SS}{\partial t^2} + \ldots \tag{116}
\]

Introducing the multiscale expansion in time and retaining terms up to second order in \( \varepsilon \), we get

\[
SS_0^{(1)} = SS \quad SS_0^{(1)} = 0 \quad i > 0
\]

\[
SS_0^{(2)} = \frac{\Delta t}{2} \frac{\partial SS}{\partial t} \quad SS_i^{(2)} = 0 \quad i > 0 \tag{117}
\]
where $SS$ is $O(\varepsilon)$. The kinetic moments of the forcing terms $SS_i$ involved in the recovery of the macroscopic PDE up to second order accuracy are

$$M_{0i}^{SS(1)} = SS$$
$$M_{0i}^{SS(2)} = \frac{\Delta t}{2} \frac{\partial SS}{\partial t_i}$$
$$M_{1i}^{SS(1)} = 0$$

where $M_{0i}^{SS(1)}$ introduces the effect of the sinks/sources; and $M_{0i}^{SS(2)}$ cancels out the numerical error introduced by $M_{0i}^{SS(1)}$.

### Forcing Term for Second Order Correction

In order to correct the error term in Eq. (113), we introduce the following forcing term:

$$F_i(x, t) = C_{\omega} \left( \frac{\tau_{a} - 1/2}{\Delta t \tau_c c^2} \left( \frac{c_{Si}^2 (x + c_i \Delta t, t) - c_{Si}^2 (x - c_i \Delta t, t)}{2} \right) \right) + C_{\omega} \left( \frac{\tau_{a} - 1/2}{\Delta t \tau_c c^2} \left( \frac{c_{Si}^2 (x + c_i \Delta t, t) - 2c_{Si}^2 (x, t) + c_{Si}^2 (x - c_i \Delta t, t)}{2} \right) \right) \quad i > 0$$

$$F_0(x, t) = 0 - \sum_{i>0} F_i(x, t)$$

Using Taylor series expansion in Eq. (119), we get

$$F_i = C_{\omega} \left( \frac{\tau_{a} - 1/2}{\Delta t \tau_c c^2} \left( \Delta t c_{ia} \frac{\partial c_{Si}^2}{\partial \alpha_i} + \frac{\Delta t}{6} c_{ia} c_{i\beta} c_{\gamma} \frac{\partial^3 c_{Si}^2}{\partial \alpha_i \partial \beta \partial \gamma} + \ldots \right) \right) + C_{\omega} \left( \frac{\tau_{a} - 1/2}{\Delta t \tau_c c^2} \left( \Delta t^2 c_{ia} c_{i\beta} \frac{\partial^2 c_{Si}^2}{\partial \alpha_i \partial \beta} + \frac{\Delta t^4}{24} c_{ia} c_{i\beta} c_{\gamma} c_{\eta} \frac{\partial^4 c_{Si}^2}{\partial \alpha_i \partial \beta \partial \gamma \partial \eta} + \ldots \right) \right) \quad i > 0$$

$$F_0 = 0 - \sum_{i>0} F_i(x, t)$$

Introducing the multiscale expansion in time and retaining terms up to second order in $\varepsilon$, we have

$$F_i^{(1)} = C_{\omega} \left( \frac{\tau_{a} - 1/2}{\tau_c c^2} \frac{\partial c_{Si}^2}{\partial \alpha_i} \right) \quad i > 0$$
$$F_0^{(1)} = 0 - \sum_{i>0} F_i^{(1)}$$

$$F_i^{(2)} = C_{\omega} \left( \frac{\tau_{a} - 1/2}{\tau_c c^2} \frac{\Delta t}{2} c_{ia} c_{i\beta} \frac{\partial^2 c_{Si}^2}{\partial \alpha_i \partial \beta} \right) \quad i > 0$$
$$F_0^{(2)} = 0 - \sum_{i>0} F_i^{(2)}$$

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Using the relationships in Eq. (108) and (109), we find that the kinetic moments of the forcing terms involved in the recovery of the macroscopic PDE up to second order accuracy are

\[ M_{0}^{F(1)} = 0 \]
\[ M_{1a}^{F(1)} = \frac{1}{\tau_a} \left( C \, \frac{\partial n D_{a\beta}}{\partial \beta} \right) \]
\[ M_{0}^{F(2)} = 0 \quad (122) \]

where \( M_{1a}^{F(1)} \) cancels out the numerical error term in Eq. (113). Then, considering Eq. (118) and Eq. (122) in the recovery procedure, the AADE is recovered up to second order accuracy.

5.1.3 Simplification

In order to make easier the implementation of the collision step, we can combine together the forcing term \( F_i \Delta t \) with the EDFs in the LTRT model. Then Eq. (114) becomes equivalent to

\[
f_i(x + c_i \Delta t, t + \Delta t) = f_i(x, t) - \frac{1}{\tau_s} (f_i^S(x, t) - f_i^{aS}(x, t)) - \frac{1}{\tau_a} (f_i^a(x, t) - f_i^{aS}(x, t)) + SS_i(x, t) \Delta t
\]

where \( f_i^{aS} \) and \( f_i^{aFeq} \) are the symmetric and anti-symmetric parts of the pseudo-equilibrium \( f_i^{Feq} \) and

\[
f_i^{Feq} = C \omega_i \left( 2\tau_s - 1 \right) \frac{c_{Seq}^2}{c^2} + \left( 2 - 2\tau_s \right) \frac{c_{Seq}^2}{c^2} + \frac{c_i \cdot q}{c^2} + \frac{3}{2} \frac{(c_i \cdot q)^2}{nc^4} - \frac{1}{2} \frac{q \cdot q}{nc^2} \right) \quad i > 0
\]
\[
f_0^{Feq} = nC - \sum_{i>0} f_i^{Feq}
\]
\[
\omega_1 = \omega_2 = \omega_3 = \omega_4 = \frac{1}{3} \quad \omega_5 = \omega_6 = \omega_7 = \omega_8 = \omega_9 = \frac{1}{12}
\]

where we have introduced the equivalent squared speed of sound \( c_{Seq}^2 \), which is

\[
c_{Seq}^2(x, t) = \frac{c_{Seq}^2(x, t) + c_{Seq}^2(x + c_i \Delta t, t)}{2}
\]

We can observe that implementing Eq. (123) with Eq.(124) is equivalent and easier than implementing Eq. (114) with Eq. (107) and Eq. (119).
5.2 LBM for Groundwater Flow Equation

In this section the LBM is extended to cope with the heterogeneous and anisotropic groundwater flow equation. The groundwater flow equation considering heterogeneous specific storage and hydraulic conductivity as follows

\[
S_h \frac{\partial h}{\partial t} = \frac{\partial}{\partial \alpha} \left( K_{aa} \frac{\partial h}{\partial \alpha} \right) + Q
\]

(126)

where \( S_h \) is the specific storage; \( K_{aa} \) represents the hydraulic conductivity tensor. we have assumed that the principal direction of the hydraulic conductivity tensor are the horizontal and vertical directions.

The recovery procedure is similar to the recovery of the AADE introduced in the previous section. The D2Q5 lattice is considered with the following EDFs

\[
f_{i}^{eq} = \frac{1}{2} h \frac{c_{S}^2}{c^2}, \quad i = 1, 2, 3, 4
\]

\[
f_{6}^{eq} = S_h h - \sum_{i=1}^{4} f_{i}^{eq}
\]

(127)

where the MSSS are

\[
c_{S1}^2 = c_{S3}^2 = c_{Sxx}^2
\]

\[
c_{S2}^2 = c_{S4}^2 = c_{Syy}^2
\]

\[
c_{Saa}^2 = \frac{K_{aa}}{\Delta t (\tau_a - 1/2)}
\]

(128)

(129)

These EDFs recover the following kinetic moments:

\[
M_0 = S_h h
\]

\[
M_{1a} = 0
\]

\[
M_{2ab} = h \delta_{ab} \frac{K_{ab}}{\Delta t (\tau_a - 1/2)}
\]

(130)
In order to recover the effect of pumping/injection terms, we introduce $SS_i$

$$SS_i(x, t) = 0; \ i > 0$$

$$SS_0(x, t) = Q(x, t) + \left( \frac{Q(x, t) - Q(x, t - \Delta t)}{2} \right)$$

(131)

where $Q$ is $O(\varepsilon)$. The kinetic moments of the forcing terms $SS_i$ involved in the recovery of the macroscopic PDE up to second order accuracy are

$$M_{i\alpha}^{SS(1)} = Q$$

$$M_{i\alpha}^{SS(1)} = 0$$

$$M_{i\alpha}^{SS(2)} = \frac{\Delta t}{2} \frac{\partial Q}{\partial t}$$

(132)

Similarly to the recovery of the AADE, we introduce the forcing term $F_i$ to cancel out the numerical error introduce by heterogeneities in the hydraulic conductivity

$$F_i(x) = h \frac{1}{2} \left( \frac{\tau_a - 1/2}{\Delta t \tau_a c^2} \right) \left( c_{Si}^2 (x + c_i \Delta t) - c_{Si}^2 (x - c_i \Delta t) \right)$$

$$+ h \frac{1}{2} \left( \frac{\tau_a - 1/2}{\Delta t \tau_a c^2} \right) \left( c_{Si}^2 (x + c_i \Delta t) - 2c_{Si}^2 (x) + c_{Si}^2 (x - c_i \Delta t) \right) \ i > 0$$

(133)

$$F_0(x) = 0 - \sum_{i>0} F_i(x)$$

Using Taylor expansion and using the multiscale expansion in time, and retaining terms up to second order in $\varepsilon$, we obtain

$$F_i^{(1)} = h \frac{1}{2} \left( \frac{\tau_a - 1/2}{\tau_a c^2} \right) \frac{\partial c_{Si}^2}{\partial \alpha_i} \ i > 0$$

$$F_i^{(2)} = h \frac{1}{2} \left( \frac{\tau_a - 1/2}{\tau_a c^2} \right) \frac{\Delta t}{2} c^2 \frac{\partial^2 c_{Si}^2}{\partial \alpha_i \partial \alpha_i} \ i > 0$$

$$F_0^{(1)} = 0 - \sum_{i>0} F_i^{(1)}$$

$$F_0^{(2)} = 0 - \sum_{i>0} F_i^{(2)}$$

(134)

The kinetic moments of the forcing terms involved in the recovery of the macroscopic PDE up to second order accuracy are
Inserting Eqs. (130), (132) and (135) into Eqs. (22) and (25) and using the multi-scale expansion, the macroscopic PDE recovered up to second order is

\[
\frac{\partial S}{\partial t} - \frac{\partial}{\partial \alpha} \left( \tau_a^{-1/2} \Delta t \frac{\partial K_{aa}}{\partial \alpha} \right) = \frac{\partial}{\partial \alpha} \left( K_{aa} \frac{\partial h}{\partial \alpha} \right) + Q
\]  

(136)

Eq. (136) is the groundwater flow equation plus the second term on the left hand side, which represents numerical error introduced by our numerical scheme. This term disappears in steady state cases.

Although an extra forcing term could be introduced to cancel out the effect of this term for transient solutions, the effect of this term is negligible. In order to select the time step for groundwater flow equation, we impose the same condition that the speed ratio is \( c_s^2 / c_{ssa}^2 \geq 1 \), which leads to \( \Delta t \leq \Delta x^2 (\tau - 1/2) / K_{aa} \). Then, the flow time step for the groundwater flow is

\[
\Delta t \leq \frac{\Delta x^2}{(K_{aa} / S_s)_{\text{max}}} \left( \tau_a - \frac{1}{2} \right)
\]  

(137)

Introducing Eq. (137) into Eq. (136), we obtain

\[
S_s \frac{\partial h}{\partial t} - \frac{\Delta x^2}{2(K_{aa} / S_s)_{\text{max}}} \left( \tau_a - \frac{1}{2} \right) \frac{\partial h}{\partial \alpha} \frac{\partial^2 K_{aa}}{\partial \alpha^2} - \frac{\Delta x^2}{2(K / S_s)_{\text{max}}} \left( \tau_a - \frac{1}{2} \right)^2 \frac{\partial^2 h}{\partial \alpha \partial t} \frac{\partial K_{aa}}{\partial \alpha} = \frac{\partial}{\partial \alpha} \left( K_{aa} \frac{\partial h}{\partial \alpha} \right) + Q
\]  

(138)

The second and third terms in the left hand side of Eq. (138) are negligible respect to

\[
S_s \frac{\partial}{\partial \alpha} h \quad \text{if} \quad \frac{K_{aa}}{(K_{aa} / S_s)_{\text{max}}} \frac{1}{S_s} \frac{\Delta x^2}{L_K^2} \ll 1
\]  

(139)
\[
\frac{K_{aa}}{(K/S_s)_{\text{max}}} \frac{1}{S_s} \frac{\Delta x^2}{L_L K} \ll 1
\]  

(140)

where \(L\) is a characteristic length of the physical domain and \(L_K\) is the characteristic length for spatial variation of hydraulic conductivity. Since the factor \((K_{aa}/S_s)/(K_{aa}/S_s)_{\text{max}} \leq 1\) and the spatial discretization must be \(\Delta x \ll L\), Eq. (138) recovers Eq. (126) if \(\Delta x < L_K\), where \(L_K\) can be estimated by the integral scale for spatially correlated hydraulic conductivity. Under this consideration, Eq.(138) recovers the groundwater flow equation given in Eq.(126).

**Simplification**

Similarly to the previous section, we can combine together the forcing term \(F_r \Delta t\) with the equilibrium in the LTRT equation, obtaining the pseudo-equilibrium \(f_i^{\text{Feq}}\)

\[
f_i^{\text{Feq}} = h \left( \frac{1}{2} \left( 2\tau_a - 1 \right) \frac{c_{\text{seq}}^2}{c^2} + \left( 2 - 2\tau_a \right) \frac{c_{\text{gi}}^2}{c^2} \right) \quad i > 0
\]

\[
f_0^{\text{Feq}} = S_s h - \sum_{i=0}^{\infty} f_i^{\text{Feq}}
\]

and \(c_{\text{seq}}^2\) is again the equivalent squared speeds of sound, which are given by

\[
c_{S1eq}^2(x) = \frac{c_{sxx}^2(x) + c_{sxx}^2(x + c_1 \Delta t)}{2}
\]

\[
c_{S2eq}^2(x) = \frac{c_{sxx}^2(x) + c_{sxx}^2(x + c_2 \Delta t)}{2}
\]

\[
c_{S3eq}^2(x) = \frac{2}{c_{sxx}^2(x)}
\]

\[
c_{S4eq}^2(x) = \frac{2}{c_{sxx}^2(x)}
\]

(141)

5.3 Specific Case: \(\tau_a = \tau_s = 1\)

In the previous sections, LBM has been extended to cope with heterogeneity in the hydraulic conductivity and the dispersion coefficient. However, the spatial variations of the hydraulic conductivity and dispersion coefficients have to be smooth enough to recover the macroscopic differential equation. If discontinuity exists, the use of Taylor series expansion is not appropriate. To overcome this problem, it is suggested to use the equivalent hydraulic
conductivity, which assumes that two nodes are connected by a material whose hydraulic conductivity is the harmonic mean the local hydraulic conductivity values at the respective nodes.

We show that when \( \tau = \tau_a = \tau_s = 1 \) and using in the pseudo-equilibrium, the harmonic mean of the squared speed of sound

\[
c_{seq}^2(x) = 2\left([c_{\delta}^2(x)]^{-1} + [c_{\delta}^2(x + c_i\Delta t)]^{-1}\right)^{-1}
\]

(143)

the equivalent hydraulic conductivity retains. The equivalent hydraulic conductivity \( K_{eq} \) is defined as the harmonic mean of the local hydraulic conductivity values between two connected nodes \( K_{eq}(x) = 2\left[K^{-1}_{aab}(x) + K^{-1}_{aab}(x + c_i\Delta t)\right]^{-1} \), where \( \alpha = x \) if \( i = 1,3 \) and \( \alpha = y \) if \( i = 2,4 \). For the sake of simplicity, we consider constant specific storage. Then, the groundwater flow equation becomes

\[
\frac{\partial h}{\partial t} = \frac{\partial}{\partial \alpha}\left(D_{aab}^{H} \frac{\partial h}{\partial \alpha}\right)
\]

(144)

where \( D_{aab}^{H} = K_{aab}/S_s \) is the hydraulic diffusion. The exchange of head between lattice nodes in one time step is

\[
\Delta h_i(x) = f_\tau^r(x, t + \Delta t) - f_i(x + c_i\Delta t, t + \Delta t)
\]

(145)

When \( \tau = \tau_a = \tau_s = 1 \), the particle distribution functions are equal to the pseudo-equilibrium values: \( f_\tau^r(x, t + \Delta t) = f_{eq}^r(x + c_i\Delta t, t) \) and \( f_i(x + c_i\Delta t, t + \Delta t) = f_{eq}^r(x, t) \). Then

\[
\Delta h_i(x) = f_{eq}^r(x + c_i\Delta t) - f_{eq}^r(x) = \left(h(x + c_i\Delta t) - h(x)\right) \frac{c_{seq}^2(x)}{2c^2}
\]

(146)

where \( \bar{i} \) represents the opposite direction to \( i \). This head exchange represents a water flux, which can be expressed as \( q_i(x) = \Delta V_{wi}(x)/\Delta x\Delta t \), where \( \Delta V_{wi}(x) \) is the volume of water
transferred in one time step through the boundary of the lattice. This volume can be expressed as a function of the head exchange by means of the specific storage. By definition, the specific storage expresses the amount of water release per unit of volume and per unit variation of head, 

\[ S_s = \Delta V_{wi}(x)/(\Delta x^2 \Delta h(x)) \].

Using this specific storage and Eq.(146), the water flux becomes

\[ q_i(x) = S_s c^2_{seqi}(x)(h(x + c_i \Delta t) - h(x))/2c \]  

(147)

when \( \tau = 1 \), the speed of sound is related to the hydraulic diffusion as

\[ D^H_{\alpha\alpha}(x) = K_{\alpha\alpha}(x)/S_s = c^2_S(x) \Delta t/2 \].

At the same time, \( c^2_{seqi}(x) = 2 \left( [c^2_{S_i}(x)]^{-1} + [c^2_{S_i}(x + c_i \Delta t)]^{-1} \right)^{-1} \).

Using \( c^2_{S_i}(x) = 2 \Delta t^{-1} K_{\alpha\alpha}(x)/S_s \), where \( \alpha = x \) if \( i = 1,3 \) and \( \alpha = y \) if \( i = 2,4 \), into \( c^2_{S_i}(x) \) leads to \( c^2_{S_i}(x) = 2cK_{eqi}(x)/S_s \). Then, inserting \( c^2_{seqi}(x) \) in Eq. (147), we obtain

\[ q_i(x) = K_{eqi}(x)(h(x + c_i \Delta t) - h(x))/\Delta x \]  

(148)

Eq.(148) is Darcy’s law considering the equivalent hydraulic conductivity. In conclusion, the directional squared speed of sound recovers the equivalent hydraulic conductivity along the lattice directions for the specific case of \( \tau = \tau_x = 1 \). This makes the equivalent squared speed of sound to be able to cope with highly discontinuous hydraulic conductivity distribution.

5.4 Boundary Conditions

The problem of implementing the boundary conditions in the LBM is equivalent to the problem of determining the values of the particle distribution functions missing in the boundary nodes. In this section, we describe how to implement two types of boundary conditions: the Dirichlet boundary condition and prescribed mass flux.

5.4.1 Dirichlet Boundary Condition

We implement the Dirichlet boundary condition as described by determining the missing distribution proportionally to the equilibrium distribution functions in their respective directions.
in a way that the specified value of the macroscopic variable in the boundary is fulfilled. Let \( f^s_i \) be the particle distribution function arriving at a boundary node after the streaming step (Figure 5.1). For the Dirichlet boundary condition, this condition is equivalent to specifying a boundary value \( A_b \) for the zero moment: \( \sum_i f^s_i = A_b \); where only some of \( f^s_i \) are known. The missing particle distribution functions \( f^s_j \) are estimated as follows:

\[
 f^s_j = \left( A_b - \sum_{k_1} f^s_{k_1} \right) \frac{f^eq_j}{\sum_{k_2} f^eq_{k_2}} 
\]

where \( k_1 \) indexes known particle distribution functions, and \( k_2 \) indexes missing particle distribution functions.

**Figure 5.1:** Known and missing particle distributions functions after streaming in a boundary node.
5.4.2 Prescribed Mass Flux Boundary Condition

Prescribed mass flux boundary conditions (BC) in the LBM were proposed in Zhang et al. (2002b). Let $\phi$ be the prescribed mass flux across the boundary. For a vertical boundary situated between nodes indexed $i$ and $i+1$ (see Figure 5.2), let the nodes indexed $i$ be the inner nodes, and then nodes indexed $i+1$ be the ghost nodes, the expressions for the missing particle distribution functions are (Zhang et al. 2002b):

\[
\begin{align*}
    f_3^*(i+1, j) &= f_1^*(i, j) + \frac{2 \phi}{3c} \\
    f_6^*(i+1, j) &= f_5^*(i, j) + \frac{\phi}{6c} \\
    f_7^*(i+1, j) &= f_6^*(i, j) + \frac{\phi}{6c}
\end{align*}
\]  

(150)

with $c = \Delta x / \Delta t$ is the lattice speed. In this way the net flux of particles across the boundary during one time step fulfills the prescribed mass flux condition. This type of boundary condition can be used to impose a no flux ($\phi = 0$) boundary condition, equivalent to an impermeable wall.

5.5 Numerical Examples

5.5.1 Two-Dimensional Transport with Anisotropic Dispersion in Uniform Flow

This case considers the mass transport of a conservative solute in a two-dimensional infinite domain. The governing equation for this problem is given by:

\[
\frac{\partial C}{\partial t} + u_x \frac{\partial C}{\partial x} + u_y \frac{\partial C}{\partial y} = D_{xx} \frac{\partial^2 C}{\partial x^2} + D_{xy} \frac{\partial^2 C}{\partial x \partial y} + 2D_{xy} \frac{\partial^2 C}{\partial x \partial y} + 2D_{xy} \frac{\partial^2 C}{\partial x \partial y} \]

(151)

The initial condition is

\[
C(x, y, t = 0) = \frac{1}{\sqrt{4\pi D_L t_0} \sqrt{4\pi D_T t_0}} \exp \left( -\frac{(x \cos \theta + y \sin \theta)^2}{4\pi D_L t_0} - \frac{(-x \sin \theta + y \cos \theta)^2}{4\pi D_T t_0} \right)
\]

(152)

where $D_L = |\mathbf{u}| \kappa_L$, $D_T = |\mathbf{u}| \kappa_T$ and $t_0 = 10/(4D_T)$.
Figure 5.2: Known and missing particle distributions functions around a vertical boundary.
The exact solution of Eq. (151) with the initial condition in Eq.(152) is

\[
C(x, y, t = 0) = \frac{1}{4\pi \sqrt{D_L D_T(t_0 + t)}} \exp \left( -\frac{(x \cos \theta + y \sin \theta - |u|(t - t_0))^2}{4\pi D_L(t_0 + t)} - \frac{(-x \sin \theta + y \cos \theta)^2}{4\pi D_T(t_0 + t)} \right)
\] (153)

In this case study, the parameter values are $\Delta x/\kappa_L = 5$, $\kappa_L/\kappa_T = 10$, $Cr = 0.5$ and $\theta = \pi/8$. We used a square lattice with $\Delta x = \Delta y = 1$, time step $\Delta t = 1$ and antisymmetric relaxation time $\tau_a = 1$. The velocity $\mathbf{u} = (u_x, u_y)$ is obtained from $|\mathbf{u}| = Cr \Delta x / \Delta t$, where $u_x = |\mathbf{u}| \cos \theta$ and $u_y = |\mathbf{u}| \sin \theta$. The components of the dispersion tensor are calculated from Eq. (106) and molecular diffusion has been assumed negligible. Then, the pseudo-equilibrium is calculated using Eq.(124) and assuming porosity equal to unity.

Figure 5.3 (a) shows iso-concentration solutions at $t = 500\Delta t$ for different choices of the symmetric relaxation time. We can observe that the optimum value $\tau_s = 0.667$ provides the best fitting to the analytical solution. This result is confirmed by looking at the evolution of errors in Figure 5.3(b), where it is shown how the amount of error increases as $\tau_s$ increases over the optimum value. However, choices of $\tau_s$ in the range of $[0.667, 1]$ provide accurate solutions based on Figure 5.3(a).

5.5.2 Steady State Groundwater Flow Equation with Smooth Hydraulic Conductivity Distribution and Sink/Source Term

To validate the LBM for solving the groundwater equation with heterogeneous hydraulic conductivity and the sink-source term, we consider steady-state groundwater flow in a domain $0 \leq x \leq 2$ and $0 \leq z \leq 1$. The hydraulic conductivity distribution in the domain is given by $K(x, z) = 0.01 + 0.009 \cos(2\pi x / 3) \sin(2\pi z)$. The sink/source term is given by $Q(x, z) = 0.009 \left( (\pi/6) \sin(2\pi x/3) - \pi \sin(2\pi z) \right)$. The boundary conditions are Dirichlet type:
h(x,0)=1+0.25x, \ h(x,1)=1.5+0.25x, \ h(0,z)=1+0.5z \ and \ h(2,z)=1.5+0.5z. \ The \ analytical
solution \ to \ this \ case \ study \ is \ h(x,z)=1+0.25x+0.5z. 

We \ use \ a \ lattice \ size \ \Delta x = \Delta z = 0.05. \ The \ time \ step \ for \ the \ required \ transient \ stage \ is
\Delta t = \Delta x^2 (\tau_a - 0.5)/(3K_{\max}), \ which \ makes \ sure \ the \ squared \ speed \ ratio \ \epsilon^2/\epsilon_S^2 \ \geq \ 3 \ at \ all \ lattice
grids. \ In \ each \ time \ step, \ we \ calculate \ the \ maximum \ nodal \ error, \ defined \ as \ the \ maximum
absolute \ value \ of \ the \ difference \ between \ the \ LBM \ solution \ and \ the \ analytical \ solution:
\[ \epsilon_{\text{max}} = \max \{ \epsilon_y \}, \text{ with } \epsilon_{i,j} = |h_{i,j}^{\text{LBM}} - h_{i,j}^{\text{a}}| \].

Figure 5.4(a) shows the evolution of the maximum nodal error for 5000 time steps when
the \ LBGK \ and \ LTRT \ model \ are \ used \ with \ arithmetic \ squared \ speed \ of \ sound \ to \ calculate \ the
directional \ squared \ speed \ of \ sound. \ When \ \tau_a = 1, \ the \ LBGK \ and \ LTRT \ obtain \ the \ best \ solution
and \ the \ LTRT \ is \ much \ more \ accurate \ than \ the \ LBGK. \ The \ solutions \ of \ the \ LBGK \ and \ LTRT \ for
\tau_a \neq 1 \ are \ almost \ similar \ and \ not \ accurate. \ Figure 5.2(b) \ shows \ that \ the \ head \ distribution \ using
the \ LTRT \ model \ with \ \tau_a = 1 \ is \ much \ better \ than \ using, \ for \ example, \ \tau_a = 0.9.

Figure 5.5(a) shows the evolution of \epsilon_{\text{max}} \ using \ \tau_a = 1 \ and \ the \ LTRT \ with \ different \ \tau_s
values. \ Arithmetic \ and \ harmonic \ approaches \ were \ considered \ to \ calculate \ the \ directional \ squared
speeds \ of \ sound. \ Using \ the \ arithmetic \ mean \ shows \ smaller \ errors \ than \ using \ the \ harmonic \ mean
in \ this \ case. \ It \ confirms \ that \ the \ optimum \ value \ \tau_s = 0.667 \ gives \ the \ smallest \ maximum \ error \ for
both \ arithmetic \ and \ harmonic \ approaches.

It \ is \ noted \ that \ the \ hydraulic conductivity \ distribution \ is \ based \ on \ trigonometric \ functions,
which \ makes \ the \ distribution \ smooth. \ Therefore, \ the \ use \ of \ arithmetic \ mean \ for \ the \ directional
squared \ speed \ of \ sound \ with \ \tau_a = 1 \ and \ the \ optimal \ \tau_s \ improves \ the \ solution \ accuracy.
Figure 5.3: Two dimensional transport with anisotropic dispersion. $\Delta x / \kappa_L = 5$, $\kappa_L / \kappa_T = 10$, $Cr = 0.5$, $\theta = \pi / 8$ and $\tau_a = 1$. 
Figure 5.4: (a) Evolution of the maximum errors using LBGK and LTRT with \( \tau_s = 0.5 + [12(\tau_a - 0.5)]^{-1} \) models. (b) Head distributions using LTRT with \( \tau_s = 0.5 + [12(\tau_a - 0.5)]^{-1} \) against the analytic solution.
Figure 5.5(b) shows the convergence analysis results using $\tau_s = 1$ and different $\tau_s$ values with the arithmetic mean. The LTRT shows second order convergence for all $\tau_s$ values, except for the optimal $\tau_s$ values that the convergence rate is almost fourth order. When using harmonic means, Figure 5.5(c) shows the convergence rates close to second order for any $\tau_s$ value and MODFLOW (Harbaugh et al. 2000). Since MODFLOW is based on the equivalent hydraulic conductivity, its similar convergence rate to LTRT using the harmonic mean is reasonable.

### 5.5.3 Steady State Groundwater Flow Equation with Discontinuous Hydraulic Conductivity

This example considers strong discontinuity in hydraulic conductivity. The boundary conditions are $h(0, z) = 1.0257, h(2, z) = 1 + 0.025(1-z), \partial_z h(x, 0) = 0$ and $\partial_z h(x, 1) = 0$. The different distributions of the hydraulic conductivity are shown in Figure 5.6. In all cases, the grid size is $\Delta x = \Delta z = 0.05$, and the time step for the LTRT is estimated based on the maximum hydraulic conductivity: $\Delta t = 0.01\Delta x^2 (\tau_a - 0.5)/3$. Results in Figure 5.6 show excellent agreement between MODFLOW and the LTRT with the harmonic mean for the directional squared speed of sound. However, the LTRT solutions with arithmetic mean is different in the areas close to the interfaces of hydraulic conductivity. In Figure 5.6(c), the use of the arithmetic mean introduces numerical errors in the vicinity of the discontinuities.

Based on the results in these two examples, we conclude that use of the arithmetic mean, $\tau_a = 1$ and the optimal $\tau_s$ can significantly improve the accuracy of the LTRT model when the variation of hydraulic conductivity is smooth. On the other hand, using the harmonic mean is recommended with $\tau_a = \tau_s = 1$ for those particles distribution functions streaming through the discontinuities.
5.6 Summary

This chapter has presented the EDFs to recover the heterogeneous and anisotropic groundwater flow and advection-dispersion equations, as well as the forcing terms to recover the effect of sinks/sources and to correct second order numerical errors. For the groundwater flow equation, it has been found that for smooth hydraulic conductivity distributions, it is more effective to use the equivalent squared speed of sound based on the arithmetic mean rather than on the harmonic mean, as well as using $\tau_a = 1$ and $\tau_s = 0.667$. However, in cases where the hydraulic conductivity has discontinuities, it is advisable to use the harmonic mean for the equivalent squared speed of sound along with $\tau_a = \tau_s = 1$. 
Figure 5.5: (a): Evolution of the maximum error using LTRT with $\tau_a = 1$, $\Delta x = 0.05$ and arithmetic mean (solid lines) or harmonic mean (dashed lines). (b) Convergence rates using LTRT with $\tau_a = 1$ and arithmetic mean. (c) Convergence rates using LTRT with $\tau_a = 1$ and harmonic mean.
Figure 5.6: LTRT solutions with $\tau_a = 1$, $\tau_s^* = 0.667$, and arithmetic mean (dashed lines); LBGK solutions with $\tau_a = \tau_s = 1$ and harmonic mean (dotted lines); MODFLOW solution (solid lines).
CHAPTER 6. NON-NEGATIVITY ANALYSIS ON EDFS

6.1 Introduction

In the previous chapters was shown how to recover accurately the advection-diffusion equation using LBM. However, no considerations about stability have been taken into account yet, which is an important issue we have to consider when choosing EDFs, relaxation times, lattice size and time step.

When using the LBGK model, some studies reported that negative values of the EDFs could quickly lead to numerical instability (Wolf-Gladrow 2000; Yu and Zhao 2000), and this is the main motivation of this section. The dimensionless forms of linear and quadratic EDFs are analyzed analytically in order to find the non-negativity domains based on the dimensionless parameters governing locally the LBM scheme.

6.2 Non-Negativity Analysis of Quadratic EDFs on D2Q9

This section analyzes the sufficient conditions in terms of $Pe_{\Delta t}^*$ and $Cr$ for obtaining non-negative values of the quadratic EDFs on a D2Q9 lattice given by Eq. (79) for any directions of the macroscopic velocity $u$. Let $S_{NL}^{DQ}$ be the set of that is conditioned on the non-negativity of second-order EDFs for any flow directions:

$$S_{NL}^{DQ} = \left\{ (Pe_{\Delta t}, Cr) \mid Pe_{\Delta t}^* > 0, Cr > 0, \forall \theta \in [0, 2\pi], \forall i : g_i^{eq}(Pe_{\Delta t}, Cr) \geq 0 \right\}$$

Due to the symmetry of the lattice directions, we can reduce our analysis to the range $\theta \in [0, \pi / 4]$. Any flow direction will give the same result for an angle in $[0, \pi / 4]$ after reordering the lattice velocities $c_i$. Therefore, Eq. (154) is rewritten as

$$S_{DQ}^{DQ} = \left\{ (Pe_{\Delta t}, Cr) \mid Pe_{\Delta t}^* > 0, Cr > 0, \forall \theta \in [0, \pi / 4], \forall i : g_i^{eq}(Pe_{\Delta t}, Cr) \geq 0 \right\}$$

Let’s consider the set of $(Pe_{\Delta t}^*, Cr)$ for individual non-negative EDFs.
\[ S_i = \{ (Pe_{\Delta x}^*, Cr) \mid Pe_{\Delta x}^* > 0, Cr > 0, \forall \theta \in [0, \pi/4], g_i^{eq}(Pe_{\Delta x}^*, Cr) \geq 0 \} \] (156)

Eq. (155) represents the intersection of all \( S_i \), i.e., \( S = \bigcap_{i=0}^{8} S_i \). The directions of the lattice structure are identified as follows: \( e_i = (\cos(\beta_i), \sin(\beta_i)) \) with \( \beta_i = (i-1)\pi/2 \) for \( i=1,2,3,4 \); \( e_i = \sqrt{2} (\cos(\beta_i), \sin(\beta_i)) \) with \( \beta_i = \pi/4 + (i-5)\pi/2 \) for \( i=5,6,7,8 \); and \( e_u = (\cos \theta, \sin \theta) \). Inserting \( e_i \cdot e_u \) into Eq. (79), we obtain the dimensionless EDFs for a given flow direction \( \alpha \):

\[
\begin{align*}
ge_1^{eq} &= \frac{1}{3} \left( \frac{Cr}{Pe_{\Delta x}^*} + Cr \cos \theta + Cr^2 \left( \frac{3}{2} \cos^2 \theta - \frac{1}{2} \right) \right) \\
ge_2^{eq} &= \frac{1}{3} \left( \frac{Cr}{Pe_{\Delta x}^*} + Cr \sin \theta + Cr^2 \left( \frac{3}{2} \sin^2 \theta - \frac{1}{2} \right) \right) \\
ge_3^{eq} &= \frac{1}{3} \left( \frac{Cr}{Pe_{\Delta x}^*} - Cr \cos \theta + Cr^2 \left( \frac{3}{2} \cos^2 \theta - \frac{1}{2} \right) \right) \\
ge_4^{eq} &= \frac{1}{3} \left( \frac{Cr}{Pe_{\Delta x}^*} - Cr \sin \theta + Cr^2 \left( \frac{3}{2} \sin^2 \theta - \frac{1}{2} \right) \right) \\
ge_5^{eq} &= \frac{1}{12} \left( \frac{Cr}{Pe_{\Delta x}^*} + Cr (\cos \theta + \sin \theta) + Cr^2 \left( \frac{3}{2} (\cos \theta + \sin \theta)^2 - \frac{1}{2} \right) \right) \\
ge_6^{eq} &= \frac{1}{12} \left( \frac{Cr}{Pe_{\Delta x}^*} + Cr (-\cos \theta + \sin \theta) + Cr^2 \left( \frac{3}{2} (-\cos \alpha + \sin \alpha)^2 - \frac{1}{2} \right) \right) \\
ge_7^{eq} &= \frac{1}{12} \left( \frac{Cr}{Pe_{\Delta x}^*} - Cr (\cos \theta + \sin \theta) + Cr^2 \left( \frac{3}{2} (\cos \theta + \sin \theta)^2 - \frac{1}{2} \right) \right) \\
ge_8^{eq} &= \frac{1}{12} \left( \frac{Cr}{Pe_{\Delta x}^*} + Cr (\cos \theta - \sin \theta) + Cr^2 \left( \frac{3}{2} (\cos \theta - \sin \theta)^2 - \frac{1}{2} \right) \right)
\end{align*}
\]
Because we only need to study the EDFs with \( \theta \in [0, \pi/4] \), the values \( \cos \theta \in [\sqrt{2}/2, 1] \), 
\( \sin \theta \in [0, \sqrt{2}/2] \), and \( \cos \theta \sin \theta \in [0, 1] \). Then Eqs.(157)-(164) render the relations: \( g_1^{eq} \geq g_3^{eq} \), 
\( g_2^{eq} \geq g_4^{eq} \), \( g_5^{eq} \geq g_7^{eq} \) and \( g_8^{eq} \geq g_6^{eq} \). Therefore, \( S_3 \subset S_1 \), \( S_4 \subset S_2 \), \( S_7 \subset S_5 \), \( S_6 \subset S_8 \), and 
\( S = S_0 \cap S_3 \cap S_4 \cap S_6 \cap S_7 \). Let \( S_i \) be \( S_3 \cap S_4 \cap S_6 \cap S_7 \). Then \( S_O^{D2Q9} = S_0 \cap S_i \).

**6.2.1 Calculation of \( S_0 \)**

By definition, \( S_0 \) is the domain where \( g_0^{eq} \) is non-negative

\[
S_0 = \left\{ (Pe_{Ax}^*, Cr) \left| Pe_{Ax}^* > 0, Cr > 0, \forall \theta \in [0, \pi/4], g_0^{eq}(Pe_{Ax}^*, Cr) \geq 0 \right. \right\} \tag{165}
\]

where for D2Q9 \( g_0^{eq} \) is

\[
g_0^{eq} = 1 - \frac{5}{3} \frac{Cr}{Pe_{Ax}^*} - \frac{2}{3} Cr^2 \tag{166}
\]

Then, \( g_0 \geq 0 \) if and only if \( 3Pe_{Ax}^* - 5Cr - 2Cr^2 Pe_{Ax}^* \geq 0 \). This leads to

\[
S_0 = \left\{ (Pe_{Ax}^*, Cr) \left| Pe_{Ax}^* > 0, Cr > 0, 3Pe_{Ax}^* - 5Cr - 2Cr^2 Pe_{Ax}^* \geq 0 \right. \right\} \tag{167}
\]

**6.2.2 Calculation of \( S_i \)**

Since the weighting factors \( \omega_i \) are positive by definition, hence \( \forall \theta \in [0, \pi/4] \) the set \( S_i \) can be redefined as

\[
S_i = \left\{ (Pe_{Ax}^*, Cr) \left| Pe_{Ax}^* > 0, Cr > 0, \frac{Cr}{Pe_{Ax}^*} \frac{Pe_{Ax}^*}{Pe_{Ax}^*} - Cr \lambda_i + Cr^2 \left( \frac{3}{2} \lambda_i^2 - \frac{1}{2} \right) \geq 0, i = 3, 4, 6, 7 \right. \right\} \tag{168}
\]

where \( \lambda_i = e_i \cdot e_u \). Hence \( \lambda_3 = \cos \theta \), \( \lambda_4 = \sin \theta \), \( \lambda_5 = \cos \theta - \sin \theta \), and \( \lambda_7 = \cos \theta + \sin \theta \). Since \( \theta \in [0, \pi/4] \), then \( \lambda_5 \in [\sqrt{2}/2, 1] \), \( \lambda_4 \in [0, \sqrt{2}/2] \), \( \lambda_6 \in [0, 1] \), and \( \lambda_7 \in [1, \sqrt{2}] \). Therefore, \( S_i \) becomes

\[
S_i = \left\{ (Pe_{Ax}^*, Cr) \left| Pe_{Ax}^* > 0, Cr > 0, \forall \lambda \in [0, \sqrt{2}]: h(Pe_{Ax}^*, Cr, \lambda) \geq 0 \right. \right\} \tag{169}
\]
where \( h(\text{Pe}_{\Delta x}^*, \text{Cr}, \lambda) = \text{Cr} / \text{Pe}_{\Delta x}^* - \text{Cr} \lambda + \text{Cr}^2 \left( 3\lambda^2 / 2 - 1/2 \right) \). According to Eq.(169), \( S_* \) is bounded by the curve \( h(\text{Pe}_{\Delta x}^*, \text{Cr}, \lambda = \sqrt{2}) = 0 \) and the envelope of the parametric family of curves \( h(\text{Pe}_{\Delta x}^*, \text{Cr}, \lambda) = 0 \) whose parameter is \( \lambda \in [0, \sqrt{2}] \). The curve \( h(\text{Pe}_{\Delta x}^*, \text{Cr}, \lambda = \sqrt{2}) = 0 \) is defined by the following equation

\[
2 - 2\sqrt{2}\text{Pe}_{\Delta x}^* + 5\text{Pe}_{\Delta x}^* \text{Cr} = 0
\]

(170)

To obtain the equation of the envelope, we need to eliminate \( \lambda \) in \( h(\text{Pe}_{\Delta x}^*, \text{Cr}, \lambda) = 0 \) via \( h_\lambda(\text{Pe}_{\Delta x}^*, \text{Cr}, \lambda) = dh/d\lambda = 0 \), which provides the value of \( \lambda^* = 1/(3\text{Cr}) \). Introducing \( \lambda^* \) into \( h(\text{Pe}_{\Delta x}^*, \text{Cr}, \lambda) = 0 \), we obtain the equation for the enveloping curve

\[
\text{Pe}_{\Delta x}^* + 3\text{Cr}^2\text{Pe}_{\Delta x}^* - 6\text{Cr} = 0
\]

(171)

The intersection of the envelop curve and \( h(\text{Pe}_{\Delta x}^*, \text{Cr}, \lambda = \sqrt{2}) = 0 \) is at \( \text{Pe}_{\Delta x}^* = 1.202 \) and \( \text{Cr} = 0.233 \). Thus, the set \( S_* \) is obtained for any \( \lambda \in [0, \sqrt{2}] \)

\[
S_* = \begin{cases}
(\text{Pe}_{\Delta x}^*, \text{Cr}) & \text{Pe}_{\Delta x}^* > 0, \text{Cr} > 0 \\
6\text{Cr} - \text{Pe}_{\Delta x}^* - 3\text{Cr}^2\text{Pe}_{\Delta x}^* \geq 0; & \text{if} \quad \text{Cr} > 0.233 \\
2 - 2\sqrt{2}\text{Pe}_{\Delta x}^* + 5\text{Pe}_{\Delta x}^* \text{Cr} \geq 0; & \text{if} \quad \text{Cr} \leq 0.233
\end{cases}
\]

(172)

6.2.3 Calculation of \( S \)

From Eq.(167) and Eq.(172), the set \( S_0^{Q99} \) is obtained as the intersection of \( S_0 \) and \( S_* \)

\[
S_0^{Q99} = \begin{cases}
(\text{Pe}_{\Delta x}^*, \text{Cr}) & \text{Pe}_{\Delta x}^* > 0, \text{Cr} > 0 \\
3\text{Pe}_{\Delta x}^* - 5\text{Cr} - 2\text{Cr}^2\text{Pe}_{\Delta x}^* \geq 0 \\
6\text{Cr} - \text{Pe}_{\Delta x}^* - 3\text{Cr}^2\text{Pe}_{\Delta x}^* \geq 0; & \text{if} \quad \text{Cr} > 0.233 \\
2 - 2\sqrt{2}\text{Pe}_{\Delta x}^* + 5\text{Pe}_{\Delta x}^* \text{Cr} \geq 0; & \text{if} \quad \text{Cr} \leq 0.233
\end{cases}
\]

(173)

Figure 6.1 shows the non-negativity domain for all EDFs regardless of the flow directions. The non-negativity domain is bounded by \( g_0^{Q99}(\text{Pe}_{\Delta x}^*, \text{Cr}) = 0 \), the envelope of the
parametric family of curves \( h(Pe_{\Delta x}^*, Cr, \lambda) = 0 \) for \( \lambda \in [0, \sqrt{2}] \), and the curve \( h(Pe_{\Delta x}^*, Cr, \lambda = \sqrt{2}) = 0 \). Outside the non-negativity domain \( S \), negative values for at least one dimensionless EDF can be obtained for some specific flow directions. Hence, to be inside the domain \( S \) is a sufficient condition for non-negativity.

Using linear EDFs (neglecting second-order terms in velocity in Eqs. (157)-(164)) has been suggested for solving the advection-diffusion equation in some specific cases, such as low Courant number (Flekkøy 1993). Hence we are also interested in investigating the non-negativity and stability when using linear EDFs.

6.3 Others Non-Negativity Analyses

6.3.1 D1Q3 Lattice with Linear EDFs

The linear dimensionless EDFs for D1Q3 lattice are

\[
\begin{align*}
    g_0^{eq} &= 1 - \frac{Cr}{Pe_{\Delta x}^*}, \\
    g_1^{eq} &= \frac{1}{2} \left( \frac{Cr}{Pe_{\Delta x}^*} + Cr \cos \alpha \right), \\
    g_2^{eq} &= \frac{1}{2} \left( \frac{Cr}{Pe_{\Delta x}^*} - Cr \cos \alpha \right)
\end{align*}
\]  

(174)

where \( g_1^{eq} \) is the dimensionless EDF for particles moving in the same direction that the flow, and \( g_2^{eq} \) is for particles moving in the opposite direction of the flow. \( g_0^{eq} \geq 0 \) results in \( Pe_{\Delta x}^* - Cr \geq 0 \); and \( g_2^{eq} \geq 0 \) results in \( 1 - Pe_{\Delta x}^* \geq 0 \). Therefore, the non-negativity set is

\[
S_{L}^{D1Q3} = \left\{ (Pe_{\Delta x}^*, Cr) \left| \begin{array}{l}
    Pe_{\Delta x}^* > 0, Cr > 0 \\
    Pe_{\Delta x}^* - Cr \geq 0 \\
    1 - Pe_{\Delta x}^* \geq 0
    \end{array} \right. \right\}
\]

(175)
Figure 6.1: Non-negativity domain for D2Q9 with quadratic EDFs (solid lines).
6.3.2 D1Q3 Lattice with Quadratic EDFs

The second-order dimensionless EDFs of D1Q3 lattice are

\[ g^q_0 = 1 - \left( \frac{Cr}{Pe^*_\Delta} + Cr^2 \right); \quad g^q_1 = \frac{1}{2} \left( \frac{Cr}{Pe^*_\Delta} + Cr \cos \alpha + Cr^2 \right); \quad g^q_2 = \frac{1}{2} \left( \frac{Cr}{Pe^*_\Delta} - Cr \cos \alpha + Cr^2 \right) \]  \hspace{1cm} (176)

\[ g^q_0 \geq 0 \text{ results in } Pe^*_\Delta - Cr - Pe^*_\Delta Cr^2 \geq 0; \quad \text{and } g^q_2 \geq 0 \text{ results in } 1 - Pe^*_\Delta + Pe^*_\Delta Cr \geq 0. \]

Therefore, the non-negativity set is

\[ S^D_{D1Q3} = \left\{ (Pe^*_\Delta, Cr) \left| \begin{array}{l}
Pe^*_\Delta > 0, Cr > 0 \\
Pe^*_\Delta - Cr - Pe^*_\Delta Cr^2 \geq 0 \\
1 - Pe^*_\Delta + Pe^*_\Delta Cr \geq 0
\end{array} \right. \right\} \]  \hspace{1cm} (177)

6.3.3 D2Q5 Lattice with Linear EDFs

For a given flow direction \( \alpha \) the linear dimensionless EDFs of D2Q5 lattice are

\[ g^q_0 = \left( 1 - 2 \frac{Cr}{Pe^*_\Delta} \right) \]
\[ g^q_1 = \frac{1}{2} \left( \frac{Cr}{Pe^*_\Delta} + Cr \cos \alpha \right); \quad g^q_2 = \frac{1}{2} \left( \frac{Cr}{Pe^*_\Delta} + Cr \sin \alpha \right) \]  \hspace{1cm} (178)
\[ g^q_3 = \frac{1}{2} \left( \frac{Cr}{Pe^*_\Delta} - Cr \cos \alpha \right); \quad g^q_4 = \frac{1}{2} \left( \frac{Cr}{Pe^*_\Delta} - Cr \sin \alpha \right) \]

The following relationships stand for any \( \alpha \in [0, \pi / 4] \): \( g^q_1 \geq g^q_3 \), \( g^q_2 \geq g^q_4 \). Therefore,

\[ S^D_{D2Q5} = \left\{ (Pe^*_\Delta, Cr) \left| \begin{array}{l}
Pe^*_\Delta > 0, Cr > 0 \\
1 - 2 \frac{Cr}{Pe^*_\Delta} \geq 0 \\
\frac{Cr}{Pe^*_\Delta} - Cr \lambda_i \geq 0, i = 3, 4
\end{array} \right. \right\} \]  \hspace{1cm} (179)

where \( \lambda_3 \in [\sqrt{2}/2, 1] \) and \( \lambda_4 \in [0, \sqrt{2}/2] \). The non-negativity set is \( S^D_{L} = \cap_{\alpha \in [0, \pi / 4]} S^D_{L, \alpha} \), which can be expressed as
\[ S_{L}^{D2Q9} = \begin{cases} 
(Pe_{\lambda x}^*, Cr) & Pe_{\lambda x}^* > 0, Cr > 0 \\
1 - 2 \frac{Cr}{Pe_{\lambda x}^*} \geq 0 & \\
\frac{Cr}{Pe_{\lambda x}^*} - Cr\lambda \geq 0, \forall \lambda \in [0,1] 
\end{cases} \tag{180} \]

And this leads to

\[ S_{L}^{D2Q9} = \begin{cases} 
(Pe_{\lambda x}^*, Cr) & Pe_{\lambda x}^* > 0, Cr > 0 \\
Pe_{\lambda x}^* - 2Cr \geq 0 & \\
Pe_{\lambda x}^* \leq 1 
\end{cases} \tag{181} \]

### 6.3.4 D2Q9 Lattice with Linear EDFs

For a given flow direction \( \alpha \), the linear dimensionless EDFs of D2Q9 lattice are

\[
g_{0}^{eq} = \left(1 - \frac{5}{3} \frac{Cr}{Pe_{\lambda x}^*}\right) 
\]

\[
g_{1}^{eq} = \frac{1}{3} \left(\frac{Cr}{Pe_{\lambda x}^*} + Cr \cos \alpha\right); \quad g_{2}^{eq} = \frac{1}{3} \left(\frac{Cr}{Pe_{\lambda x}^*} + Cr \sin \alpha\right) 
\]

\[
g_{3}^{eq} = \frac{1}{3} \left(\frac{Cr}{Pe_{\lambda x}^*} - Cr \cos \alpha\right); \quad g_{4}^{eq} = \frac{1}{3} \left(\frac{Cr}{Pe_{\lambda x}^*} - Cr \sin \alpha\right) 
\]

\[
g_{5}^{eq} = \frac{1}{12} \left(\frac{Cr}{Pe_{\lambda x}^*} + Cr(\cos \alpha + \sin \alpha)\right); \quad g_{6}^{eq} = \frac{1}{12} \left(\frac{Cr}{Pe_{\lambda x}^*} + Cr(-\cos \alpha + \sin \alpha)\right) 
\]

\[
g_{7}^{eq} = \frac{1}{12} \left(\frac{Cr}{Pe_{\lambda x}^*} - Cr(\cos \alpha + \sin \alpha)\right); \quad g_{8}^{eq} = \frac{1}{12} \left(\frac{Cr}{Pe_{\lambda x}^*} + Cr(\cos \alpha - \sin \alpha)\right) 
\]

The following relationships \( g_{1}^{eq} \geq g_{3}^{eq}, g_{2}^{eq} \geq g_{4}^{eq}, g_{5}^{eq} \geq g_{7}^{eq} \) and \( g_{6}^{eq} \geq g_{8}^{eq} \) are valid for any \( \alpha \in [0, \pi / 4] \). Therefore, we have

\[ S_{L}^{D2Q9} = \begin{cases} 
(Pe_{\lambda x}^*, Cr) & Pe_{\lambda x}^* > 0, Cr > 0 \\
1 - 5Cr / (3Pe_{\lambda x}^*) \geq 0 & \\
Cr / Pe_{\lambda x}^* - Cr\lambda_i \geq 0, i = 3, 4, 6, 7 
\end{cases} \tag{183} \]
The non-negativity set is $S_{L}^{D2Q9} = \bigcap_{\alpha \in [0, \pi/4]} S_{\Lambda_{\alpha}}^{D2Q9}$, which can be expressed as:

$$
S_{L}^{D2Q9} = \{(P_{\alpha x}^{*}, Cr) \mid \begin{align*}
&P_{\alpha x}^{*} > 0, Cr > 0 \\
&1 - \frac{Cr}{3 P_{\alpha x}^{*}} \geq 0 \\
&\frac{Cr}{P_{\alpha x}^{*}} - Cr \lambda \geq 0, \forall \lambda \in [0, \sqrt{2}] 
\end{align*} \} \quad (184)
$$

which leads to

$$
S_{L}^{D2Q9} = \{(P_{\alpha x}^{*}, Cr) \mid \begin{align*}
&P_{\alpha x}^{*} > 0, Cr > 0 \\
&3 P_{\alpha x}^{*} - 5 Cr \geq 0 \\
&P_{\alpha x}^{*} \leq \sqrt{2}/2
\end{align*} \} \quad (185)
$$

6.4 Summary

In this chapter, analytical expressions for the non-negativity domain of EDFs have been found. Different types of lattices (D1Q3, D2Q5 and D2Q9) as well as different types of EDFs (linear and quadratic) have been studied.
CHAPTER 7. LINEAR STABILITY FOR THE ADVECTION-DIFFUSION EQUATION

7.1 Introduction

One of the earlier works on investigating the stability problem in the LBM was provided by Sterling and Chen (1996), where the LBGK was linearized for the fluctuating quantities of particle distribution functions with respect to the EDFs. The von Neumann analysis was carried out to identify the most unstable directions and wave numbers, and their relationship with the mean flow field, relaxation time and mass distribution parameters. Worthing et al. (1997) extended the work of Sterling and Chen (1996) to non-uniform flows. In particular to the case of a shear background flow was studied and some stability boundaries were found.

In this work, we focus on the stability of the LBM when solving the advection-diffusion equation. To our knowledge, the stability problem of using LBM to solve the advection-diffusion equation is not fully discussed and most works in the stability of the LBM mainly focus on hydrodynamics equations and to date no clear stability boundaries have been provided when solving the advection-diffusion equation.

In this study, we carry out linear stability analysis of the LBGK and investigate the relationship between the stability and non-negativity of EDFs. Suga (2006) carried out linear stability analysis on the LBGK for the advection-diffusion equation and stability boundaries were delineated for several two dimensional lattices. However, only linear EDFs were considered and the ratio between the lattice speed and the speed of sound was constrained to a specific value, which creates a dependency among the lattice Peclet number, Courant number and the relaxation time. In this study, we eliminate this constraint and extend the linear stability analysis to the LTRT and EDFs other than linear EDFs.
7.2 Linear Stability of LTRT for Advection-Diffusion Equation

The LTRT in Eq. (5) can be written as follows

\[
f_i(x, t + \Delta t) = f_i(x - c_i \Delta t, t) - \frac{1}{\tau_s} \left( \frac{f_i(x - c_i \Delta t, t) + f_i(x - c_i \Delta t, t)}{2} - \frac{f_i^{eq}(x, t + \Delta t) + f_i^{eq}(x, t + \Delta t)}{2} \right)
- \frac{1}{\tau_a} \left( \frac{f_i(x - c_i \Delta t, t) - f_i(x - c_i \Delta t, t)}{2} - \frac{f_i^{eq}(x, t + \Delta t) - f_i^{eq}(x, t + \Delta t)}{2} \right)
\]  

(186)

where \( \vec{i} \) represents the opposite direction of \( i \), and hence \( \vec{f}_i = f_i \). This equation represents the evolution of the particle distribution functions to the next time step as a function of the particle distribution functions and EDFs at the present time step. In this section, we adopt the von Neumann analysis to study the linear stability of Eq.(186). Due to the streaming step and mass conservation at the collision operator, \( C(x, t + \Delta t) \) can be written as

\[
C(x, t + \Delta t) = \sum_j f_j(x - c_j \Delta t, t)
\]

(187)

Introducing dimensionless EDFs, \( g_i^{eq}(x, t) = f_i^{eq}(x, t)/C(x, t) \), and Eq.(187) into Eq.(186), we obtain

\[
f_i(x, t + \Delta t) = \left( 1 - \frac{1}{2\tau_s} - \frac{1}{2\tau_a} \right) f_i(x - c_i \Delta t, t) - \left( \frac{1}{2\tau_s} - \frac{1}{2\tau_a} \right) f_i(x - c_i \Delta t, t)
+ \left[ \frac{1}{\tau_s} g_i^{eq}(x, t + \Delta t) + \frac{1}{\tau_a} g_i^{acq}(x, t + \Delta t) \right] \sum_j f_j(x - c_j \Delta t, t)
\]

(188)

Eq. (188) becomes a linear system of equations when the dimensionless EDFs are constant for each direction and in time. This condition is fulfilled under the assumption of uniform and steady flow when linear and quadratic EDFs are used. Then, a discrete Fourier series solution for the particle distribution functions is introduced to perform the von Neumann analysis:
\[ f_i(x, t) = \sum_m b_m(t)e^{-ik_mx} \]  \hspace{1cm} (189)

where \( I \) is the complex number; \( b_m(t) \) represents the amplitude; and \( k_m \) represents the wave number. Introducing the Fourier series solution into Eq.(188), we obtain the following equation for each wave number

\[ b_m(t + \Delta t) = \left(1 - \frac{1}{2\tau_s} - \frac{1}{2\tau_a}\right)b_m(t)e^{-ik_m\Delta t} - \left(\frac{1}{2\tau_s} - \frac{1}{2\tau_a}\right)b_m(t)e^{ik_m\Delta t} \]

\[ + \left[\frac{\tau_s}{\tau_s} g_{i}^{\text{eq}}(x, t + \Delta t) + \frac{\tau_s}{\tau_a} g_{i}^{\text{eq}}(x, t + \Delta t)\right] \sum_j b_{jm}(t)e^{-ik_m\Delta t} \]  \hspace{1cm} (190)

which can be written in vector-matrix form as follows

\[ \mathbf{b}(t + \Delta t) = \mathbf{A}\mathbf{b}(t) \]  \hspace{1cm} (191)

where \( \mathbf{A} \) is the amplification matrix

\[ \mathbf{A} = \left(1 - \frac{1}{2\tau_s} - \frac{1}{2\tau_a}\right)\mathbf{M} - \left(\frac{1}{2\tau_s} - \frac{1}{2\tau_a}\right)N + \frac{1}{\tau_s} \mathbf{G}'\mathbf{M} + \frac{1}{\tau_a} \mathbf{G}''\mathbf{M} \]  \hspace{1cm} (192)

with \( \mathbf{M} \) the diagonal matrix whose diagonal elements are given by \( M_{ii} = e^{-ik_m\Delta t} \); \( \mathbf{N} \) is a matrix with elements \( N_{ij} = \delta_{ij} e^{ik_m\Delta t} \); and \( \mathbf{G}' \) and \( \mathbf{G}'' \) are given respectively by \( G'_{ij} = g_{i}^{\text{eq}} \) and \( G''_{ij} = g_{i}^{\text{eq}} \). Therefore, the linear stability of the system depends on the module of the eigenvalues of matrix \( \mathbf{A} \). The LTRT will be stable as long as the module of all the eigenvalues are less than unity for any wave number \( k_m \).

### 7.3 Linear Stability of LBGK Model

For the specific case in which \( \tau = \tau_a = \tau_s \), the LTRT becomes the LBGK model and the amplification matrix is

\[ \mathbf{A} = \left(1 - \frac{1}{\tau}\right)\mathbf{M} + \frac{1}{\tau}(\mathbf{G}' + \mathbf{G}'')\mathbf{M} \]  \hspace{1cm} (193)
7.3.1 Linear Stability on D1Q3

In this section, the eigenvalue problem is solved for the one-dimensional lattice with three velocities D1Q3. Since the system has only three velocities \((Q = 3)\), the matrix \(\mathbf{A}\) is a 3 by 3 matrix. The eigenvalues of \(\mathbf{A}\) are governed by the three parameters \(\prod = (Pe_{\Delta x}^*, Cr, \tau)\) and the direction of the flow is given by either \(\theta = 0\) or \(\theta = \pi\) in the one-dimensional case. The dimensionless EDFs for D1Q3 are

\[
\begin{align*}
    g_1^{eq} &= \frac{1}{2} \left( \frac{Cr}{Pe_{\Delta x}^*} + Cr + Cr^2 \right), \\
    g_2^{eq} &= \frac{1}{2} \left( \frac{Cr}{Pe_{\Delta x}^*} - Cr + Cr^2 \right), \\
    g_0^{eq} &= 1 - \frac{Cr}{Pe_{\Delta x}^*} + Cr^2
\end{align*}
\]

where \(g_1^{eq}\) is the dimensionless EDFs for particles moving in the same direction as the flow, \(g_2^{eq}\) is for particles moving in the opposite direction of the flow, and \(g_0^{eq}\) represents rest particles. Due to the complexity of getting the eigenvalues of the matrix \(\mathbf{A}\) analytically as an explicit function of \(\tau\), \(Pe_{\Delta x}^*\) and \(Cr\), they are obtained numerically. We use the dimensionless wave number \(\beta_n = k_m c_{js} \Delta t = n \pi / N\), where \(n\) is from 1 to \(N\), and \(N\) is the number of \(\beta_n\) used in the analysis. Since the values of particle distribution functions are real numbers, the eigenvalue problem for \(k_m\) gives the same eigenvalue when solving for \(-k_m\); therefore, \(\beta_n\) are only considered from zero to \(\pi\).

The number of dimensionless wave numbers used is \(N = 36\). The eigenvalue problem is solved twice, based on the pair \((Pe_{\Delta x}^*, Cr)\) and based on \((Pe_{\Delta x}, Cr)\), using a grid of 100 by 100 points in each case. We test different values of the relaxation time: \(\tau = 0.51, 0.6, 0.7, 0.8, 0.9,\) and \(1.0\).

Figure 7.1(a) shows the stability domain in term of \(Pe_{\Delta x}^*\) and \(Cr\) for \(\tau = 0.7\). We observe that the stability domain is bounded by two stability boundaries (stability boundary 1 and
stability boundary 2). Stability boundary 1 corresponds to the condition \( g^q_0 = 0 \). There is no direct relationship between stability boundary 2 and the non-negativity of the dimensionless EDFs. Actually, stability boundary 2 lies on the area where \( g^q_2 < 0 \) for \( \tau = 0.7 \). Therefore, it can be concluded that negative EDF values do not necessarily lead to linear instabilities. Figure 7.1(b) shows that the stability domain grows with increasing relaxation time and that the stability domain using a value of relaxation time includes the stability domain when using smaller values of relaxation time.

The non-negativity domain for D1Q3 with second-order EDFs is also shown in Figure 7.1(b) to be compared with the stability domains. The non-negativity domain is bounded by two non-negativity boundaries, \( g^q_0 = 0 \) and \( g^q_2 = 0 \), obtained in Eq.(177).

Figure 7.1 presents two important remarks. First, stability boundary 2 approaches the non-negativity boundary of \( g^q_2 = 0 \) as the relaxation time decreases, and the non-negativity domain becomes the stability domain when the relaxation time is very close to 0.5. Second, if the pair \((Pe^*_\text{Ax}, Cr)\) lies in the stability domain for a given value of the relaxation time, the pair also lies in the stability domain if larger values of the relaxation time are used. In other words, given \( Pe^*_\text{Ax} \) and \( Cr \) values there exists a minimum value of the relaxation time \( \tau \) for stable solutions.

Figure 7.2 redraws the stability domains provided by Figure 7.1(b) in terms of \( Pe^*_\text{Ax} \) and \( Cr \). Because of decoupling the relaxation time from the lattice Peclet number, a larger value of the relaxation time does not necessarily result in stable solutions. This shows the advantage of using \( Pe^*_\text{Ax} \) instead of \( Pe^*_\text{Ax} \) for the analysis.

If only linear terms are considered, the dimensionless EDFs become

\[
\begin{align*}
g^q_1 &= \frac{1}{2} \left( \frac{Cr}{Pe^*_\text{Ax}} + Cr \right), \\
g^q_2 &= \frac{1}{2} \left( \frac{Cr}{Pe^*_\text{Ax}} - Cr \right), \\
g^q_0 &= 1 - \frac{Cr}{Pe^*_\text{Ax}}
\end{align*}
\]
Figure 7.1: Linear stability boundaries for LBGK in D1Q3 with quadratic EDFs: (a) specific case $\tau = 0.7$; (b) different $\tau$ values (solid lines) and non-negativity boundaries (dash lines) for dimensionless EDFs.
Figure 7.2: Linear stability boundaries for LBGK model in D1Q3 with quadratic EDFs.
Figure 7.3 shows the stability boundaries for different values of relaxation time for the linear EDFs. The stability domain is bounded by stability boundary 1 and stability boundary 2 for a given relaxation time. Stability boundary 1 is given by \( g_0^{\text{eq}} = 0 \) and stability boundary 2 moves and enlarges the stability domain when the relaxation time increases. Comparing Figure 7.3 with Figure 7.1(b), we can observe that the stability domains with quadratic EDFs are larger than those with linear EDFs for a given \( \tau \). The non-negativity domain with second-order EDFs is also much larger than that when using linear EDFs; and as \( Pe_{\Lambda}^* \) increases, stable solutions will only be found for low Courant number.

### 7.3.2 Linear Stability Analysis on D2Q9 and D2Q5

In this section, we analyze the LBGK stability for D2Q9 and D2Q5 lattices. We first consider D2Q9. Since both lattices have symmetry respect to the horizontal, vertical and diagonal directions, we can reduce our study to the flow direction \( \theta \in [0, \pi / 4] \), and any other directions will be equivalent to the one in this interval.

The procedure is the same as in the one-dimensional case, but \( A \) is a 9 by 9 matrix instead of 3 by 3. In this problem, the angle \( \alpha \) of flow velocity with respect to the lattice grid will be an additional factor in the analysis. For different values of \( \Pi = (Pe_{\Lambda}^*, Cr, \tau, \theta) \), the eigenvalues of the matrix \( A \) are calculated numerically. When solving the eigenvalue problem numerically in 2D, we use the dimensionless wave number \( \beta_n = k_n c_j \Delta t \) and \( \gamma_p = k_p c_j \Delta t \).

Then, \( \exp(k_m \cdot c_j \Delta t) = \exp(\beta_n) \exp(\gamma_p) \), where \( \beta_n = n \Delta \pi / N \) and \( \gamma_p = p \Delta \pi / N \). \( n \) and \( p \) go from 1 to \( N \). \( N \) is the number of \( \beta_n \) and \( \gamma_p \) that we use to discretize the range \([0, 2\pi]\).

Similar to the one-dimensional case, we test different values of the relaxation time, \( \tau = 0.51, 0.6, 0.7, 0.8, 0.9, \) and 1.0, to determine the stability domain. The number of the
The dimensionless wave numbers used is $N = 72$. The eigenvalue problem is solved twice based on the pairs $(Pe_{\Delta x}, Cr)$ and $(Pe_{\Delta x}, Cr)$, using a grid of 100 by 100 points in each case.

**Figure 7.3:** Stability and non-negativity domains of D1Q3 lattice with linear EDFs. The stability domain is the area underneath the stability boundaries (solid lines). The non-negativity domain is the area underneath the non-negativity boundaries (dash lines).

The stability domains shown in Figure 7.4 are for the D2Q9 lattice with quadratic EDFs. For a specific flow direction $\theta = 22.5^\circ$ (Figures 7.4(a)-7.4(b)), the non-negativity domain shown in Figure 7.4(a) is delineated using Eq.(167) and Eq.(168). Figure 7.4(a) shows growing stability domains based on $Pe_{\Delta x}^*$ and $Cr$ when the relaxation time increases. Moreover, we can observe
that the stability domain becomes the non-negativity domain when the relaxation time is very close to 0.5.

Similar to the one-dimension case, given \((Pe^*_{\Delta t}, Cr, \theta)\) in Figure 7.4(a) there is a minimum value of the relaxation time for stable solutions. However, if \(Pe_{\Delta t}\) is used, the stability boundaries for different values of relaxation time can intersect each other (Figure 7.4(b)). Hence, given \((Pe_{\Delta t}, Cr, \theta)\) increasing the relaxation time does not guarantee stable solution in general.

Figures 7.4(c) and 7.3(d) show the domain resulting from intersecting the stability domains for five flow directions \(\theta = (i - 1)\pi / 16, \ i = 1, 2, ..., 5\). The non-negativity domain in Figure 7.4(c) is also obtained by considering intersection of the non-negativity domains for those flow directions. Figure 7.4 has been obtained as an approximation to the stability domain for any direction of the flow, which would result from the intersection of stability domains for \(\forall \theta \in [0, \pi / 4]\).

Next, we consider the case of neglecting the second-order terms in the EDFs. It is noted that D2Q5 with linear EDFs can recover the same moments as D2Q9 with linear EDFs, and therefore the same macroscopic equation. Hence our interest is in comparing these two lattices. Figure 7.5 shows the non-negativity and stability domains using linear EDFs for D2Q5 and D2Q9 lattices with the five flow directions \(\theta = (i - 1)\pi / 16, \ i = 1, 2, ..., 5\). The stability domains of the D2Q9 are slightly larger than those for the D2Q5. However, the D2Q9 non-negativity domain is slightly smaller than that for the D2Q5.

Comparing Figure 7.5 with Figure 7.4, we observe that quadratic EDFs give larger non-negativity and stability domains than those given by linear EDFs. Linear EDFs only offer stable solutions for low Courant number as \(Pe^*_{\Delta t}\) increases while quadratic EDFs can produce stable solution at higher Courant number.
Figure 7.4: Stability and non-negativity domains for D2Q9 lattice with quadratic EDFs. (a) and (b) are for specific case \( \theta = 22.5^\circ \). (c) and (d) consider five flow directions \( (\theta = 0^\circ, 11.25^\circ, 22.5^\circ, 37.75^\circ, 45^\circ) \) simultaneously. The stability domain is the area underneath the stability boundaries (solid lines). The non-negativity domain is the area underneath the non-negativity boundaries (dash lines).
Figure 7.5: Stability and non-negativity domains for D2Q9 and D2Q5 lattices with linear EDFs, considering five flow directions (θ = 0°, 11.25°, 22.5°, 37.75°, 45°) simultaneously. The stability domain is the area underneath the stability boundaries (solid lines). The non-negativity domain is the area underneath the non-negativity boundaries (dash lines).
7.3.3 Verification and Validation Examples

7.3.3.1 One-Dimensional Transport with Gaussian Initial Condition

This section conducts numerical experiments to demonstrate the stability problem of using the LTRT to solve the one-dimensional advection-diffusion equation. The set up of this case study is described in section 3.4.1.

Figure 7.6 shows the numerical results using quadratic EDFs, for the relaxation time $\tau = 0.51, 0.6, 0.7, 0.8, 0.9, 1.2, \text{ and } 3$ for $Pe_{\Delta x} = 50$ and $Cr = 0.8$. By simulating one thousand time steps, $\tau = 0.51$ and 0.7 provide unstable solutions as we observe in Figure 7.6 (a). The unstable solutions are confirmed by Figure 7.2, in which the pair of $Pe_{\Delta x} = 50$ and $Cr = 0.8$ lies in the unstable domains for $\tau = 0.51$ and 0.7. On the other hand, the pair of $Pe_{\Delta x} = 50$ and $Cr = 0.8$ gives the module of the eigenvalues of matrix $A$ less than unity for $\tau = 0.6, 0.8, 0.9, 1.0, 2.0, \text{ and } 3.0$ and results in stable solutions (Figure 7.6 (a)). The stability when $\tau = 0.6, 0.8, 0.9, \text{ and } 1.0$ can be checked in Figure 7.2. Furthermore, total errors for relaxation times larger than one greatly increase, indicating that more numerical dispersion has been introduced.

None of the relaxation times considered in Figure 7.6 (a) makes the pair of $Pe_{\Delta x} = 50$ and $Cr = 0.8$ to lie in the non-negativity domain except for $\tau = 0.6$. This confirms that using negative EDFs does not necessarily lead to unstable solutions.

Figure 7.6 (b) shows normalized concentration distributions after one thousand time steps. Figure 7.6 (b) also shows that numerical dispersion greatly increases for relaxation times larger than one. The greater the numerical dispersion, the greater the total errors (see Figure 7.6 (a)). Based on Figure 7.6, we find that the most accurate solution is obtained for values of the relaxation time $\tau \approx 0.8$. 

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7.3.3.2 Two-Dimensional Mass Transport in Uniform Flow

The one-dimensional mass-transport in uniform flow was already introduced in section 3.4.2 to compare the performance of linear, linear with second order correction and quadratic EDFs. In this section, we use the same transport problem, but with different values of Peclet and Courant numbers, to corroborate the correctness of the 2D linear stability analysis.

This case tests the stability of the solutions with relaxation times $\tau = 0.51, 0.6, 0.7, 0.8, 0.9, 1.0, 2.0, \text{ and } 3.0$ when $Pe_{\Delta x} = 20$, $Cr = 0.5$ and $\theta = 22.5^\circ$. None of these $\tau$ values places the pair of $Pe_{\Delta x} = 20$ and $Cr = 0.5$ in the non-negativity domain. Figure 7.4(b) implies stable solutions for $\tau = 0.6, 0.8, 0.9,$ and $1.0$ and unstable solutions for $\tau = 0.51$ and $0.7$. Moreover, the module of the eigenvalue of the matrix $A$ is less than unity for $\tau = 2$ and $3$. The numerical results in Figure 7.7 confirm these implications.

Figure 7.7(a) shows the evolution of the total errors for each case up to 500 time steps. Unstable solutions for $\tau = 0.51$ and $0.7$ are obvious. Figures 7.7(b)-(h) show the normalized
concentration distribution after five hundreds time steps for the analytical solution (Figure 7.7(b)) and the LBM results (Figure 7.7(c)-(h)). In this case, we observe that \( \tau = 0.8 \) provides the best solution as it happened in the one-dimensional cases. Moreover, numerical dispersion increases as \( \tau \) is larger than 0.8. While \( \tau = 1 \) produced a good solution with moderate numerical dispersion (Figure 7.7(f)), using \( \tau \) values larger than unity introduce too much numerical dispersion (Figures 7.7(g)-(h)).

### 7.4 LTRT Model vs LBGK Model

#### 7.4.1 Linear Stability with Quadratic EDFs

##### 7.4.1.1 Linear Stability Analysis on D1Q3

In the one dimensional case, the dimensionless EDFs are

\[
\begin{align*}
    g_1^{\text{eq}} &= g_2^{\text{eq}} = \frac{1}{2} \left( \frac{Cr}{Pe_{\Delta t}(\tau_a - 1/2)} + Cr^2 \right), \\
    g_0^{\text{eq}} &= 1 - \frac{Cr}{Pe_{\Delta t}(\tau_a - 1/2)} - Cr^2 \\
    g_1^{\text{aco}} &= -g_2^{\text{aco}} = \frac{1}{2} Cr, \\
    g_0^{\text{aco}} &= 0
\end{align*}
\]

where \( g_1^{\text{eq}} \) represents the particle distribution function streaming in the direction of the flow.

Figure 7.8 shows the linear stability boundaries for the LBGK and LTRT with different \( \tau_a \) values. The stability domains were obtained by varying systematically the values of the lattice Peclet number and the Courant number, and calculating the maximum modulus of the eigenvalues of the amplification matrix.

The linear stability domain is located between the upper and lower stability boundaries. The upper stability boundaries remain the same for both LBGK and LTRT while the lower boundary changes. The stability domain for the LTRT decreases with respect to the LBGK when \( \tau_a > 0.789 \).
7.4.1.2 Linear Stability of Quadratic EDFs on D2Q9

In the two dimensional case, the dimensionless EDFs are given by Eq.(79). Regarding the flow direction, due to the lattice symmetry with respect to the horizontal, vertical and diagonal directions, we can reduce our study to \( \theta \in [0, \pi/4] \).

Figure 7.9 shows the linear stability boundaries of the LBGK and LTRT for \( \theta = \pi/8 \). Similarly, we observe that the linear stability domain of the LTRT decreases with respect to the LBGK for \( \tau_a > 0.789 \). Figure 7.10 shows the linear stability boundaries for the LBGK and LTRT for any flow directions. The stable domains lie under the stability boundaries.

7.4.2 Stability of Linear EDFs with Second Order Correction on D2Q5

The dimensionless linear EDFs for symmetric and anti-symmetric parts are given in Eq. (78). The EDFs and the forcing term under uniform and steady flow can be expressed as

\[
\begin{align*}
 f_i^{\text{seq}}(t+\Delta t) &= C^{\prime+\Delta t} g_i^{\text{seq}} \\
 f_i^{\text{a}eq}(t+\Delta t) &= C^{\prime+\Delta t} g_i^{\text{a}eq} \\
 F_i(t+\Delta t) &= g_i^{\text{a}eq} \frac{1}{\tau_a} \left( \tau_a - \frac{1}{2} \right) \frac{C^{\prime+\Delta t} - C'}{\Delta t}
\end{align*}
\]

(197)

According to Eq.(187), Eq. (197) becomes

\[
\begin{align*}
 f_i^{\text{seq}}(t+\Delta t) &= g_i^{\text{seq}} \sum_j f_j(x - c_j \Delta t, t) \\
 f_i^{\text{a}eq}(t+\Delta t) &= g_i^{\text{a}eq} \sum_j f_j(x - c_j \Delta t, t) \\
 F_i(t+\Delta t) &= \frac{1}{\Delta t \tau_a} g_i^{\text{a}eq} \left( \tau_a - \frac{1}{2} \right) \left( \sum_j f_j(x - c_j \Delta t, t) - \sum_j f_j(x, t) \right)
\end{align*}
\]

(198)

Introducing Eq. (198) and (189) into the LTRT model, the linear system is obtained

\[
\begin{align*}
 b_{im}(t+\Delta t) &= \left( 1 - \frac{1}{2\tau_s} - \frac{1}{2\tau_a} \right) b_{im}(t) e^{-\kappa_{im} \tau_s \Delta t} - \left( 1 - \frac{1}{2\tau_s} - \frac{1}{2\tau_a} \right) b_{im}(t) e^{\kappa_{im} \epsilon_s \Delta t} \\
 &+ \left[ \frac{1}{\tau_a} g_i^{\text{seq}} + \frac{1}{\tau_a} \left( \tau_a + \frac{1}{2} \right) g_i^{\text{a}eq} \right] \sum_j b_{jm}(t) e^{-\kappa_{ij} \epsilon_s \Delta t} - \frac{1}{\tau_a} \left( \tau_a - \frac{1}{2} \right) g_i^{\text{a}eq} \sum_j b_{jm}(t)
\end{align*}
\]

(199)
which can be written in vector-matrix form $\mathbf{b}(t + \Delta t) = \mathbf{A}\mathbf{b}(t)$, where the amplification matrix $\mathbf{A}$ is

$$
\mathbf{A} = \left(1 - \frac{1}{2\tau_s} - \frac{1}{2\tau_a}\right)\mathbf{M} - \left(\frac{1}{2\tau_s} - \frac{1}{2\tau_a}\right)\mathbf{N} + \frac{1}{\tau_s} \mathbf{G}'\mathbf{M} + \frac{1}{\tau_a} \left(\tau_a + \frac{1}{2}\right) \mathbf{G}''\mathbf{M} - \frac{1}{\tau_a} \left(\tau_a - \frac{1}{2}\right) \mathbf{G}''
$$

(200)

where $\mathbf{M}$, $\mathbf{N}$, $\mathbf{G}'$ and $\mathbf{G}''$ have been defined in section 7.3.

Figure 7.11 shows the linear stability boundaries for the LBGK and LTRT for any flow directions. Comparing Figure 7.10 and Figure 7.11, we observe that the quadratic EDFs on D2Q9 provide larger linear stability domains than linear EDFs with second order correction on D2Q5. Nevertheless, using D2Q5 with linear EDFs still has advantages for solving the advection-diffusion equation because fewer directions are needed than quadratic EDFs.

7.4.3 Verification and Validation Examples

7.4.3.1 One-Dimensional Transport with Gaussian Initial Condition

This section conducts numerical experiments to demonstrate the stability problem of using the LTRT to solve the one-dimensional advection-diffusion equation. The set up of this case study is described in section 3.4.1.

Figures 7.12(a) and (b) show the normalized results at $t = 1000\Delta t$ for $Pe_{\Delta x} = 40$ and $Cr = 0.8$ using the LBGK and LTRT with different stable values of $\tau_a$. Figures 7.12(c) and 14(d) show the total error evolution up to one thousand time steps for stable and unstable solutions. Based on Figure 7.12(c), the LBGK model at $Pe_{\Delta x} = 40$ and $Cr = 0.8$ is stable for $\tau_a = 0.6$, $0.8$, $0.9$, and $1.0$ and unstable for $\tau_a = 0.51$ and $0.7$. Figure 7.12(d) also shows that LTRT model at $Pe_{\Delta x} = 40$ and $Cr = 0.8$ is stable for $\tau_a = 0.6$, $0.7$, $0.8$, and $0.9$ and unstable for $\tau_a = 0.51$ and $1.0$. These stability results are confirmed by Figure 7.8.
Figure 7.7: (a) Evolution of total errors for $Pe_{\Delta t} = 20$, $Cr = 0.5$ and $\theta = 22.5^\circ$ using D2Q9 with quadratic EDFs; (b) analytic solution; (c)-(h) normalized concentration distributions after five hundreds time steps.
Figure 7.8: Linear stability boundaries on D1Q3. Solid line: LBGK, $\tau_s = \tau_a$; Dash line: LTRT with $\tau_s = 0.5 + \left[12\left(\tau_a - 1/2\right)\right]^{-1}$. 
7.4.3.2 Two-Dimensional Transport with Gaussian Initial Condition

In section 4.3.2 the two dimensional mass-transport problem in uniform flow was studied with $Pe_x = 40$, $Cr = 0.2$ and $\theta = \pi / 8$. From Figure 4.2(c) and (d) we can notice that unstable solutions are obtained for $\tau_a = 0.6$ and 0.7 when using the LBGK model, and $\tau_a = 0.51, 0.6$ and 0.7 when using the LTRT model, as they are predicted by the linear stability analysis in Figure 7.9.

![Graph](image1.png)

**Figure 7.9:** Linear stability analysis on D2Q9 with $\theta = \pi / 8$. (a) LBGK; (b) LTRT with $\tau_s = 0.5 + [12(\tau_a - 1/2)]^{-1}$. 
Figure 7.10: Linear stability analysis on D2Q9 with quadratic EDFs for any flow direction. (a) LBGK; (b) LTRT with $\tau_s = 0.5 + \left[12(\tau_a - 1/2)\right]^{-1}$
Figure 7.11: Linear stability analysis on D2Q5 with linear EDFS and second order correction for any flow direction. (a): LBGK; (b): LTRT with $\tau_s = 0.5 + [12(\tau_a - 1/2)]^{-1}$
Figure 7.12: 1D Transport problem: $Pe_{\Delta x} = 40$, $Cr = 0.8$. (a) and (c): LBGK, $\tau_s = \tau_a$; (b) and (d): LTRT with $\tau_s = 0.5 + [12(\tau_a - 1/2)]^{1/2}$.
7.5 Linear Stability for AADE

In this section, we carry out the linear stability analysis on the LTRT when solving the AADE using D2Q9 lattice. We assume uniform and steady flow and uniform porosity in order to make the dimensionless EDFs constant for each direction. For uniform and steady flow, the dispersion tensor remains the same at any location and any time. Hence, the AADE can be written as:

\[
\frac{\partial C}{\partial t} + u_\alpha \frac{\partial C}{\partial \alpha} = D_{\alpha\beta} \frac{\partial^2 C}{\partial \alpha \partial \beta}
\]  

(201)

The dimensionless EDFs to solve Eq. (201) become:

\[
g_{i}^{eq} = \omega_i \left( \frac{c^2_{si}}{c^2} + \frac{\mathbf{c} \cdot \mathbf{u}}{c^2} + \frac{3}{2} \left( \frac{\mathbf{c} \cdot \mathbf{u}}{c} \right)^2 - \frac{1}{2} \frac{\mathbf{u} \cdot \mathbf{u}}{c^2} \right) \quad i > 0
\]

\[
g_{0}^{eq} = 1 - \sum_{i>0} f_i^{eq}
\]

(202)

where \( c^2_{si} \) are given by Eq.(108) and Eq.(109). The amplification matrix is given by Eq. (192). Then, the linear stability boundaries are obtained by solving the eigenvalue problem with the dimensionless EDFs in Eq. (202).

When using the LBM to solve the advection-diffusion equation, the linear stability analysis of the LTRT model depends on \( Pe_\Delta x \), \( Cr \), \( \tau_a \), \( \tau_s \) and \( \theta \). However, when considering the AADE, there are two new parameters that need to be taken into account: the longitudinal and transversal dispersivities (\( \kappa_L \) and \( \kappa_T \)). In this section, we carry out linear stability analysis for the AADE considering that there is no molecular diffusion, and then the dispersion tensor depends on the flow as \( D_{\alpha\beta} = \delta_{\alpha\beta} \kappa_T (\mathbf{u} \cdot \mathbf{u})/|\mathbf{u}| + (\kappa_L - \kappa_T) (u_\alpha u_\beta)/|\mathbf{u}| \). Hence, the linear stability depends on the following parameters: \( Cr \), \( \tau_a \), \( \tau_s \), \( \theta \), \( \kappa_L/\Delta x \) and \( \kappa_T/\kappa_T \). Figure 7.13 shows the
linear stability boundaries for the specific case of using $\tau_a = 1$ and $\tau_s = 0.6, 0.667, 0.7, 0.8, 0.9$ and 1. Figures 7.13 (a), (b), (c) and (d) provide the stability boundaries for $\kappa_L / \kappa_T = 1$, $\kappa_L / \kappa_T = 10$, $\kappa_L / \kappa_T = 20$ and $\kappa_L / \kappa_T = 50$ respectively.

7.6 Summary

In this chapter the Von Neumann analysis has been applied to the lattice Boltzmann Equation. The dimensionless approach has provided linear stability boundaries based on the dimensionless parameters governing the LBM. This is useful to reduce the number of variables involved in the linear stability analysis and therefore allows representing linear stability boundaries in a compact manner.

Linear stability boundaries have been found for different types of lattices (D1Q3, D2Q5 and D2Q9), different types of EDFs (linear, quadratic and linear with second order correction), and different types of collision operators (BGK and TRT). Moreover, the relationship between non-negativity of EDFs and the linear stability has been found.
Figure 7.13: Linear stability analysis of LTRT on D2Q9 with quadratic EDFs.
CHAPTER 8. APPLICATION EXAMPLES: LBM FOR SALTWATER INTRUSION

8.1 Literature Review on Saltwater Intrusion Modeling

Modeling saltwater intrusion has been extensively studied through the sharp-interface model and density-dependent model. The employment of the sharp-interface model assumes that the width of the freshwater-saltwater mixing zone is much smaller than the thickness of the aquifer, and therefore it can be assumed that freshwater and saltwater are two immiscible fluids of different but constant densities separated by an interface. Essaid (1990) developed a quasi three-dimensional finite difference model to study layered coastal aquifer systems. The main idea was to solve vertically integrated groundwater equations for each aquifer using the sharp interface approach, and to allow vertical leakage through confined layers including the effect of density differences. Dispersion of saltwater was neglected. The earliest development of the sharp-interface model is the Ghyben-Herzberg model, where the interface location is explicitly determined by the hydrostatic pressure balance between the seawater and freshwater (Segol 1994). Significant improvements were reached on the sharp-interface model under the Dupuit assumption, which assumes that equipotential lines are vertical, the flow is horizontal, and the specific discharge is uniform along the vertical direction. Shamir and Dagan (1971) presented an implicit numerical scheme to solve the linearized equations of the seawater motion in a vertical section under the Dupuit assumption and the sharp interface approach, taking into consideration the vertical geometry of the aquifer. Wilson and da Costa (1982) applied a one dimensional finite element scheme for solving two-layer flow involving the lower and upper toe of the seawater-freshwater interface, which is assumed to be a straight line. This numerical scheme was presented as an alternative to the moving boundary model, which was computationally expensive because of the need of remeshing to track the sharp interface.
The density-dependent model better describes the real saltwater intrusion mechanism due to strong saltwater hydrodynamic dispersion and the existence of a wide transition zone, which is evident in real coastal aquifers. Kohout (1964) reported an investigation on a real aquifer in the Miami area. This investigation showed that numerical predictions were far from accurate because, among other factors, the saltwater is moving instead of remaining steady as it was supposed. Moreover, a saltwater intrusion zone was reported, and this zone corresponds to the intrusion area of the saltwater due to the higher pressures at the bottom of the aquifer in the seaside. The seawater intrudes through the lower part and later on moves upwards and returns to the sea. This was demonstrated by the net flow discharged in the shoreline, which is higher than the freshwater discharge at the inland side. The hydrodynamic dispersion is an important factor developing saltwater circulation at the seaside of the aquifer. Cooper (1964) focused on the fact that if there is a diffusion zone, the salt must return to the sea by means of a circulation, which makes the saltwater intrude from the bottom and return somewhere around the diffusion zone. The density-dependent model considers freshwater and saltwater mixing and allows change in water density by solving coupled flow and transport equations simultaneously. Pinder and Cooper (1970) successfully applied the method of characteristics to track the saltwater front for saline concentrations no larger than concentration in the seawater. Lee and Cheng (1974) applied the finite element method to calculate the steady state solution of the saltwater encroachment in a two dimensional coastal aquifer. Results were in good agreement with the Henry analytical solution (Henry 1964), and they compared qualitatively well with field data in the Biscayne area (Kohout 1964). Segol et al. (1975) solved the transient saltwater intrusion problem in a two dimensional coastal aquifer using the finite element method. The groundwater flow equation was written for zero specific storage, which means that the propagation of head is much faster than the salt transport. Problems were found to specify Dirichlet boundary conditions with the finite
element method at the sea boundary where the water is flushed out, which was solved imposing a Neumann boundary condition.

Numerical instabilities are often encountered when the convective term in the transport equation become dominant, which was supposed to be due to the discontinuous velocity field. Frind (1982) proposed a finite element formulation that lessens the computational cost with the governing equations formulated in term of freshwater head instead of pressure, which reduces the computational cost. Results for the transient solution in the Henry problem were compared with those in Segol et al. (1975), and good agreement was found. Huyakorn et al. (1987) developed a three dimensional finite element model for saltwater intrusion in either confined or phreatic aquifers. The formulation is based on hydraulic head and concentration instead of pressure and density. Voss and Souza (1987) applied a finite element method capable of dealing with narrow transition zones with minimum numerical dispersion. In addition, discussion was provided regarding the validity of the Henry problem to test buoyancy driven flows, and the Peclet number in the mesh was found have to be less than four to guarantee numerical stability.

The Henry problem (Henry 1964) was the primary benchmark to validate those numerical models, and with advancing capability in computation, the accuracy of the Henry analytical solution was greatly improved. Segol (1994) recomputed the Henry analytical solution finding out that the solution of Henry was not accurate enough. Although Segol solution was a good improvement, values of concentration near the upper boundary were still hard to compute, and non-smooth isochlors lines were obtained. Simpson and Clement (2004) presented an improved computation of the Henry analytical solution, in which the isochlors are smooth and reach the upper boundary. Moreover, a decrease in the freshwater inflow was proposed to improve the worthiness of the Henry problem as a test of buoyancy effects due to the variability of density.
8.2 Derivation of Density-Dependent Groundwater Flow Equation

Darcy’s law for density-dependent groundwater flow is (Hubbert 1954)

\[
q = -\frac{k}{\mu} (\nabla p - \rho g)
\]

(203)

where \( k \) is the intrinsic permeability tensor; \( \mu \) is the dynamic viscosity of formation water; \( \rho \) is the density of formation water; \( p \) is the pore water pressure; \( g \) is the gravity vector; and \( \nabla \) is the gradient operation in the vertical plane.

Although the Darcy velocity is a function of the formation water density and viscosity when the dissolved salt is present, only variations of density are considered in this work. Besides, the groundwater flow equation is formulated in terms of freshwater head. To do so, the freshwater head is defined as \( h_f = \rho / \rho_f g + z \) and freshwater hydraulic conductivity is defined as \( K_f = k \rho_f g / \mu_f \). Then, the Darcy velocity in \( x \) and \( z \) directions are

\[
q_x = -K_{xf} \frac{\partial h_f}{\partial x}
\]

(204)

\[
q_z = -K_{zf} \left( \frac{\partial h_f}{\partial z} + \phi - 1 \right)
\]

(205)

where \( \phi = \rho / \rho_f \) is the ratio of actual density to freshwater density. This study focuses on the saltwater intrusion problem, where the maximum salinity is as much as seawater. At the temperature 20°C, the linear relationship between the water density ratio and salt (NaCl) concentration, \( \phi = 1 + EC \) over the concentration range 0–35 parts per thousands (ppt) is observed (Weast and Astle 1982), where \( \rho_f = 998 \text{kg/m}^3 \) is the freshwater density, \( C \) is the salt concentration in \( \text{g/L} \) or in ppt, and \( E = 6.614 \times 10^{-4} \text{L/g} \). The mass conservation of the formation water leads to the following PDE
\[
\frac{\partial (n\rho)}{\partial t} + \nabla \cdot (\rho \mathbf{q}) = \rho_{ss} Q_{ss}
\]  \hspace{1cm} (206)

where \( n \) is porosity, \( \rho_{ss} \) is the water density at the sinks/sources; and \( Q_{ss} \) is the flow rate per unit aquifer volume at the sinks/sources. The total mass in the mass conservation equation (Eq.(206)) includes the mass of freshwater and mass of dissolved salt, i.e., \( \rho = \rho_f + C \). The dispersion process of the salt concentration is considered negligible in the water mass balance equation. However, it will be a significant component in the salt transport equation. Moreover, when the salt concentration does not exceed the seawater concentration, the total fluid volume is considered unchanged while additional dissolved salt is added into the freshwater. The saltwater compressibility is considered the same as the freshwater compressibility. We recognize that the flux \( \mathbf{q} \) in Eq.(206) should include additional flux due to concentration gradient when high salinity, e.g., brine, is considered in the flow problem (Hassanizadeh and Leijnse 1988; Oldenburg and Pruess 1995). However, using only convection due to Darcy’s velocity is sufficient when the maximum salinity is up to seawater concentration.

Due to the consideration of slight compressibility in water and soil matrix and the presence of the dissolved salt, the local change term in Eq. (206) becomes

\[
\frac{\partial (n\rho)}{\partial t} = \phi \rho_f S_{sf} \frac{\partial h_f}{\partial t} + n \frac{\partial \rho}{\partial C} \frac{\partial C}{\partial t} + \frac{\partial}{\partial x} \left( \phi \frac{\partial h_f}{\partial x} \right) + \frac{\partial}{\partial z} \left( \phi k_{fz} \frac{\partial h_f}{\partial z} \right) + \frac{\partial}{\partial z} \left( \phi (\phi - 1) k_{fzz} \right) + \frac{\rho_{ss} Q_{ss}}{\rho_f} \]  \hspace{1cm} (207)

where \( S_{sf} = \rho_f g (\alpha + n\beta) \) is the freshwater specific storage, \( \alpha \) is the soil compressibility, and \( \beta \) is the water compressibility. Substituting the Darcy velocity and the local change term into the mass conservation equation, the density-viscosity-dependent groundwater flow equation is obtained:

\[
\phi S_{sf} \frac{\partial h_f}{\partial t} + nE \frac{\partial C}{\partial t} = \frac{\partial}{\partial x} \left( \phi K_{fxx} \frac{\partial h_f}{\partial x} \right) + \frac{\partial}{\partial z} \left( \phi K_{fzz} \frac{\partial h_f}{\partial z} \right) + \frac{\partial}{\partial z} \left( \phi (\phi - 1) K_{fzz} \right) + \frac{\rho_{ss} Q_{ss}}{\rho_f} \]  \hspace{1cm} (208)
8.3 LBM for Saltwater Intrusion Problems

8.3.1 Groundwater Flow Equation for Saltwater Intrusion

Saltwater intrusion problems are governed by Darcy’s law, the density dependent groundwater flow equation (Eq.(208)), the AADE (Eq.(105)), and the equation of state \( \phi = \rho / \rho_f = 1 + EC \). Therefore, our mathematical model for the saltwater intrusion problem consists of the aforementioned governing equations.

On one hand, if \( L \) is a characteristic length in our case study, a characteristic time scale for the groundwater flow can be estimated by \( T_g = L^2 / (K^c / S^c_s) \), where \( K_g \) and \( S_g \) are characteristic values for the hydraulic conductivity and specific storage. On the other hand, the characteristic time for the salt transport problem can be estimated by \( T_s = L^2 / D^c \) where \( D_s \) is a characteristic value for the dispersion. If we compare both time scales, we get that \( T_g / T_s = D^c S^c_s / K^c \). In this work, we consider cases where due to very small values of specific storages, the time scales are very small \( (T_g / T_s \ll 1) \). This means that the redistribution of freshwater head (or pressure) over the domain occurs in a much shorter period of time than the time required to see small changes in concentrations. Hence we can assume that the groundwater flow basically reaches the steady state within one transport time step. Therefore, the groundwater flow equation can be simplified to a Poisson type equation for each transport time step as follows

\[
0 = \frac{\partial}{\partial x} \left( \phi K_{f,xx} \frac{\partial h_f}{\partial x} \right) + \frac{\partial}{\partial z} \left( \phi K_{f,zz} \frac{\partial h_f}{\partial z} \right) + \frac{\partial}{\partial z} \left( \phi (\phi - 1) K_{f,z} \right) + \frac{\rho_s}{\rho_f} Q_{ss} + nE \frac{\partial C}{\partial t} \tag{209}
\]

Since the LBM is a time-marching method, we obtain the solution of equation Eq.(209) as the steady state solution of

\[
\frac{\partial h}{\partial t'} = \frac{\partial}{\partial x} \left( \phi K_{f,xx} \frac{\partial h_f}{\partial x} \right) + \frac{\partial}{\partial z} \left( \phi K_{f,zz} \frac{\partial h_f}{\partial z} \right) + \frac{\partial}{\partial z} \left( \phi (\phi - 1) K_{f,z} \right) + \frac{\rho_s}{\rho_f} Q_{ss} + nE \frac{\partial C}{\partial t} \tag{210}
\]

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where $t'$ is a fictitious time and $\partial_t C$ represents the variation of concentration but in the transport time scale, which can be assumed to be a constant value during one transport time step. The latter approach has been effectively used and was named as lattice Poisson by Wang et al. (2006) to obtain steady-state solutions.

In order to solve Eq. (210), we use the following EDFs

$$
\begin{align*}
    f_1^{eq} &= h \frac{c^2_{xx}}{2c^2}, \\
    f_2^{eq} &= h \frac{c^2_{zz}}{2c^2} - \frac{\phi(\phi-1)K_{fz}}{2c}, \\
    f_3^{eq} &= h \frac{c^2_{zz}}{2c^2}, \\
    f_4^{eq} &= h \frac{c^2_{zz}}{2c^2} + \frac{\phi(\phi-1)K_{fz}}{2c}, \\
    f_0^{eq} &= h - \sum_{i=1}^{4} f_i^{eq}
\end{align*}
$$

(211)

with

$$
    c^2_{Saa} = \frac{\phi K_{aa}}{\Delta t (\tau_a - 1/2)}
$$

(212)

The EDFs fulfill the following moments

$$
\begin{align*}
    M_0 &= h, \\
    M_{1a} &= -\delta_{aa} \phi(\phi-1)K_{fz}, \\
    M_{2ab} &= h \delta_{ab} \frac{\phi K_{ab}}{\Delta t (\tau_a - 1/2)}
\end{align*}
$$

(213)

In order to cancel out the effect of the heterogeneity, the forcing term $F_i$ is introduced as in Eq. (133) with $c^2_{S1} = c^2_{S3} = c^2_{Sx}$, $c^2_{S2} = c^2_{S4} = c^2_{Sz}$. Then, the forcing term fulfills the following moments
\[ M_0^{F(k)} = 0 \quad k \geq 1 \]
\[ M_{1a}^{F(1)} = \frac{1}{\tau_a} \frac{h \partial f \partial \alpha}{\Delta t} \quad M_{1a}^{F(2)} = 0 \]
\[ M_{2a}^{F(1)} = 0 \]

The fourth and fifth terms on the right hand side of Eq. (210) are recovered by the forcing term \( SS_i \)

\[ SS_i(x) = 0; \quad i > 0 \]
\[ SS_0(x) = Q_{SS}(x) \rho_{SS}(x) / \rho_f(x) + nE \partial_t C \]  

The kinetic moments of the forcing terms \( SS_i \) are

\[ M_0^{SS(1)} = Q \rho_{SS} / \rho_f + nE \partial_t C \quad M_0^{SS(k)} = 0 \quad k \geq 2 \]
\[ M_{1a}^{SS(k)} = 0 \quad k \geq 1 \]
\[ M_{2a}^{SS(k)} = 0 \quad k \geq 1 \]

**Steady State Limit**

In the asymptotic case of steady state, Eqs. (18), (25) and (31) become

\[ O(\varepsilon): \quad \frac{\partial M_{1a}}{\partial \alpha_i} = M_{0}^{F(1)} + M_{0}^{SS(1)} \]  

\[ O(\varepsilon^2): \quad 0 = \Delta t \left( \tau_a - \frac{1}{2} \right) \frac{\partial^2 M_{2a_{ab}}}{\partial \alpha_i \partial \beta_i} - \Delta t \tau_a \frac{\partial (M_{1a}^{F(1)} + M_{1a}^{SS(1)})}{\partial \alpha_i} + M_{0}^{F(2)} + M_{0}^{SS(2)} \]  

\[ O(\varepsilon^3): \quad 0 = -\Delta t^2 h_2(\tau_a, \tau_s) \frac{\partial^3 M_{3a_{ab}}}{\partial \alpha_i \partial \beta_i \partial \gamma_i} + M_{0}^{F(3)} + M_{0}^{SS(3)} \]

\[ -\Delta t^2 \tau_a \frac{\partial (M_{1a}^{F(2)} + M_{1a}^{SS(2)})}{\partial \alpha_i} + \Delta t^2 \tau_s \left( \tau_a - \frac{1}{2} \right) \frac{\partial^2 (M_{2a_{ab}}^{F(1)} + M_{2a_{ab}}^{SS(1)})}{\partial \alpha_i \partial \beta_i} \]  

Introducing Eqs. (213), (214) and (216), and choosing the symmetric relaxation time such that \( h_2(\tau_a, \tau_s) = 0 \), Eqs. (217), (218) and (219) become

\[ O(\varepsilon): \quad -\delta_{\alpha a} \frac{\partial (\phi(\phi-1)K_{Fz})}{\partial \alpha_i} = Q \rho_{SS} / \rho_f + nE \partial_t C \]  

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\[ O(\varepsilon^2): \quad 0 = \frac{\partial^2 h\phi K_{faa}}{\partial \alpha \partial \alpha_i} - \frac{\partial}{\partial \alpha_i} \left( h \frac{\partial \phi K_{aa}}{\partial \alpha} \right) \]  

(221)

\[ O(\varepsilon^3): \quad 0 = 0 \]  

(222)

Then, using the multiscale expansion, the macroscopic PDE recovered in the asymptotic limit of steady state is Eq. (209) up to third order in \( \varepsilon \).

### 8.3.2 Salt Transport Equation for Saltwater Intrusion

For the sake of simplicity, uniform porosity and no sinks or sources are considered in the case studies in this chapter. Then the governing equation for the salt transport problem is

\[ \frac{\partial C}{\partial t} + \frac{\partial (u_{\alpha} C)}{\partial \alpha} = \frac{\partial}{\partial \alpha} \left( D_{\alpha \beta} \frac{\partial C}{\partial \beta} \right) \]  

(223)

The EDFs to solve Eq. (223) can be obtained from Chapter 5 using \( n = 1 \) and substituting \( q \) by \( u \).

### 8.3.3 Implementation procedure

In order to implement the LBM to solve saltwater intrusion problem, the groundwater flow and salt transport equation have to be solved simultaneously. Moreover, the flow field has to be updated before solving the salt transport equation and the density distribution has to be updated before solving the groundwater flow equation. This coupling between the two governing equations is described in Figure 8.1 and Figure 8.2. Figure 8.1 represents a flow chart for the main loop of an LBM based program. Each loop iteration show the evolution of one transport time step. Figure 8.2 shows how Eq. (209) is solved for the steady state solution of Eq. (210).

### 8.4 Validation and Verification

This section is aimed to validate the LBM introduced in the previous sections to solve the saltwater intrusion problem in coastal aquifers. We use the Henry problem as the basic case study. Since the Henry problem model the saltwater intrusion problem in a very simple manner,
we study new versions that incorporate heterogeneity and anisotropy in the hydraulic conductivity and dispersion tensors. Moreover, a prescribed salt flux boundary condition at the sea side is also taken into account in order to increase the realism of the simulations. The numerical results obtained by the LBM are compared with analytical and experimental results solutions, and with SUTRA (Voss and Provost 2002), a finite element code developed specifically for saltwater intrusion problems.

8.4.1 The Henry Problem

The Henry problem (Henry 1964) considers the seawater intrusion in a rectangular confined aquifer of 2 meters long and one meter deep (Figure 8.3). A constant freshwater flux is applied to the inland side at a rate of $Q_{in} = 5.702 \text{ m}^3/\text{day}$. At the seaside, the boundary conditions are hydrostatic pressure and seawater concentration $C_s = 35 \text{ kg/m}^3$. The upper and lower sides are impermeable boundaries, so that no-flow boundary conditions are applied. The parameter values used in the Henry problem are provided in Table 8.1.

The LTRT is implemented to solve the Henry problem using $\tau_a = 0.789, 0.9$ and 1, $\tau_s = 0.5 + [12(\tau_a - 0.5)]^{-1}$. Grid size is $\Delta x = 0.05 \text{ m}$ and time step is $\Delta t = 13.3 \text{s}$. The maximum average pore velocity obtained was $u_{max} \approx 0.0013 \text{ m/s}$, which gives a maximum lattice Peclet $Pe_{\Delta x} = 3.45$ and maximum Courant number $Cr = 0.345$. Using these parameter values in Figure 7.10(b), we find that the solutions are linearly stable.

Figure 8.4 compares the LTRT solutions to the analytical solutions computed by Segol (1994) and Simpson and Clement (2004). The solutions show no significant difference between LTRT solutions and Henry’s analytical solution in the area $z < 0.8 \text{ m}$. However, in the area located at the upper-right corner, the analytical solution does not converge due to the imposition of a constant concentration boundary condition, high out-flowing velocity, and high gradient of
the concentration. Figure 8.4(b) presents a close up view of the top-right corner. While smaller anti-symmetric relaxation times introduce numerical oscillations, $\tau_a = 1$ does not have this problem. Hence we recommend the use of $\tau_a = 1$ and $\tau_s = 0.667$ for the salt transport equation.

Figure 8.1: Flow chart to implement LBM to solve saltwater intrusion problems
Figure 8.2: Flowchart for groundwater flow subroutine
Table 8.1 Parameter values for the Henry problem.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$ : dispersion coefficient, [m$^2$/sec]</td>
<td>$1.8857 \times 10^{-5}$</td>
</tr>
<tr>
<td>$K_f$ : freshwater hydraulic conductivity, [m/sec]</td>
<td>0.01</td>
</tr>
<tr>
<td>$Q_m$ : inflow flux, [m/sec]</td>
<td>$6.6 \times 10^{-5}$</td>
</tr>
<tr>
<td>$n$ : porosity, [-]</td>
<td>0.35</td>
</tr>
<tr>
<td>$\rho_f$ : freshwater density, [kg/m$^3$]</td>
<td>1000</td>
</tr>
<tr>
<td>$\rho_s$ : seawater density, [kg/m$^3$]</td>
<td>1025</td>
</tr>
<tr>
<td>$C_s$ : seawater concentration, [kg/m$^3$]</td>
<td>35</td>
</tr>
<tr>
<td>$E$ : $\rho_f^{-1} \frac{\partial \rho}{\partial C}$ [m$^3$/kg]</td>
<td>0.714</td>
</tr>
</tbody>
</table>

Figure 8.3: Henry problem

Although the Henry problem seems to reproduce the saltwater intrusion problem in a sand box, its applicability can be extended to much larger aquifers by simply using a dimensionless analysis over the parameters involved. Table 8.2 shows that we can consider the Henry problem depending on 8 variables, and three dimensions are involved (length, mass and...
time). Then five dimensionless variables govern the Henry problem. After applying the Pi theorem, we find the following dimensionless numbers: porosity $n$; aquifer Peclet number $Pe = Q_{in} H / D$; aquifer aspect ratio $\xi = L / H$; density contrast parameter $E_{\rho} = (\rho_s - \rho_f) / \rho_f$; and the ratio $\psi = Q_{in} / K_f$. Then the solution to the saltwater intrusion problem should be determined by the aforementioned five dimensionless parameters. However, Henry (1964) found that the analytical solution only depends on three dimensionless numbers, which are combinations of the those dimensionless variables. Those dimensionless parameters are: $a = \psi / E_{\rho}, b = n / Pe$ and $\xi$.

Table 8.2 Parameters involved in Henry problem

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D$ : dispersion coefficient,</td>
<td>$[L^2T^{-1}]$</td>
</tr>
<tr>
<td>$K_f$ : freshwater hydraulic conductivity,</td>
<td>$[LT^{-1}]$</td>
</tr>
<tr>
<td>$Q_{in}$ : inflow flux,</td>
<td>$[LT^{-1}]$</td>
</tr>
<tr>
<td>$n$ : porosity,</td>
<td>$[-]$</td>
</tr>
<tr>
<td>$\rho_f$ : freshwater density</td>
<td>$[ML^{-3}]$</td>
</tr>
<tr>
<td>$\rho_s$ : seawater density</td>
<td>$[ML^{-3}]$</td>
</tr>
<tr>
<td>$H$ : aquifer thickness</td>
<td>$[L]$</td>
</tr>
<tr>
<td>$L$ : aquifer length</td>
<td>$[L]$</td>
</tr>
</tbody>
</table>

Table 8.3 compares the Henry values with the values of a similar aquifer. We observe that although the similar aquifer is ten times bigger in size, the value of the hydraulic conductivity and inland freshwater flux are ten times smaller, while having the rest of the values similar. These set of values lead to equal dimensionless values and therefore they will share similar solutions.
Figure 8.4: Henry problem: (a) LTRT solutions with $\tau_s = 0.5 + [12(\tau_s - 0.5)]^{-1}$ versus analytical solutions. (b) Close up view of the outflow area.
We can also compare time scales between similar cases. A characteristic time can be estimated as \( T_c = H / K_f \). Then, comparing the characteristic times between the Henry problem and the similar aquifer described in Table 8.3, we find out that the ratio between time scales is 
\[
T_{\text{SA}} / T_H = (H_{\text{SA}} / K_{f,\text{SA}})(K_{f,H} / H_H) = 100,
\]
where the subscript H refers to Henry values and SA refers to similar aquifer values. In conclusion, the time scale for the similar aquifer is hundred times slower than the time scale for the Henry problem. Therefore, one hour in the time scale of the Henry problem is equivalent to 100 hours in the similar aquifer.

**Table 8.3** Parameter values for the Henry problem and similar aquifer

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Henry</th>
<th>Similar aquifer</th>
</tr>
</thead>
<tbody>
<tr>
<td>( D ) [m(^2)/s]</td>
<td>( 1.8857 \times 10^{-5} )</td>
<td>( 1.8857 \times 10^{-5} )</td>
</tr>
<tr>
<td>( K_f ) [m/s]</td>
<td>0.01</td>
<td>0.001</td>
</tr>
<tr>
<td>( Q_{\text{in}} ) [m/s]</td>
<td>( 6.6 \times 10^{-5} )</td>
<td>( 6.6 \times 10^{-6} )</td>
</tr>
<tr>
<td>( n ) [-]</td>
<td>0.35</td>
<td>0.35</td>
</tr>
<tr>
<td>( \rho_f ) [Kg/m(^3)]</td>
<td>1000</td>
<td>1000</td>
</tr>
<tr>
<td>( \rho_s ) [Kg/m(^3)]</td>
<td>1025</td>
<td>1025</td>
</tr>
<tr>
<td>( H ) [m]</td>
<td>1</td>
<td>10</td>
</tr>
<tr>
<td>( L ) [m]</td>
<td>2</td>
<td>20</td>
</tr>
<tr>
<td>( a )</td>
<td>0.263</td>
<td>0.263</td>
</tr>
<tr>
<td>( b )</td>
<td>0.1</td>
<td>0.1</td>
</tr>
<tr>
<td>( \xi )</td>
<td>2</td>
<td>2</td>
</tr>
</tbody>
</table>

**8.4.2 Modified Henry Problem**

This example compares the LTRT solution in a modified Henry problem (Simpson and Clement 2004) that halves the inland freshwater flux. We used three different types of lattice size to test grid convergence: \( \Delta x_1 = 0.1 \text{ m}, \Delta x_2 = 0.05 \text{ m} \) and \( \Delta x_3 = 0.025 \text{ m} \). The time steps are \( \Delta t_1 = 70 \text{ s}, \Delta t_2 = 30 \text{ s} \) and \( \Delta t_3 = 10 \text{ s} \). We use \( \tau_a = 1 \) and \( \tau_s = 0.667 \). In all simulations,
\[ u_{\text{max}} \approx 0.001, \text{ which leads to the maximum Peclet numbers } Pe_{\Delta x_1} = 5.3, \ Pe_{\Delta x_3} = 1.32, \text{ and } \]
\[ Pe_{\Delta x_2} = 2.65, \text{ and Courant numbers } Cr_1 = 0.7, \ Cr_2 = 0.6 \text{ and } Cr_3 = 0.4. \]
Based on Figure 7.10(b), these parameters provide linearly stable solutions.

Figure 8.5(a) compares the LTRT results with the analytical solution obtained by Simpson and Clement (2004). Numerical results obtained with the LTRT agree with the analytical solution and show good grid convergence. Figure 8.5(b) shows the temporal evolution of the toe intrusion. The comparison between LTRT and the analytical solution (Simpson and Clement 2004) are made for 25%, 50% and 75% of the seawater concentration. It shows good agreement between the LTRT and the analytical solution for the transient period.

### 8.4.3 Henry Problem with Prescribed Mass Flux at Seaside

In this section, we present a variation of the Henry problem, in which the only difference from the original Henry problem is the mass flux boundary condition at the seaside (Abarca et al. 2007). We believe that this type of boundary condition is more suitable for the real saltwater intrusion problem and has been considered in some works (Sanz and Voss 2006; Abarca et al. 2007). At the seaside, the flux \( nu_s C_s \) is applied to the boundary segment where the saltwater intrudes the aquifer and the flux \( nu_s C \) is applied to the boundary segment where the groundwater flows out of the aquifer.

We use \( \tau_a = 1, \ \tau_s = 0.667, \ \Delta x = 0.05 \text{ m, and } \Delta t = 25 \text{ s.} \) At the seaside, the prescribed salt flux BC is implemented using the mesoscopic approach explained in section 5.4. The maximum average pore velocity obtained was \( u_{\text{max}} \approx 0.0015 \text{ m/s,} \) which gives a maximum lattice Peclet \( Pe_{\Delta x} = 3.97 \) and maximum Courant number \( Cr = 0.75. \) According to Figure 7.10(b), the LTRT solutions are linearly stable. Figure 8.6 compares the LTRT solutions with the solutions obtained
with SUTRA with the same grid resolution (Sanz and Voss 2006). It was found a good agreement between both numerical solutions.

**Figure 8.5:** Modified Henry problem (Simpson and Clement 2004). (a) Convergence study of LTRT with $\tau_a = 1$ and $\tau_s = 0.667$. (b) Temporal evolution of the toe of isoconcentration lines.
8.4.4 Dispersive Henry Problem

This example solves the saltwater intrusion problem with the velocity-dependent dispersion coefficient in the ADE and neglecting the molecular diffusion. We consider the dispersivity \( \kappa_L = \kappa_T = D/Q_m = 0.1 \text{ m} \). We use \( \tau_x = 1, \quad \tau_z = 0.667, \quad \Delta x = 0.0125 \text{ m}, \) and \( \Delta t = 0.195 \text{ s} \). At the seaside, the prescribed salt flux BC is implemented using the mesoscopic approach explained in section 5.4.2. The lattice Peclet number is defined as

\[
Pe_{\Delta x} = \frac{u \Delta x}{D} = \frac{u \Delta x}{(u \kappa)} = \Delta x / \kappa.
\]

For this case study, \( Pe_{\Delta x} = 0.125 \). The maximum average pore velocity obtained was \( u_{\text{max}} \approx 0.00195 \text{ m/s} \), which leads to a maximum Courant number of \( Cr = 0.0305 \). Based on Figure 7.10(b), this value of the Courant number guarantee linear stability when \( Pe_{\Delta x} = 0.125 \).

Figure 8.7 shows the isoconcentration lines. Comparing Figure 8.6 and Figure 8.7, we observe that the use of a velocity dependent dispersion coefficient produces more intrusion than in the diffusive case.
8.4.5 Dispersive Henry Problem in Anisotropic Porous Medium

So far, all the previous cases studies have used isotropic hydraulic conductivity. In order to make the simulations one step closer to reality, we consider in the following case studies that the hydraulic conductivity tensor is anisotropic and with principal directions the horizontal and vertical directions. Then, we assume the hydraulic conductivity tensor to be such that

$$K_{xx} / K_{zz} = 3/2$$ and $$K_{xy} = 0$$.

We consider the saltwater intrusion described in the previous section but with anisotropic hydraulic conductivity. In order to be able to compare with previous results, we use

$$\sqrt{K_{xx} K_{zz}} = K_{Henry} = 0.01 \text{ m/s}.$$ Then, the aforementioned assumption leads to $$K_{xx} = 1.225 \cdot 10^{-2} \text{ m/s},$$

$$K_{zz} = 8.165 \cdot 10^{-3} \text{ m/s}.$$ We use $$\tau_0 = 1,$$ $$\tau_s = 0.667,$$ $$\Delta x = 7.813 \cdot 10^{-3} \text{ m},$$ and $$\Delta t = 0.1017 \text{ s}.$$ The lattice Peclet number is defined as $$Pe_{\Delta x} = \Delta x / \kappa_L = 7.813 \cdot 10^{-2}.$$ The maximum average pore velocity obtained was $$u_{max} \approx 0.00225 \text{ m/s},$$ which leads to a maximum Courant number of
\( Cr = 0.030 \). Based on Figure 7.10(b), this value of the Courant number guarantees linear stability.

Figure 8.8 compares the isoconcentration lines obtained by the LBM and by SUTRA (Abarca et al. 2007) for the whole mixing zone. Both numerical solutions compare well. Comparing Figure 8.8 to Figure 8.7, we observe that more saltwater intrusion happens in Figure 8.8. The reason is because the larger value of the horizontal component of the hydraulic conductivity enhances the intrusion of saltwater, while the lower value of the vertical component opposes the recirculation of the intrusion water to the outflow area, resulting in an increase of the intrusion area.

**8.4.6 Anisotropic and Dispersive Henry Problem in Anisotropic Porous Medium**

Another step further to increase the capability of the simulations to represent actual saltwater intrusion problems is to take into consideration that hydrodynamic dispersion is anisotropic. In dispersive processes, dispersion happening along streamlines (longitudinal dispersion) is often stronger than the dispersion happening across streamlines (transverse dispersion) as a result of the heterogeneity and anisotropy of the porous medium. Hence in this work we assume that the dependency on the flow field of the longitudinal and transverse dispersion is as in Eq. (106) (Bear 1972). In the following examples, we solve the saltwater intrusion in an anisotropic porous medium introduced in the previous section 8.4.5, but considering the anisotropic dispersion tensor.

Boundary conditions for LBM were introduced in section 5.4.2 based on a mesoscopic approach. This approach is based on determining the specific values of the missing particle distribution functions to impose the boundary condition at a mesoscopic level. While this type of BC has worked well so far, we found that this mesoscopic approach fails to implement the prescribed salt flux BC at the seaside in the zone where the flow neither intrudes nor leaves the
aquifer. This is a transition zone where the prescribed flux changes based on whether the flow intrudes or leaves when the dispersion tensor is anisotropic. In this zone, the imposition of complex BC such as prescribed mass flux with anisotropic dispersion are very likely to create numerical instabilities.

In order to overcome this difficulty, we introduce a macroscopic approach for the prescribed salt flux BC at the seaside. The macroscopic approach is based on estimating the values of the macroscopic variables at the ghost nodes that fulfill the macroscopic BC. These values are estimated by implementing the BC based on second order finite differences. Then, the concentration values at the boundary nodes depend on the concentration values within the domain. Once the values of the macroscopic variables are known at the boundary nodes, we implement them as Dirichlet BC using the mesoscopic approach described in section 5.4 (Eq.(149)).

![Figure 8.8: Dispersive Henry problem in anisotropic porous medium with prescribed salt flux boundary condition at seaside.](image_url)
Figure 8.9 compares LBM solutions with solutions obtained with SUTRA (Abarca et al. 2007) for different values of the longitudinal and transversal dispersivities. In order to fairly compare the results, we use the same grid resolution that was used in Abarca et al. (2007). The numerical parameters used in each case are provided in Table 8.4. In particular Figure 8.9(d) shows the result for a case in which the transverse dispersion is larger than the longitudinal dispersion. Although this is not realistic, this case has been included for validation purposes by intercode comparison. In the saltwater intrusion problem, there are two main parameters describing the intrusion: the toe penetration and the width of the mixing zone. In Figure 8.9, we observe that the numerical results obtained by the LBM and SUTRA present almost similar results for the toe intrusion and width of the transition zone.

8.4.7 Anisotropic and Dispersive Henry Problem in Anisotropic and Heterogeneous Porous Medium

In this section, we demonstrate the application of the LBM to solve a case that considers spatially correlated hydraulic conductivity and velocity-dependent dispersion. We assume a spatial covariance for the logarithmic freshwater hydraulic conductivity ($\log_{10} K_f$) described by an exponential model:

$$\text{Cov}(\delta_x, \delta_z) = \sigma^2 \exp\left[-\sqrt{\left(\frac{\delta_x}{I_x}\right)^2 + \left(\frac{\delta_z}{I_z}\right)^2}\right]$$

(224)

where $\delta_x$ and $\delta_z$ are the distance lags in x and z directions, respectively; $I_x$ and $I_z$ are the integral scales for x and z directions, respectively; and $\sigma^2$ is the unconditional variance. We generate values of the hydraulic conductivity such that $Y = \log_{10} K_f = -2$ is the same as the $\log_{10} K_f$ value in the Henry problem. Moreover, we give $\sigma = 0.5$ m/s, $I_x = 0.5$ m, and $I_z = 0.1$ m.

We study the anisotropic and dispersive Henry problem in an heterogeneous and anisotropic aquifer with the following set of parameters: $\kappa_L = 0.1$, $\kappa_L / \kappa_T = 10$, $D_m = 0$, $\gamma = 0.1$, and $\kappa_T = 0.01$. The results for the toe penetration and width of the mixing zone are shown in Figure 8.9, and they suggest that the LBM and SUTRA solutions are in good agreement.
\( K_{xx}/K_{zz} = 3/2, \ K_{xy} = 0 \) and \( \sqrt{K_{xx}K_{zz}} = K_f \). We use a grid with 258x128 lattices, which implies \( \Delta x = 7.8125 \times 10^{-3} \text{m}, \ \Delta t = 0.1 \text{s}, \ \tau_a = 1 \) and \( \tau_s = 0.667 \). The generated \( K_f \) values ranges between \( 5.86 \times 10^{-4} \text{m/s} \) and \( 1.449 \times 10^{-1} \text{m/s} \). Then imposing \( K_{xx}/K_{zz} = 3/2, \ K_{xy} = 0 \) and \( \sqrt{K_{xx}K_{zz}} = K_f \), we obtain \( K_{xx} = 1.2247 K_f \) and \( K_{zz} = 0.8165 K_f \).

**Table 8.4** Parameter values for the anisotropic and dispersive Henry problem in anisotropic porous medium

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Case (a)</th>
<th>Case (b)</th>
<th>Case (c)</th>
<th>Case (d)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \kappa_L ) [m]</td>
<td>0.1</td>
<td>1</td>
<td>0.5</td>
<td>0.1</td>
</tr>
<tr>
<td>( \kappa_L / \kappa_T ) [m]</td>
<td>10</td>
<td>10</td>
<td>50</td>
<td>0.2</td>
</tr>
<tr>
<td>( \Delta x ) [m]</td>
<td>7.8125 \times 10^{-3}</td>
<td>7.8125 \times 10^{-3}</td>
<td>7.8125 \times 10^{-3}</td>
<td>7.8125 \times 10^{-3}</td>
</tr>
<tr>
<td>( \Delta t ) [s]</td>
<td>0.1017</td>
<td>0.007629</td>
<td>0.02034</td>
<td>0.03391</td>
</tr>
<tr>
<td>( \tau_a ) [-]</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( \tau_s ) [-]</td>
<td>0.667</td>
<td>0.667</td>
<td>0.8</td>
<td>0.667</td>
</tr>
</tbody>
</table>

In order to make it possible to compare the results with the homogeneous case (Figure 8.9(a)), we impose a different BC condition for the groundwater flow equation at the inland side. Instead of imposing constant freshwater discharge, we impose a constant freshwater head value of \( h_f = 1.0238 \text{m} \), which is a value close to the freshwater head values obtained in the homogeneous case at the inland side. All the others BC remain the same.

Figure 8.10 shows the isoconcentration lines, equipotential, flow field and hydraulic conductivity field for the anisotropic and dispersive Henry problem in the heterogeneous and anisotropic porous medium. We can observe that preferential flow paths are formed by the connected areas of high hydraulic conductivity. The maximum average pore velocity happens in the outflow area, and \( u_{\text{max}} \approx 0.00253 \text{m/s} \), which implies a maximum Courant number of \( C_{r_{\text{max}}} \approx 0.033 \). Considering that \( \Delta x / \kappa_L \approx 0.078 \), based on Figure 7.10(b), the solution is stable.
Figure 8.9: Anisotropic and dispersive Henry problem in anisotropic porous medium with prescribed salt flux boundary condition at the seaside.
Figure 8.9 (cont.): Anisotropic and dispersive Henry problem in anisotropic porous medium with prescribed salt flux boundary condition at the seaside.
8.4.8 Experimental Saltwater Intrusion Problem

Goswami and Clement (2007) investigated the transport patterns of saltwater intrusion wedges at laboratory-scale. The experiments were carried out in a tank filled with uniform silica beads with average diameter 1.1 mm. In the experiments, at one side of the tank there was a freshwater reservoir while at the opposite side there was a saltwater reservoir. While the saltwater head was kept constant and equal to 25.5 cm during all the experiments, the freshwater head was not. First, they fixed the freshwater head at the freshwater reservoir at 26.7 cm and let the saltwater intrude until the steady state was reached (SS1). Second, the freshwater head was changed from 26.7 cm to 26.2 cm, calling to this transient period as the intruding wedge stage, until a second steady state was reached (SS2). Third, the freshwater head was changed from 26.2 cm to 26.5 cm, calling to this transient period as the receding wedge stage, until a third steady state was reached (SS3).

The porosity of the porous medium was measured and it was obtained $n=0.385$. The hydraulic conductivity of the porous media was measured by setting up a uniform flow and
measuring the gradient and the corresponding flow discharge. The averaged hydraulic conductivity obtained was 1050 m/day. In order to estimate the dispersivity values, a tracer test was carried out and the spreading of the tracer was measured. Then, simulations were carried out with a transport model with a longitudinal dispersivity of 1mm and transverse dispersivity estimated in one tenth of the longitudinal dispersivity. The simulations were able to predict the average spreading observe.

Goswami and Clement (2007) reported that a narrow mixing zone is observed in the experiments, and therefore a well defined wedge appears. They provided results regarding the location of the saltwater wedge under different conditions. They also carried out numerical simulations of the experiments using SEAWAT, and compared the location of the 50% isochlors with the experimental saltwater wedge.

Simulations using the LBM model were carried out using $\Delta x = \Delta z = 0.25$, $\Delta t = 0.25$ sec, $\tau_a = 1$ and $\tau_s = 0.667$. At the saltwater reservoir side, a prescribed flux BC was applied using the macroscopic approach as discussed in the previous sections.

Figure 8.11 compares the results obtained with the LBM, SEAWAT and the laboratory results for the three steady states for the three different values of the freshwater head at the freshwater reservoir. The numerical models predict fairly well the location of the saltwater wedge. The deviations of the LBM model and SEAWAT from the experimental results are of the same order of magnitude, and the deviation is largest for the case of SS2.

From the experiments and the numerical simulations, we can observe that low values of dispersivity lead to narrow mixing zones. When this happens, the saltwater intrusion can be well simulated using the sharp interface model. In the sharp interface model, saltwater and freshwater are considered as two immiscible fluids with different densities (saltwater and freshwater densities). The main advantage of the sharp interface model is that there is no transport equation
for the salt because the fluid density is considered not to depend on the salt concentration. Instead, it is necessary to implement a tracking method for the interface to identify in each time step the location of the wedge. On the other hand, sharp interface models are not suitable when mixing zones are not narrow and in those cases, the salt transport equation needs to be solved.

Figure 8.12 compares the results obtained with the LBM, SEAWAT and the laboratory results for intruding wedge and receding wedge stages. The numerical models predict again fairly well the location of the saltwater wedge. The deviations of the LBM model and SEAWAT from the experimental results are in the same order of magnitude, and the deviation is largest for the case of the receding wedge. When carrying out the receding wedge stage, Goswami and Clement (2007) reported problems in keeping the freshwater head value at the freshwater reservoir fix to 26.5 cm for the first five minutes of this stage. Hence, this might be the reason why the numerical predictions advance behind the experiments.

8.5 Summary

In this chapter, the LBM has been implemented to simulate saltwater intrusion problems. The implementation has been carried out by means of coupling an LBM code for the groundwater flow equation with an LBM code for the salt transport equation through an equation of state that relates changes in density with changes in salt concentration. A variety of cases based on the Henry problem have been tested. Comparisons with analytical solutions and experimental results, and the intercode comparison have validated tools the LBM based code.
Figure 8.11: Experimental saltwater intrusion problem. (a) SS1; (b) SS2; (c) SS3.
**Figure 8.12:** Experimental saltwater problem. (a) Advancing wedge; (b) Receding wedge.
CHAPTER 9. CONCLUSIONS

The PDE recovered by the LTRT has been obtained in a general form, including the effect of the forcing term, up to third order. This general expression guides the LBM user to tailor customized equilibrium distribution functions (EDFs) and forcing terms, and to select relaxation times in order to recover a specific PDE.

The LTRT model outperforms the LBGK model in terms of accuracy. The extra degree of freedom offered by using an extra relaxation time can be used to improve the accuracy of the LTRT over the LBGK. In particular, we found an optimum value of the symmetric relaxation time as a function of the antisymmetric relaxation time that can be used to reduce third order numerical errors.

When developing an LBM based code, one of the most important tasks is the selection the EDFs. The general PDE recovered depends greatly on the kinetic moments of the EDFs. We have shown how the advection-diffusion equation can be recovered with different order of accuracy by different selections of the EDFs.

LBM has been extended to cope with anisotropic and heterogeneous dispersion tensors in porous media. On one hand, anisotropy is handled by means of the directional squared speed of sound, which allows introducing into the EDFs the anisotropic properties that will be recovered in the second order dispersion tensor. On the other hand, the use of the equivalent speed of sound has been shown to be an effective way to introduce into the EDFs the information regarding how the properties of the media change across one lattice.

The linear stability of LTRT has been investigated. The dimensionless analysis introduced in this dissertation is a key point to understand the dependency of linear stability on the governing dimensionless parameters, as well as to reduce the number of variables involved and therefore to make easier to obtain linear stability boundaries. It has been found that the non-
negativity of the EDFs is a sufficient condition for linear stability when the LBGK model is used in the absence of forcing terms.

LBM has been implemented to simulate saltwater intrusion in the porous medium. We found that LBM results agree well with the analytical solution of the Henry problem as well as with numerical solutions obtained by SUTRA. Different scenarios were considered from the original Henry problem to anisotropic and dispersive saltwater intrusion problems in anisotropic and heterogeneous porous media. Moreover, the LBM developed in this work has shown good agreement with the experimental results of saltwater intrusion carried out at a laboratory scale for steady-state and transient cases.
REFERENCES


APPENDIX: ACRONYMS

AADE: Anisotropic Advection-Dispersion Equation

BC: Boundary Condition

BGK: Bhatnagar-Gross-Krook Collision Operator

EDF: Equilibrium Distribution Function

FDM: Finite Difference Method

FEM: Finite Element Method

FVM: Finite Volume Method

LBE: Lattice Boltzmann Equation

LBGK: Lattice Boltzmann Equation with Bhatnagar-Gross-Krook Collision Operator

LTRT: Lattice Boltzmann Equation with Two-Relaxation-Times Collision Operator

LBM: Lattice Boltzmann Method

LGA: Lattice Gas automata

MOC: Method of Characteristics

MSSS: Multidirectional Squared Speeds of Sound

PDE: Partial Differential Equation

PDF: Probability Density Function

REV: Representative Elementary Volume

TRT: Two Relaxation Times Collision Operator
VITA

Borja Serván Camas was born in San Fernando, Cádiz, Spain, in March, 1976, to Angel Serván Martínez and Josefa Camas Ramírez. He grew up in Huelva, where he pursued his high school education. In September 1994 he moved to Madrid, where he obtained his degree in naval engineering at the Escuela Técnica Superior de Ingenieros Navales, Universidad Politécnica de Madrid, graduating in 2002. In the period between November 2003 and April 2005 he worked as Research Engineer in the model basin facilities at the Escuela Técnica Superior de Ingenieros Navales in Madrid. In May 2005 he moved to Baton Rouge (USA) and started graduate studies in the Civil and Environmental Engineering Department at Louisiana State University. Under the advice of Dr. Frank T-C. Tsai, he conducted research in the field of hydrology, focusing on numerical modeling using lattice Boltzmann techniques. In May 2007, he finished his Master of Science in Civil Engineering while pursuing his doctoral studies.