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MAICON VINICIUS RITTER DEGGERONI

FLOW OF THE DRILLING MUD INSIDE AN ANNULUS USING THE LATTICE BOLTZMANN METHOD

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Master thesis submitted to the Mechanical Engineering Department at the College of Technological Science of Santa Catarina State University in fulfillment of the partial requirement for the Master's degree in Mechanical Engineering. Advisor: Luiz Adolfo Hegele Júnior, Ph. D.

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Dissertação apresentada ao Programa de Pós-Graduação em Engenharia Mecânica do Centro de Ciências Tecnológicas, da Universidade do Estado de Santa Catarina, como requisito parcial para obtenção do Título de Mestre em Engenharia Mecânica.

BANCA EXAMINADORA

Luiz Adolfo Hegele Júnior, Dr. Universidade do Estado de Santa Catarina

Membros:

Paulo Sergio Berving Zdanski, Dr. Universidade do Estado de Santa Catarina

Diogo Nardelli Siebert, Dr. Universidade Federal de Santa Catarina

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Dedico este trabalho a Deus, minha esposa Náthila, meus pais Orivaldi e Rose, minha madrasta Jane, e meu irmão Tiago.

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ABSTRACT

The drilling mud has an important role in Drilling Engineering because, during the wellbore drilling, the drilling mud is required to be chemically stable, to cool, and lubricate the bit, to stabilize the wellbore walls, and especially to carry the cuttings from the bottom-hole wellbore to the surface. The flow of drilling mud inside the wellbore annulus is a knowledge target all around the world since it is not completely comprehended. As the presence of cuttings inside the annulus and drilling mud rheology leads to a robust model to solve the problem, simplifications were applied and the study was developed focusing on the Reynolds number. A literature review is performed to list previous works related to flow between cylinders especially the Taylor-Couette, and the lattice Boltzmann method. There are appointments and characteristics about the methodology using velocity set D3Q19, explicitly the regularization process to boundary conditions, new boundary sites, Chapman-Enskog analysis to enlighten the LB approach on solving the Navier-Stokes equations, as well as the use of forces in methodology. First results are presented and compared with analytical solutions of White (2006) for both flows inside parallel plates and concentric cylinders with the use of forces in the lattice Boltzmann, where both forcing magnitude $F_{g_{\tau}} = 1 \times 10^{-7}$ and relaxation time $\tau = 0.8$ are fixed. Both velocity and total volume rate present closer values for the numerical solution to the analytical one as the mash is higher. Then, compared with the analytical solution of Mohammadipour, Succi, and Niazmand (2018) establishing a bi-dimensional flow with different mesh grids at Re = 10 and radius ratio $\eta = 5/7$, obtaining good results for the tangential velocity and pressure, despite the tangential tensor derivatives equal to zero at inner cylinder were not be implemented. Finally, a study of the Taylor-Couette flow contrasting with Ostilla et al. (2013) leads to the emergency of rolls (toroidal vortices) at Taylor numbers 2.44×10^5 and 7.04×10^5 . Values of the wavelength of the rolls seem to be consistent. Thus, the obtained final results were satisfying, despite some discrepancies and considering computational difficulties. Future works should focus on boundary conditions with zero tangential tension at the inner cylinder wall and implementing simulations for greater computational domains to improve results, verifying temperature behavior in the flow, as well as including cuttings to obtain better knowledge about the mud flow inside the wellbore annulus with its presence.

Keywords: Drilling mud. Wellbore annulus. Lattice Boltzmann method. Taylor-Couette flow.

RESUMO

O fluido de perfuração tem papel importante na Engenharia de Perfuração, pois durante a perfuração do poço o fluido precisa ser quimicamente estável, resfriar e lubrificar a broca, estabilizar as paredes do poço, e especialmente carregar o cascalho do fundo do poço à superfície. O escoamento do fluido de perfuração no anular do poço é alvo de conhecimento em âmbito mundial, uma vez que não está completamente compreendido. Como a presença de cascalho no anular do poço e a reologia do fluido de perfuração determinam um robusto modelo para solução do problema, simplificações foram feitas e o trabalho foi desenvolvido com foco no número de Reynolds. Uma revisão de literatura é realizada para elencar trabalhos desenvolvidos com estudos de escoamento entre cilindros - especialmente o de Taylor-Couette, e o método do reticulado de Boltzmann. São apontadas considerações e características do método para solução numérica utilizando conjunto de distribuição de velocidades D3Q19, explicitando o processo de regularização para condições de contorno, novas condições de fluido, análise de Chapman-Enskog na solução das equações de Navier-Stokes, bem como aplicação de forças na metodologia. Os primeiros resultados são dados em função de comparativos de soluções analíticas de White (2006) para ambos escoamentos entre placas paralelas e cilindros concêntricos, tendo o uso de forças no reticulado de Boltzmann e fixos a magnitude de força $F_{g_z} = 1 \times 10^{-7}$ e tempo de relaxação $\tau = 0.8$. Ambas velocidade e volume de vazão total apresentam valores para solução numérica cada vez mais próximos da solução analítica, na medida que os tamanho de malha aumentam. Em seguida, comparou-se com a solução analítica de Mohammadipour, Succi e Niazmand (2018) um escoamento bi-dimensional em diferentes malhas a Re = 10 e razão de raio $\eta = 5/7$, obtendo-se bons resultados para velocidade tangencial e pressão, apesar de não ser implementada a derivada igual a zero dos tensores tangenciais no cilindro interno. Finalmente, um estudo do escoamento de Taylor-Couette contrastando com Ostilla et al. (2013) traz a formação esperada de rolos (vórtices toroidais) para ambos número de Taylor 2.44×10^5 e 7.04×10^5 . Valores para comprimento de onda dos rolos demonstram estar consistentes. Desse modo, os resultados finais obtidos foram satisfatórios, apesar de discrepâncias pontuais e considerando dificuldades computacionais. Trabalhos futuros devem focar em aplicar derivadas de tensores tangenciais iguais a zero na parede do cilindro interno e implementar simulações para domínios computacionais maiores para aprimorar resultados, verificar o comportamento da temperatura no escoamento, bem como levar em consideração a presença de cascalho para que seja conhecido como se dá efetivamente o escoamento do fluido de perfuração no anular do poço.

Palavras-chave: Fluido de perfuração. Anular do poço. Método do reticulado de Boltzmann. Escoamento de Taylor-Couette.

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LIST OF ABBREVIATIONS AND ACRONYMS

- BGK Bhatnagar-Gross-Krook
- CFD Computational Fluid Dynamics
- DdQq *d*-Dimensional set of *q* velocities
- FDM Finite Difference Method
- FEM Finite Element Method
- FVM Finite Volume Method
- IC Inner cylinder
- LBM Lattice Boltzmann Method
- NSE Navier-Stokes Equations
- OC Outer cylinder

LIST OF SYMBOLS

A	dependent term on radius ratio and rotational speed of the inner cylinder in Taylor-Couette flow; model dependent parameter (related to Forces)
a_s	scaling factor
В	dependent term on radius ratio and rotational speed of the inner cylinder in Taylor-Couette flow
b_C	proportional term for the zero-order moments at the corners boundary conditions
b_E	proportional term for the zero-order moments at the edges boundary conditions
c_i	particle velocity
Cs	speed of sound
D	gap between two concentric cylinders; pipe diameter
d_C	disproportionate term for the zero-order moments at the corners boundary conditions
d_E	disproportionate term for the zero-order moments at the edges boundary conditions
$\frac{\mathrm{d}p}{\mathrm{d}x}$	pressure gradient
F	force vector
\boldsymbol{F}_{g}	force density vector
F_i	forcing term
\boldsymbol{F}_{lpha}	forcing term component
f_i	discrete-particle distribution
$f_i^{(1)}$	first-order distribution perturbation
$f_i^{(eq)}$	equilibrium particle distribution
$f_i^{(neq)}$	non-equilibrium particle distribution
$\widehat{f_i}$	regularized particle distribution
$\widehat{f}_i^{(neq)}$	regularized non-equilibrium particle distribution

$\overline{f_i}$	modified discrete-particle distribution
g	gravitational acceleration vector
<i>g</i> _i	particle distribution or regularized particle distribution
h	distance from the origin to a plate
$\mathscr{H}^{(2)}_{\alpha\beta,i}$	second-order velocity expansion in the Hermite polynomials
I_s	incoming velocity set
k	wavenumber vector
k	wavenumber
<i>k_{crit}</i>	critical wavenumber
L	cylinder length
l	macroscopic length scale
Ма	Mach number
Ν	number of mean spacing
n	integer number of waves around the annulus
O_s	outgoing velocity set
$P_{pqr}^{(1)}$	coefficients associated to the zeroth-order moment
$P_{pqr}^{(m)}$	coefficients associated to the second-order moment
$P_{pqr}^{(u)}$	coefficients associated to the first-order moment
р	pressure
p^{\star}	non-dimensional pressure
Q	total volume rate flow
${\cal Q}_{pq}^{(1)}$	coefficients associated to the zeroth-order moment
$Q_{pq}^{(m)}$	coefficients associated to the second-order moment
$Q_{pq}^{(u)}$	coefficients associated to the first-order moment
q	rate or amplification factor for the disturbance; number of populations in a $DdQq$ model

q_a	analytical simulation in L_2 error norm
q_n	numerical simulation in L_2 error norm
R*	non-dimensional radius
R_1	inner cylinder radius
R_2	outer cylinder radius
$R_{pqr}^{(1)}$	coefficients associated to the zeroth-order moment
$R_{pqr}^{(u)}$	coefficients associated to the first-order moment
Re	Reynolds number
<i>Re_{crit}</i>	critical Reynolds number
Re_z	axial Reynolds number
Re_{θ}	azimuthal Reynolds number
r	particle position vector
r	radial coordinate
\widetilde{r}	normalized radius
S_i	source term
$S_{pqr}^{(m)}$	coefficients associated to the second-order moment
$S_{pqr}^{(u)}$	coefficients associated to the first-order moment
Та	Taylor number
Ta _{crit}	critical Taylor number
t	time
Ur	radial component of velocity in Taylor-Couette flow
$U_{ heta}$	azimuthal component of velocity in Taylor-Couette flow
U_z	axial component of velocity in Taylor-Couette flow
\overline{U}	mean velocity flow
\overline{U}_{max}	maximum mean velocity flow
и	fluid velocity vector

<i>u_{pipe}</i>	velocity of the inner cylinder R_1
u ^{eq}	equilibrium velocity vector
$u_{ heta}$	tangential velocity
$u_{ heta}^{\star}$	non-dimensional tangential velocity
Wi	quadrature weights
x	space vector
x	horizontal Cartesian coordinate
У	vertical Cartesian coordinate
	Greeks
Г	aspect ratio
Δt	lattice time-step; time variation
$\delta_{lphaeta}$	Kronecker delta
$\widetilde{\delta}_{l_k}$	modified Kronecker delta
ϵ_q	L_2 error norm
ϵ_{q_p}	L_2 error norm for the pressure
ϵ_{q_p}	L_2 error norm for the total volume rate
ϵ_{q_u}	L_2 error norm for the tangential velocity
η	radius ratio
heta	azimuthal component
λ	wavelength
μ	dynamic or Newtonian viscosity
ν	kinematic viscosity
ρ	specific mass or absolute density of fluid; zeroth-order moment
ρ_I	zero-order moment of incoming set
ρu_{α}	first-order moment

	Subscripts
$\langle \overline{\omega} \rangle_z$	normalized <i>z</i> -averaged angular velocity
ω_{LB}	modified collision frequency
ω	angular velocity
Ω_i	BGK collision operator
Ω_1	rotational speed of the inner cylinder
$\overline{ au}$	modified relaxation time
τ	relaxation time
$ ho m^{(2)}_{lphaeta}$	second-order moment

Subscripts

 α, β, γ components of tensors

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1 INTRODUCTION

The petroleum industry comprehends a great and massive conglomerate of areas, as reservoir engineering, onshore and offshore structures, production and completion engineering, and one of most important, drilling engineering. Prospecting formations and exploring petroleum, and considering offshore structures especially, is a hard and complex challenge that any oil company has to meet.

Speaking particularly of drilling engineering, significant equipment, and human expertise are required to explore the desired petroleum area. It is important to acquire knowledge about rotary drilling, bits, drilling hydraulics, drilling mud, and other considerations that involves this complex task. Considering drilling engineering, after all the definitions on the use of equipment and considerations are made, while the bit is drilling inside the wellbore, cuttings result from it, which have to be taken up to the surface.

The wellbore basically consists in the wall of the formation and the drill pipes which are drilling and exploring it. Between this wall and the drill pipes, there is an empty space, which we call annulus wellbore or just annulus. The cuttings mentioned above that results from the drilling are brought to the surface through this space. Figure 1 shows, as an example, the drilling system. Carrying the cuttings from the bottom-hole requires the right drilling mud because it is necessary to evaluate the pressure, depth, and other characteristics that are going to facilitate it.

Even after more than a hundred years of petroleum exploration and advanced technologies, full characterization of the flow of the drilling mud inside the annulus is yet to be accomplished. As it is not completely established, and especially considering the presence of the cuttings, it may be laminar or turbulent, and even the fluid may assume a Newtonian or non-Newtonian behavior. Between main characteristics, the drilling mud must be chemically stable, stabilize wellbore walls, cool and lubricate the bit and, especially, carry the cuttings from the bottom-hole to the surface (THOMAS, 2004).

According to Mme and Skalle (2012, p. 130), the cuttings tend to sink through the ascending fluid because of the gravity influence, withal when a sufficient volume of mud flows fast enough to get over this effect, the cuttings are carried to the surface. Removing the cuttings from the hole depends on some important factors, as fluid viscoelastic properties, annular velocity, angle of inclination, drilled cuttings size and their shape.

To solve problems of Computational Fluid Dynamics (CFD), there are some known methods to be evaluated here. Among them, we can enumerate the Finite Difference Method (FDM), the Finite Volume Method (FVM), the Finite Element Method (FEM) and the Lattice Boltzmann Method (LBM). The oldest method for a numerical solution is FDM (18th century), and it is also the easiest to implement in simple geometries. According to Ferziger and Perić (2001, p. 40), "in FDM discretization methods the grid is usually locally structured, i.e., each grid node may be considered the origin of a local coordinate system, whose axes coincide with gridlines".



Figure 1 – Drilling scheme of a petroleum wellbore.

Source: Adapted from Mme and Skalle (2012).

The FVM appeared in the 1970s with strength on its connection to physical flow properties. The basis of the method relies on the direct discretization of the integral form of the conservation law (HIRSCH, 2007, p. 209). Compared to FDM, the great difference between them is that on FDM the discretization is on the *differential* form, as opposed to FVM which discretizes the *integral* form.

In the FEM, "the domain is broken into a set of discrete volumes or finite elements that are generally unstructured; in 2D, they are usually triangles or quadrilaterals, while in 3D tetrahedra or hexahedra are most often used" (FERZIGER; PERIĆ, 2001, p. 36). The method uses a set of functions as base (elements), that are "located in space", to describe the solution. Here a weight function is considered multiplied to the equations before they are integrated over the entire domain.

The LBM consists basically of representing the fluid through particles, which themselves may represent atoms, molecules, collections or distributions of molecules, or portions of the macroscopic fluid, instead of attempting to solve the equations of fluid mechanics directly (KRÜGER et al., 2017, p. 55).

To Krüger et al. (2017), the problem of solving equations of fluid mechanics is that it represents a nonlinear simultaneous system where solutions can behave complexly, especially when related to turbulent flow or complex geometries.

It is important to say that here we will only consider the influence of the Reynolds number on the drilling mud flow. The constitution (made by oil, water, and other compounds) will not be taken into account in the analysis. That is because Reynolds number already has some physical considerations, such as viscosity and velocity. In addition, for objectivity and to facilitate the complexity of implementing this problem, at the first moment, we will not consider the presence of the cuttings in the drilling mud. We must evaluate Reynolds number before we analyze other complex factors such as particulate flow (cuttings) and rheology (non-Newtonian behavior).

The geometry with concentric cylinders is, at first sight, simple to implement and evaluate the flow in the annulus. So, it could be done using other method to solve the problem, as commented before. But, we use LBM in this work because it is the beginning of a long study, where after the boundary sites and boundary conditions are defined, expressive knowledge about the flow, especially the Taylor-Couette one and its instabilities are clear, the transition from laminar to turbulent flow. The simulations will allow to insert the cuttings in the drilling mud flow, and at this last mentioned step, is that LBM will take a robust advantage.

1.1 OBJECTIVES

The main objective in this thesis is to understand the behavior as a function of the Reynolds number inside the wellbore annulus using the Lattice Boltzmann Method as a computational solution method. To reach it, the specific objectives are as follows:

- To present a literature review and theoretical foundation to express the methodology that will be used. Thus, it is possible to note what researchers are studying about similar problems related to this work and comprehend how to use the lattice Boltzmann method specifically to drilling mud flow inside the annulus;
- To determine boundary sites of the flow. As we are interested in what is happening inside the annulus, and since the inner pipe rotates, we must consider a three-dimensional case to observe the complex phenomena in more detail;
- To implement a high performance code for fluid flow simulation. With the use of the Lattice Boltzmann Method, we have some advantages because it deals very well with complex fluid flow, since the method does not solve the Navier-Stokes equations directly;
- To evaluate the potential and limitations of the computational solution for general cases. Once the boundary conditions are determined, it is possible to generalize this current case, allowing their application to different problems.

1.2 THESIS OUTLINE

The thesis consists of 5 chapters, divided as follow:

- **Chapter 1**: presents the introductory theoretical context and the main objective, describing some numerical methods usually applied to fluid dynamics, as well as presents the main and specific objectives of the study.
- Chapter 2: describes previous studies related to the flow inside an annulus and the use of the LBM to solve similar problems. Also, a contextualization about Taylor-Couette flow is presented.
- **Chapter 3**: in this chapter, the LBM is described, and consequently the concepts of particle are also presented. The Chapman-Enskog analysis is explained in order to clarify the lattice Boltzmann method as a tool for obtaining numerical solution to the Navier-Stokes equations. Forces are discussed, since they perform an important role in the present study.
- Chapter 4: the obtained results are presented and discussed in this chapter, introducing the use of forces in the modeling and contrasting the analytical solutions to numerical ones, bi-dimensional annulus flow at low *Re* comparing analytical to the numerical solution, and a Taylor-Couette flow comparison with another study.
- Chapter 5: finally, in this chapter, we point out the general considerations about the current study, and suggestions for future works.

2 LITERATURE REVIEW

In this chapter, we bring a literature review of existing researches about drilling mud flow, the use of LBM related to the same idea, and definitions that will be used throughout the work. Approaches to rheology and the flow of fluids, as well as all the important definitions necessary to comprehend this study, are given.

2.1 REYNOLDS NUMBER AND FLUIDS FLOW

There are two known main types of fluid flow regimes, which are laminar flow and turbulent flow. Between those, there is the transitional flow. But, before we explain each one, it is important to define what is the Reynolds number, which characterizes directly these types of flow.

2.1.1 Reynolds Number

Osborne Reynolds (1842-1912), a British engineer, was who first proposed experimentally the existence of the two types of flows. His experiment showed that fluid flowing in a circular pipe of small-diameter or low-velocity, flows as laminar (or viscous flow). In high-velocity or through a large-diameter pipe, the flow is characterized as turbulent (MACHADO, 2002, p. 13).

According to White (2008), the Reynolds number is always important, both with or without a free surface, and can be neglected only in flow regions away from high-velocity gradients (solid surfaces, jets, or wakes). It is highlighted in the Navier-Stokes Equation as a dimensionless parameter. The following equation shows its expression as a kinematic viscosity function, relating the inertial effect with the viscous effect, as:

$$Re = \frac{D\overline{U}}{\gamma}.$$
 (2.1)

where *D* is the channel dimension of flow (pipe diameter), \overline{U} the mean axial velocity flow, and *v* the kinematic viscosity. Here, it is possible to see that the flow tends to be turbulent when the velocity increases or the fluid viscosity decreases. For a particular velocity and viscosity, there will be a turbulent flow if the pipe diameter increases and, conversely, it will be laminar.

2.1.2 Laminar Flow in a pipe

In the laminar flow, the fluid layers move through streamlines, straights, or curves, parallel to flow direction, without macroscopic mixture (MACHADO, 2002, p. 14). The maximum velocity is concentrated in the axial axis (shear stress is zero) and equal to zero at the wall of the pipe (shear stress is maximum). It is important to say that the necessary strength to maintain the velocity gradient in a laminar flow increases with the viscosity of the fluid.

2.1.3 Turbulent Flow in a pipe

The characteristic of turbulent flow is that a small mass of fluid has chaotic displacement all along the pipe. There is a mixture between the layers, and velocity fluctuates around an average value (MACHADO, 2002, p. 16). Fluid particles move randomly through curved trajectories. Thus, point velocities change their values and direction all time.

In Figure 2, we can see the velocity profile for both profiles. It is possible to observe that in laminar flow, the velocity profile is parabolic. The \overline{U} parameter represents the local flow velocity and \overline{U}_{max} represents the maximum velocity.





Source: Adapted from White (2008).

As the Reynolds number classifies the corresponding flow, Table 1 shows how the petroleum industry categorizes the fluid flow, considering drilling and completion fluids, slurry density, fracturing fluids, petroleum, and derivatives:

Table 1 –	Critical Reynol	ls number o	of fluids flow	used in the	petroleum	industry
	2				1	2

5		1		
Critical Reynolds Number	Flow Type	Fluid Type		
2,100	laminar (<)	Newtonian		
3,000	turbulent (>)	Newtonian		
3,000-8,000	turbulent	non-Newtonian		
Source: Adapted from Machado (2002).				

2.1.4 Transitional Flow in a pipe

Transitional flow is related to laminar and turbulent flow at the same time, with turbulence acting in the center of the pipe and laminar flow near the edges (ENGINEERING TOOLBOX,

2004). The fluid particles move with both flows. And, viscous and Reynolds stresses, are of approximately equal magnitude. As we see in Table 1, the transitional flow is placed amidst 2,100 and 3,000, but in certain petroleum industry branches, the actual turbulent flow occurs when Reynolds number overcomes 8,000, especially when it flows with non-Newtonian fluids.

2.2 PREVIOUS WORK

Differently of the flow in pipes of petroleum wellbores, e.g., churn and annular, the behavior of the flow that takes place in the annulus is, up to this date, not very well understood due to its flow complexity, including the presence of cuttings from drilling formation.

In 1993, Reed and Pilehvari (1993, p. 469) developed a new model for the flow of drilling mud. According to them, "the method is valid in any flow regime and can be used to determine whether a non-Newtonian flow is laminar, transitional, or turbulent". The model makes use of an "effective" diameter, which is the "diameter of a circular pipe with the presence of a non-Newtonian flow, that would have the identical pressure drop for the flow of a Newtonian fluid with a viscosity equal to the "apparent" viscosity and the same average velocity as the non-Newtonian flow" (REED; PILEHVARI, 1993, p. 470).

On the other hand, Ramadan, Skalle, and Johansen (2003) developed a mechanistic model to determine the critical flow velocity required to initiate the movement of a spherical bed of particles in inclined channels. The particles are the drilled cuttings, and the considerations made here embrace a complex task because the angle of the wellbore will affect directly on the carrying of these particles.

Accordingly to Hall, Thompson, and Nuss (1950, p. 45), "turbulence due to restrictions, drill pipe vibration, and rotations, etc., may tend to alter the path of cuttings moving upward in the annulus, but the ability of a drilling mud to effectively lift cuttings is not affected by these factors". Then, if the drilling mud velocity is greater than the calculated slip velocity (of the cuttings), cuttings between a size range will be lifted and not allowed to settle back down the hole. It can be noted that the velocity and particle size ranges affect directly the flow of the drilling mud(WILLIAMS JR.; BRUCE, 1951; EPELLE; GEROGIORGIS, 2018).

As a foundation to the present study, Hegele et al. (2018) developed a study of high-Reynolds-number turbulent cavity flow (ALBENSOEDER; KUHLMANN, 2005; LERICHE, 2006; BOUFFANAIS; DEVILLE; LERICHE, 2007). The study uses the LBM to perform a direct numerical simulation of the flow with Reynolds number up to 50,000. For two-dimensional flows (MONTESSORI et al., 2014), they noted that as the Reynolds number are not so elevated, the velocity profile is presented uniformly.

As the Reynolds number increases considerably, the regime changes to transient. Consequently, the vortex center created by the fluid moves towards the center of the cavity. That justifies the difficulty of implementing a numerical simulation for confined flows, that is because the fluid does not have where to flow (it needs to deform itself), producing an unstable model, using LBM. But, Hegele et al. (2018) found a boundary modeling that solves the problem of this numerical instability.

2.2.1 Taylor-Couette Flow

An important factor that must be considered in this work is the Taylor-Couette flow. According to Lueptow (2009), it "is the name of a fluid flow and the related instability that occurs in the annulus between deferentially rotating concentric cylinders, most often with the inner cylinder rotating and the outer cylinder fixed, when the rotation rate exceeds a critical value."

The flow between two concentric cylinders is of interest earlier than the petroleum industry. In the 16th century, Isaac Newton used it to describe the circular motion of fluids in his Principia. George G. Stokes, in the 18th century, considered this simple flow noting the difficulty in modelling the boundary conditions at the wall of the cylinder, now taken for granted as the no-slip boundary condition.

There are some crucial applications aspects concerning this flow, such as linear stability analysis, low dimensional bifurcation phenomena, chaotic advection, absolute and convective instabilities, and a host of other fundamental physical phenomenon and analytic approaches. These instabilities can be related to the toroidal Taylor vortices stacked in the annulus and the theoretical framework that describes them.

The stable flow for this geometry is known as cylindrical Couette flow. Lueptow (2009) states that "as with all Couette-type flows, the flow is driven by the motion of one wall bounding a viscous liquid." With the application of the Navier-Stokes Equations for an incompressible Newtonian fluid, the accurate solution for infinite-length long cylinders is of the form (in cylindrical coordinates (r, θ, z)):

$$U_r = 0, \tag{2.2}$$

$$U_{\theta} = Ar + \frac{B}{r},\tag{2.3}$$

$$U_z = 0, \tag{2.4}$$

$$\frac{\partial p}{\partial r} = \rho \frac{U_r^2}{r},\tag{2.5}$$

where U_r , U_{θ} , and U_z are the radial, azimuthal, and axial components of velocity, p is the pressure, and ρ is the fluid density. A and B depend on the radius ratio $\eta = R_1/R_2$ of the inner cylinder radius R_1 and the outer cylinder radius R_2 , and the rotational speed of the inner cylinder Ω_1 , as:

$$A = -\Omega_1 \frac{\eta^2}{1 - \eta^2},\tag{2.6}$$

$$B = \Omega_1 \frac{R_1^2}{1 - \eta^2}.$$
 (2.7)

Instability in the cylindrical Couette flow begins to appear as the rotational speed of the inner cylinder increases resulting in pairs of counter-rotating, axisymmetric, toroidal vortices that fill the annulus superimposed on the Couette flow (LUEPTOW, 2009). Figure 3 illustrates these vortices. Each pair of vortices has a wavelength of approximately 2*D*, where $D = R_2 - R_1$ is the gap between the cylinders.



Figure 3 – Vortex formation of Taylor-Couette flow.

Source: Adapted from Lueptow (2009).

High-speed fluid close to the rotating inner cylinder is carried outward in the outflow regions between vortices, while low-speed fluid close to the fixed outer cylinder is carried inward in the inflow regions between vortices, redistributing angular momentum of the fluid in the annulus, because of the vortices. A small percentage of the surface speed of the inner cylinder is related to the axial and radial velocities, with Taylor vortices (WERELEY; LUEPTOW, 1998).

The vortical flow comes from a centrifugal instability (stable cylindrical Couette flow is geostrophic - when Coriolis' force and pressure gradient are in balance), this centrifugal force due to the azimuthal velocity is balanced by the radial pressure gradient force set up due to the azimuthal velocity. If a fluid particle is perturbed (moved slightly) outward from its initial radius, it reaches a region where the local restoring force due to the pressure gradient is slightly less than the outward inertia of the particle, which is based on the particle's initial position because its angular momentum is conserved. As a consequence, a fluid particle perturbed outward will continue outward. Analogously, if a fluid particle moved slightly inward from its initial radius will continue inward as the local restoring force due to the pressure gradient is smaller than the inward inertia of the particle (LUEPTOW, 2009). If the mass conservation guarantees a return

flow with a toroidal vortex of Taylor-Couette flow-form, does not matter whether the initial perturbation is inward or outward.

The viscosity can suppress the instability at low rotational speeds, damping out the perturbations. This instability occurs only when the pressure gradient force decreases (because of the decreasing azimuthal velocity) with increasing radius, as is the case for the inner cylinder rotating with the outer cylinder fixed. If the only rotating cylinder is the outer one, the pressure gradient force increases with increasing radius, and the flow remains stable (LUEPTOW, 2009).

Rayleigh (1917) quoted in Lueptow (2009) first put forth the inviscid (no viscosity) approach to the instability based on an imbalance of the centrifugal force and pressure gradient force. He explained that if the value for $(r^2\Omega)^2$ decreases in the radial direction, as it does for an inner rotating cylinder and a fixed outer cylinder, the flow should be unstable in cyclones taking a fluid angular velocity $\Omega(r)$, for example. Rayleigh's stability criterion predicts that regardless of the speed of the inner cylinder, as long as the inner cylinder rotates within a stationary outer cylinder, the flow should be unstable. That is not the case, since viscosity damps the perturbations for low rotational speeds, preventing the vortices from forming (LUEPTOW, 2009).

Taylor (1923) quoted in Lueptow (2009) first showed how viscosity stabilizes the flow at low rotational speeds using linear stability analysis. The analysis is based on small perturbations of the velocity and pressure fields considering a perturbation including a sinusoidal variation of the disturbance in the z-direction with axial wavenumber k (describes the axial periodicity of the perturbation) and $U_r = U_z = 0$, a growth rate or amplification factor q for the disturbance, and amplitudes of the disturbance which are dependent on the radial position. The axial component of the perturbation is zero where the other perturbations are maximum, and vice versa.

When applying those small perturbations expressions into the NSE followed by linearizing the equations (discarding higher-order terms) results in a set of ordinary differential equations. One way to solve these equations is transforming them into an eigenvalue problem, setting the amplification factor to zero, so it will correspond to the onset of the instability. As a result, the critical wavenumber, k_{crit} , and the critical Taylor number, Ta_{crit} (non-dimensional number above which the instability occurs), are taken. (LUEPTOW, 2009). Below the critical Taylor number, the flow is stable with no vortical structure; above, it is unstable with toroidal vortices. It is possible to express the Taylor number when the inner cylinder rotates within a fixed outer cylinder as follows:

$$Ta = \left[\frac{1-\eta}{\eta}\right] Re_{\theta}^{2}, \tag{2.8}$$

where $Re_{\theta} = \Omega_1 R_1 D/\nu$ is an azimuthal Reynolds number based on the surface velocity of the inner cylinder as the velocity scale and the gap width as the length scale. It is essential to say that Ta can also be measured as a function of Equation 2.1, which leads this parameter to two degrees of freedom. In our case, we are considering that the axial Reynolds number $Re_z = 0$, this because mean axial velocity \overline{U}_z averaged over the annular cross-section, is in our parameter range, independent of time and axial position, and given by the total through-flow.

The critical Reynolds number, Re_{crit} , which corresponds to the both critical Taylor number and the associated wavenumber (defines the axial spacing of the vortices or wavelength, $\lambda = 2\pi/k_{crit}$) for the onset of vortices, depends on the radius ratio as can be observed in Table 2. "Thus, since $k_{crit} = 3.13$ for $\eta = 0.9$, $\lambda \approx 2D$, indicating that a counter-rotating pair of vortices (one wavelength) has an axial wavelength that is twice the radial gap width. Thus, each vortex tends to be circular (as opposed to elliptical), filling a region that is $D \times D$, consistent with experiments" (LUEPTOW, 2009).

η	Ta _{crit}	R e _{crit}	k _{crit}
0.975	1,746.00	260.9	3.1270
0.900	1,924.69	131.6	3.1288
0.800	2,243.59	94.7	3.1326
0.700	2,708.02	79.5	3.1389
0.600	3,428.73	71.7	3.1483
0.500	4,649.33	68.2	3.1625

Table 2 – Critical Taylor and Reynolds number for transition to vortical flow.

Source: Adapted from Recktenwald, Lücke, and Müller (1993) quoted in Lueptow (2009).

As the Taylor number becomes larger than the critical Taylor number, more instabilities appear (higher-order) inside the annulus, with modified vortices. Wavy vortex flow appears first, which is characterized by the azimuthal waviness of the vortices. We can see this transition in Figure 4, which compared to Figure 3, neatly presents higher instabilities.

Figure 4 – Higher instabilities in the Taylor-Couette flow.



Source: Adapted from Lueptow (2009).

King et al. (1984) quoted in Lueptow (2009) explain that "the waves travel around the annulus at a speed that is 30-50% of the surface speed of the inner cylinder, depending on the Taylor number and other conditions".

The perturbation is, theoretically, the sum of many normal modes, "but in practice, the mode that dominates is the one for which the Taylor number at the stability limit is lowest" (LUEPTOW, 2009). When considering the transition from axisymmetric toroidal Taylor vortices to wavy vortices, is it known that its Taylor number is not tightly established. Serre, Sprague, and Lueptow (2008) quoted in Lueptow (2009) proposed that the transition is theoretically predicted to occur at $Ta/Ta_{crit} = 1.1$ for $\eta = 0.85$ for infinitely long cylinders, whereas experiments indicate a range of higher values between 1.14 and 1.31 for $\eta = 0.80 - 0.90$, depending on experimental conditions. As said Coles (1965) quoted in Lueptow (2009), the number of azimuthal waves is usually less than 6 or 7.

Depending on the direction of deformation of a wavy vortex (upward or downward), it will correspond to the direction of the (upward or downward) axial flow. Consequently, stream tubes are destroyed leading to chaotic particle paths with intra-vortex mixing. We can observe this phenomenon in Figure 5, where velocity vectors measured using particle image velocimetry in a meridional $(r - \theta)$ plane is showing intra-vortex flow between counter-rotating wavy vortices. The vortical flow is strong enough to wrap the azimuthal velocity contours around the vortex centers slightly and create relatively large regions across the annular gap where the azimuthal velocity does not vary substantially (AKONUR; LUEPTOW, 2003).

By contrast, Lueptow (2009) states that "the axisymmetric cellular structure of non-wavy Taylor vortex flow results in a set of nested stream tubes for each vortex with a dividing invariant stream surface between adjacent vortices. The only mechanism for transport within a vortex or between vortices is molecular diffusion."

The wavy vortices transition to modulated wavy vortices, evident upon flow visualization as a slight flattening of the outflow boundary when the flow is at higher Taylor numbers. Lueptow (2009) explains that the transition is easily distinguished from spectral analysis of a velocity or reflected light measurement at a particular point in the flow. The Wavy vortex flow holds a solitary peak at a frequency related to the passage of the azimuthal wave. Still, "the waviness gives way to turbulence, which raises the spectral level at all frequencies. The vortices become axisymmetric, but the flow is turbulent at small scales. At high enough Taylor number, the turbulent vortices disappear, and the flow is fully turbulent" (LUEPTOW, 2009).

2.2.1.1 Taylor-Couette Flow Studies

Following the Taylor-Couette flow studies, Di Prima and Swinney (1985) proposed many considerations about the stability and transitions of viscous incompressible flow between concentric rotating cylinders for the increasing speed of one or both cylinders. They presented a complex and robust study about the Taylor-Couette flow, comparing experiments and numerical Figure 5 – Velocity vectors in a meridional plane overlaid with azimuthal velocity. Color corresponds to the azimuthal (θ) velocity, with red corresponding to the velocity of the inner cylinder (IC) on the left, and blue corresponding to the velocity of the outer cylinder (OC) on the right. The azimuthal velocity contours are equally spaced between 0 at the OC and $1.0R_1\Omega$ at the IC.



Source: Lueptow (2009).

models, especially evaluating the growth of Taylor vortices, wavy vortex flow, instability of Couette flow, and higher instabilities and turbulence.

Other authors also have studied the instability of Taylor–Couette flow between concentric rotating cylinders, such as Dou, Khoo, and Yeo (2008). Their study used the energy gradient theory (proposed in their previous work), seeking the instability of Taylor–Couette flow between concentric rotating cylinders. One important conclusion was that the energy gradient theory can serve to relate the condition of transition in Taylor–Couette flow to that in plane Couette flow, and also possibly for analysis of flow instability and turbulent transition.

Through a 3D direct numerical simulation of turbulent Taylor–Couette flow, Dong (2007) investigated the dynamical and statistical features of turbulent Taylor–Couette flow ($\eta = 0.5$) at Reynolds numbers ranging from 1,000 to 8,000. In the three-dimensional space, they evidenced a random distribution of Görtler vortices - secondary flows that show up in a boundary layer flow along a concave wall (SARIC, 1994), in banded regions on the wall. These Görtler vortices lead to streaky structures that form herringbone-like patterns near the wall.

Another approach related to Taylor–Couette flow, was studied, with an imposed pressure-driven axial flow considering radius ratio $\eta = 0.83$ and aspect ratio $\Gamma = 47$, experimentally using particle image velocimetry in a meridional plane of the annulus

(WERELEY; LUEPTOW, 1999). For both toroidal and helical vortices with the absence of waviness, they demonstrate the axial flow winding around vortices in velocity vector fields.

Ostilla et al. (2013) implemented direct numerical simulations to reproduce turbulent Taylor–Couette flow with inner and outer cylinders rotating independently, evaluating analogously to a turbulent Rayleigh–Bénard flow. They found effective scaling laws for the torque and other system responses. Also, it was possible to reach an optimum transport for rotation at non-zero counter-rotation considering large enough Ta in the numerically accessible range. Between many considerations, their study shows a comparison between different Ta simulations, where boundary layers for the angular velocities ω transport become thinner with increasing Ta indicating increased angular velocity transport, which will be discussed more of in Chapter 4.

To prove the robustness of their boundary conditions in complex geometries, Mohammadipour, Niazmand, and Succi (2017) simulated a laminar flow between two rotating circular cylinders using LBM. It is visible that their approach for the boundary conditions provided more accurate velocity prediction when compared to other studies. This because the non-equilibrium component of distribution functions was approximated as a third-order power series in the lattice velocities, and also, they formulated a procedure to obtain boundary node distributions by using fluid variables.

Mohammadipour, Succi, and Niazmand (2018) simulated a flow governed by the force balance between the centrifugal force and the pressure gradient in the radial direction using LBM, presenting a comparison between their results with analytical solutions, which are the tangential velocity and the pressure in dimensionless form, respectively:

$$u_{\theta}^{\star} = \frac{u_{\theta}}{R_1 \omega} = \frac{1}{1 - \eta^2} \left(\frac{1}{R^{\star}} - \eta^2 R^{\star} \right), \tag{2.9}$$

where ω is the angular velocity, $R^* = \frac{r}{R_1}$ the dimensionless radial distance, $r = \sqrt{x^2 + y^2}$ is the radial coordinate and function of *x* (horizontal) and *y* (vertical) Cartesian coordinates, and

$$p^{\star} = \frac{p}{\rho R_1^2 \omega^2} = p_{R=R_1}^{\star} + \frac{1}{(1-\eta^2)^2} \left[\frac{\eta^4}{2} (R^{\star 2} - 1) - 2\eta^2 \ln R^{\star} - \frac{1}{2} \left(\frac{1}{R^{\star 2}} - 1 \right) \right], \quad (2.10)$$

where p is the pressure, ρ the zero-order moment in LBM (will be discussed further) and $p_{R=R_1}^{\star}$ the pressure in the inner cylinder.

White (2006, p. 110) presents many viscous flow solutions, but a pure Poiseuille flow between plates is going to be a good similarity to validate the use of forces (will be presented further in section 3.3) in our annulus study case. With a constant pressure gradient $(\frac{dp}{dx})$ as presented in Figure 6, simple equations to express the velocity and total volume rate of flow are obtained, respectively, as follow:

$$\overline{U} = \overline{U}_{max} \left(1 - \frac{y^2}{h^2} \right), \tag{2.11}$$

where \overline{U}_{max} is given by:

$$\overline{U}_{max} = \left(-\frac{\mathrm{d}p}{\mathrm{d}x}\right)\frac{h^2}{2\mu},\tag{2.12}$$

and

$$Q = \frac{4}{3}h\overline{U}_{max}.$$
(2.13)

Figure 6 – Pure Poiseuille flow between parallel plates.



Source: Adapted from White (2006, p. 98).

On the other hand, applying the viscous flow from White (2006, p. 114) studies directly to concentric circular annulus (what we are most interested in), it is possible to express the solutions to the velocity and total volume rate of flow, respectively:

$$\overline{U} = \frac{\mathrm{d}p/\mathrm{d}x}{4\mu} \left[R_2^2 - r^2 + (R_2^2 - R_1^2) \frac{\ln(R_2/r)}{\ln(R_1/R_2)} \right],\tag{2.14}$$

and

$$Q = \frac{\pi}{8\mu} \left(-\frac{\mathrm{d}p}{\mathrm{d}x} \right) \left[R_2^4 - R_1^4 - \frac{(R_2^2 - R_1^2)^2}{\ln(R_2/R_1)} \right].$$
 (2.15)

The Taylor-Couette flow presented in this subsection is similar to the problem found in the petroleum industry. We are considering that the inner cylinder is rotating, all along its length, just like in drilling engineering. The outer cylinder will not rotate because, of course, represents the formation (wellbore wall).

3 METHODOLOGY

The methodology that is applied in this thesis is the LBM, especially because it has a solid physical foundation, is stable, and seeks to connect its dynamics to macroscopic conservation equations of fluids, apart from having simple and efficient implementations (KRÜGER et al., 2017). To present all the methodology development, we will divide this chapter into sections, each one with its importance and contribution to the analysis.

3.1 THE LATTICE BOLTZMANN EQUATION

In this section, we will describe the particle distribution, velocity set, moments, and important basic particularities that are required to understand the LBM.

3.1.1 Particle Populations

The density of particles are represented by the particle populations, also called as discrete-particle distribution function $f_i(\mathbf{r}, t)$ according to Equation (3.1), which is related to velocity c_i at position \mathbf{r} and time t. Moreover, there are velocity sets that are used to solve the NSE, denoted by DdQq (where d is the number of spatial dimensions and q is the velocity set number), among which the most commonly used are D1Q3, D2Q9, D3Q15, D3Q19, and D3Q27 (KRÜGER et al., 2017):

$$f_i(\mathbf{r} + \mathbf{c}_i, t+1) = f_i^{(eq)}(\mathbf{r}, t) + (1 - \tau^{-1}) \hat{f}_i^{(neq)}(\mathbf{r}, t),$$
(3.1)

considering that $f_i^{(eq)}$ is the equilibrium particle distribution and $\hat{f}_i^{(neq)}$ is the regularized non-equilibrium particle distribution, and τ is the relaxation time. The last term in Equation 3.1 is the Bhatnagar-Gross-Krook (BGK) regularized collision operator (Ω_i). In this work the D3Q19 velocity set was used, this because we intend to study the 3D fluid flow inside the annulus.

It is also essential to express that, according to Hegele et al. (2018), the relaxation time (τ) is tuned to set the Reynolds number through the viscosity:

$$v = \frac{\tau - \frac{1}{2}}{a_s^2}.$$
 (3.2)

Still, another indispensable parameter we use is the pressure (isothermal), which is calculated by:

$$p = c_s^2 \rho, \tag{3.3}$$

where c_s is the speed of sound.

The equilibrium depends on the local quantities density and fluid velocity \boldsymbol{u} , which is found by:

$$\boldsymbol{u}(\boldsymbol{r},t) = \frac{\rho \boldsymbol{u}(\boldsymbol{r},t)}{\rho(\boldsymbol{r},t)},\tag{3.4}$$

where we can write:

$$\rho = \sum_{i} f_i = \sum_{i} f_i^{eq}, \qquad (3.5)$$

and

$$\rho \boldsymbol{u} = \sum_{i} f_i \boldsymbol{c}_i = \sum_{i} f_i^{eq} \boldsymbol{c}_i.$$
(3.6)

3.1.2 Particle Regularization and its Moments

To regularize the particle distribution function, Equation (3.7) define the moments of this distribution, being zeroth-order (ρ), first-order (ρu_{α}) and second order ($\rho m_{\alpha\beta}^{(2)}$), respectively. The $\delta_{\alpha\beta}$ term is the Kronecker delta, a_s the scaling factor ($\sqrt{(3)}$ for the D3Q19 velocity set), and g_i is the particle distribution function or regularized particle distribution function (LATT; CHOPARD, 2006; MONTESSORI et al., 2014):

$$\left\{\rho,\rho u_{\alpha},\rho m_{\alpha\beta}^{(2)}\right\} = \sum_{i} g_{i}\left\{1,c_{i\alpha},c_{i\alpha}c_{i\beta}-\delta_{\alpha\beta}/a_{s}^{2}\right\}.$$
(3.7)

The equilibrium particle distribution function $f^{(eq)}$, is expressed by Equation (3.8) applying Einstein notation (STOVER; WEISSTEIN, 2021) and considering the second-order velocity expansion in the Hermite polynomials (\mathcal{H}) (PHILIPPI et al., 2006; SHAN; YUAN; CHEN, 2006):

$$f_i^{(eq)}(\boldsymbol{r},t) = \rho w_i (1 + a_s^2 u_\alpha c_{i\alpha} + \frac{1}{2} a_s^4 u_\alpha u_\beta \mathscr{H}_{\alpha\beta,i}^{(2)}), \qquad (3.8)$$

where w_i are the quadrature weights that depend on the direction c_i . The second-order moments are expressed by:

$$\widehat{f}_{i}^{(neq)}(\boldsymbol{r},t) = \frac{1}{2}\rho w_{i}a_{s}^{4} \left[m_{\alpha\beta}^{(2)} - u_{\alpha}u_{\beta}\right] \mathcal{H}_{\alpha\beta,i}^{(2)}.$$
(3.9)

Finally, the regularization procedure is completed as Equation (3.10) (MATTILA; PHILIPPI; HEGELE JR., 2017; COREIXAS et al., 2017):

$$\widehat{f}_i(\boldsymbol{r},t) = f_i^{(eq)}(\boldsymbol{r},t) + \widehat{f}_i^{(neq)}(\boldsymbol{r},t).$$
(3.10)

One fundamental point to be highlighted is that in regularization, the particle distributions are allocated to the subspace where they arrange themselves. It is a process that gives information to each neighboring distribution. In addition, the high-order moments are filtered in this process. So, e.g., the third- and fourth-order moments, when summed, respectively, they are equal to zero. Taking all these considerations into account makes the use of the regularization process a great advantage in dealing with high-Reynolds number simulations.

On the other hand, for the f_i (non-regularized), we do not modify the terms we use in the way it arrives at the site. And, of course, the high-order moments are not filtered. When summed,
they are not equal to zero, e.g., the third- and fourth-order moments. The non-regularized particle distributions make use of the "pure" BGK.

We must say that LBM solves the Boltzmann equation, which is at least in theory, more general than the NSE. The NSE describes the behavior of fluid flow in the continuum approximation, but the Boltzmann equation is a more detailed description of the behavior since it is based on a statistical over the movement of fluid molecules. Therefore, it can be applied to cases where the NSE are no longer accurate. Generally, the LBM has advantages over the NSE solver for multi-phase flows, non-Newtonian flows, and small-scale flows where the continuity approximation in the NS equation does not hold (KRÜGER et al., 2017).

Still, another point in the use of LBM is the Chapman-Enskog analysis, which we will not describe in a detailed way, but can be generally described as the analysis that shows the lattice Boltzmann equation can be actually used to simulate the behavior of fluids, as described above. While it was previously looked at the macroscopic behavior of the undiscretized Boltzmann equation, and found that it behaves according to the continuity equation and a general Cauchy momentum equation with an unknown stress tensor, Chapman-Enskog analysis developed similar methods of finding macroscopic equations from the Boltzmann equation with Boltzmann's original collision operator (KRÜGER et al., 2017). We can say that this analysis establishes the connection between the "mesoscopic" LBE and the macroscopic mass and momentum equations.

3.1.3 D3Q19 and Boundary Sites

By itself, the regularization procedure of LB does not necessarily address boundaries (HEGELE et al., 2018). Thus, from the regularization procedure of particle distribution function, boundary conditions may be found. (LATT et al., 2008; MALASPINAS; CHOPARD; LATT, 2011). With the sum of the still-unknown regularized distribution at the boundaries node, it is possible to obtain the second-order particle moment from Equation (3.11), which is also expressed with the regularized particle distribution function, as shows Equation (3.12).

$$\sum_{i \in I_s} f_i \mathcal{H}^{(2)}_{\alpha\beta,i} + \sum_{i \notin I_s} \widehat{f}_i \mathcal{H}^{(2)}_{\alpha\beta,i} = \rho m^{(2)}_{\alpha\beta}.$$
(3.11)

$$\rho m_{\alpha\beta}^{(2)} = \sum_{i \in I_s} \widehat{f}_i \mathscr{H}_{\alpha\beta,i}^{(2)} + \sum_{i \notin I_s} \widehat{f}_i \mathscr{H}_{\alpha\beta,i}^{(2)}, \qquad (3.12)$$

where I_s is the incoming velocity set. Through second-order moment decomposition to regularized particle distribution function (considering belonging and not belonging particle distribution to an I_s) combined to Equation (3.11), equivalence is established between the sum of f_i function (regularized and not-regularized), according to Equation (3.13), leading to a set of seven equations when using D3Q19 distribution.

$$\sum_{i \in I_s} f_i \mathscr{H}^{(2)}_{\alpha\beta,i} = \sum_{i \in I_s} \widehat{f}_i \mathscr{H}^{(2)}_{\alpha\beta,i}.$$
(3.13)

In a nutshell, LBM consists of collision and streaming. The collision is simply an algebraic local operator, which calculates the density (zeroth-order moment) and the macroscopic velocity (first-order moment) to find the equilibrium distributions $f_i^{(eq)}$ and then the post-collisional distribution functions. After that, the resulting distribution is streamed to neighboring nodes (KRÜGER et al., 2017).

When considering Dirichlet boundaries, the velocity \boldsymbol{u} is known, in principle. Then, with mass conservation during the process of particles collision, the boundaries are given by:

$$\sum_{i \in I_s} f_i(\mathbf{r}, t) = \sum_{i \in O_s} f_i(\mathbf{r} + \mathbf{c}_i, t+1) = (1 - \tau^{-1}) \sum_{i \in O_s} \widehat{f_i}(\mathbf{r}, t) + \tau^{-1} \sum_{i \in O_s} f_i^{(eq)}(\mathbf{r}, t).$$
(3.14)

It is possible to see in Figure 7 the 3D simulation of hydrodynamic velocity set of D3Q19. Compared to D3Q27, requires 40% less memory and computing power. Thus, its velocities and weights are presented in Table 3.

Figure 7 – D3Q19 velocity sets. The cube origin of the system of coordinates is situated at the center of the grid.



Source: Hegele et al. (2018).

i	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
\boldsymbol{w}_i	$\frac{1}{3}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{18}$	$\frac{1}{36}$											
\boldsymbol{c}_{ix}	0	+1	-1	0	0	0	0	+1	-1	+1	-1	0	0	+1	-1	+1	-1	0	0
\boldsymbol{c}_{iy}	0	0	0	+1	-1	0	0	+1	-1	0	0	+1	-1	-1	+1	0	0	+1	-1
\boldsymbol{c}_{iz}	0	0	0	0	0	+1	-1	0	0	+1	-1	+1	-1	0	0	-1	+1	-1	+1
	Source: Krüger et al. (2017).																		

Table 3 – D3Q19 velocity set in explicit form.

The incoming particles to the site index set I_s are defined by $I_s = \{i \mid \mathbf{r} - c_i \text{ is a fluid site}\}$, and in the opposite direction we have the outgoing particles from the site index set O_s is given by $O_s = \{j \mid c_j = -c_i, i \in I_s\}$ (HEGELE et al., 2018). An example of an outgoing corner boundary site is shown in Figure 8, which is located at the point (x, y, z) = (0, 0, 0) with normal vectors given by $\hat{n}_1 = (0, 0, -1)$, $\hat{n}_2 = (-1, 0, 0)$ and $\hat{n}_3 = (0, 1, 0)$. It is expressed by an intersection of three perpendicular planes defined by these normals.

Figure 8 – Outgoing vectors of a corner boundary site. Seen vectors set: $I = \{0, 2, 4, 6, 12, 14, 17\}$ and $O_s = \{0, 1, 3, 5, 8, 10, 15\}.$



Source: Hegele et al. (2018).

It is possible to see an example of an edge boundary site, which is located at the point (x, y, z) = (0, 0, 0) with normal vectors given by $\hat{n}_1 = (0, 0, -1)$ and $\hat{n}_2 = (-1, 0, 0)$, on Figure 9. It comprehends the intersection of two perpendicular planes, with these two normals.

Figure 10 and Figure 11 present an example of a face boundary site, which are located at the point (x, y, z) = (0, 0, 0) with only one normal vector given by $\hat{n}_1 = (0, 0, -1)$, such that are outgoing and incoming vectors, respectively.

3.1.4 General Explicit Equations for the Moments

As explained by Hegele et al. (2018), Dirichlet-type of boundary conditions lead to a system of equations for the unknown moments ρ and $m_{\alpha\beta}^{(2)}$, and the known moments u_{x_1} , u_{x_2} and u_{x_3} , since \hat{f} is only a function of ρ , u_β and $m_{\alpha\beta}^{(2)}$. Then, we can observe that a nonlinear system of equations will be created, that is why we consider $\rho m_{\alpha\beta}^{(2)}$.

Diagonal moments $\rho_I m_{x_1 x_1, I}^{(2)}$, $\rho_I m_{x_1 x_1, I}^{(2)}$ and $\rho_I m_{x_1 x_1, I}^{(2)}$, and non-diagonal moments $\rho_I m_{x_1 x_2, I}^{(2)}$, $\rho_I m_{x_1 x_3, I}^{(2)}$ and $\rho_I m_{x_2 x_3, I}^{(2)}$ come from Equation (3.13). For the first diagonal one, $\rho_I m_{x_1 x_1, I}^{(2)}$, considering the right-hand side of Equation (3.13), is solved relating the geometrical parameters that form the boundaries, so:

Figure 9 – Outgoing vectors of an edge boundary site. Seen vectors set: $I = \{0, 2, 4, 5, 6, 12, 14, 16, 17, 18\}$ and $O_s = \{0, 1, 2, 3, 5, 7, 8, 9, 10, 15\}$.



Source: Hegele et al. (2018).

Figure 10 – Outgoing vectors of a face boundary site, which the set is $O_s = \{0, 1, 2, 3, 4, 5, 7, 8, 9, 10, 12, 13, 15, 16\}.$



Source: Hegele et al. (2018).

$$\rho_{I}m_{x_{1}x_{1},I}^{(2)} = \rho(P_{123}^{(1)} + u_{x_{1}}P_{123}^{(u)} + u_{x_{2}}S_{123}^{(u)} + u_{x_{3}}S_{132}^{(u)}) + \rho m_{x_{1}x_{1}}^{(2)}P_{123}^{(m)} + \rho m_{x_{2}x_{2}}^{(2)}S_{123}^{(m)} + \rho m_{x_{3}x_{3}}^{(2)}S_{132}^{(m)} + \rho m_{x_{1}x_{2}}^{(2)}\frac{1}{6}l_{1}l_{2} + \rho m_{x_{1}x_{3}}^{(2)}\frac{1}{6}l_{1}l_{3} - \rho m_{x_{2}x_{3}}^{(2)}\frac{1}{12}l_{2}l_{3},$$
(3.15)

where:

$$P_{pqr}^{(1)} = -\frac{1}{12} + \frac{2}{27} \widetilde{\delta}_{l_p} + \frac{1}{54} \widetilde{\delta}_{l_p} (\widetilde{\delta}_{l_q} + \widetilde{\delta}_{l_r}) - \frac{1}{108} (\widetilde{\delta}_{l_q} + \widetilde{\delta}_{l_r} + \widetilde{\delta}_{l_q} \widetilde{\delta}_{l_r}),$$
(3.16)

Figure 11 – Incoming vectors of a face boundary site, which the set is $I_s = \{0, 1, 2, 4, 5, 6, 7, 10, 11, 12, 14, 16, 17, 18\}.$



Source: Hegele et al. (2018).

$$P_{pqr}^{(u)} = l_p \left(\frac{2}{9} + \frac{\tilde{\delta}_{l_q}}{18} + \frac{\tilde{\delta}_{l_r}}{18} \right),$$
(3.17)

$$S_{pqr}^{(u)} = l_q \left(\frac{\tilde{\delta}_{l_p}}{18} - \frac{1}{36} - \frac{\tilde{\delta}_{l_r}}{36} \right),$$
 (3.18)

$$P_{pqr}^{(m)} = \frac{11}{24} + \frac{2}{9}\widetilde{\delta}_{l_p} + \frac{7}{72}(\widetilde{\delta}_{l_q} + \widetilde{\delta}_{l_r}) + \frac{\delta_{l_p}}{18}(\widetilde{\delta}_{l_q} + \widetilde{\delta}_{l_r}) + \frac{1}{72}\widetilde{\delta}_{l_q}\widetilde{\delta}_{l_e},$$
(3.19)

$$S_{pqr}^{(m)} = \frac{1}{12} - \frac{1}{36} (\widetilde{\delta}_{l_p} + \widetilde{\delta}_{l_q} + \widetilde{\delta}_{l_r}) - \frac{1}{36} (\widetilde{\delta}_{l_p} + \widetilde{\delta}_{l_q}) \widetilde{\delta}_{l_r} + \frac{1}{18} \widetilde{\delta}_{l_p} \widetilde{\delta}_{l_q},$$
(3.20)

and the modified function δ is given by:

$$\widetilde{\delta}_{l_k} = \begin{cases} 1, & \text{if } l_k = 0, \\ 0, & \text{otherwise,} \end{cases}$$
(3.21)

where k = 1, 2, 3 assumes any permutation of the coordinates and $l_j = \pm 1$ expresses the orientation of the planes.

The Equations (3.16) to (3.20) depend exclusively on geometrical parameters given by the definition of the boundary, and the indices $\{p, q, r\}$ can assume all of the permutations of the set $\{1, 2, 3\}$. Similarly, the two other diagonal moments can be determined, expressed as:

$$\rho_{I}m_{x_{2}x_{2},I}^{(2)} = \rho(P_{213}^{(1)} + u_{x_{2}}P_{213}^{(u)} + u_{x_{1}}S_{213}^{(u)} + u_{x_{3}}S_{213}^{(u)}) + \rho m_{x_{2}x_{2}}^{(2)}P_{213}^{(m)} + \rho m_{x_{1}x_{1}}^{(2)}S_{213}^{(m)} + \rho m_{x_{1}x_{2}}^{(2)}\frac{1}{6}l_{1}l_{2} + \rho m_{x_{2}x_{3}}^{(2)}\frac{1}{6}l_{2}l_{3} - \rho m_{x_{1}x_{3}}^{(2)}\frac{1}{12}l_{1}l_{3},$$
(3.22)

$$m_{x_{3}x_{3},I}^{(2)} = \rho(P_{312}^{(1)} + u_{x_{3}}P_{312}^{(u)} + u_{x_{1}}S_{312}^{(u)} + u_{x_{2}}S_{312}^{(u)}) + \rho m_{x_{3}x_{3}}^{(2)}P_{312}^{(m)} + \rho m_{x_{1}x_{1}}^{(2)}S_{312}^{(m)} + \rho m_{x_{1}x_{3}}^{(2)}\frac{1}{6}l_{1}l_{3} + \rho m_{x_{2}x_{3}}^{(2)}\frac{1}{6}l_{2}l_{3} - \rho m_{x_{1}x_{2}}^{(2)}\frac{1}{12}l_{1}l_{2}.$$
(3.23)

In sequence, the non-diagonal moment, $\rho_I m_{x_1x_2,I}^{(2)}$, can be found as:

$$\rho_{I}m_{x_{1}x_{2},I}^{(2)} = \rho(Q_{12}^{(1)} + u_{x_{1}}Q_{12}^{(u)} + u_{x_{2}}Q_{21}^{(u)}) + \rho m_{x_{1}x_{1}}^{(2)} \frac{1}{12}l_{1}l_{2} + \rho m_{x_{2}x_{2}}^{(2)} \frac{1}{12}l_{1}l_{2} - \rho m_{x_{3}x_{3}}^{(2)} \frac{1}{24}l_{1}l_{2} + \rho m_{x_{1}x_{2}}^{(2)}Q_{12}^{(m)},$$
(3.24)

where

$$Q_{pq}^{(1)} = \frac{1}{36} l_p l_q, \tag{3.25}$$

$$Q_{pq}^{(u)} = \frac{1}{12} (1 + \tilde{\delta}_{l_p}) l_q, \qquad (3.26)$$

$$Q_{pq}^{(m)} = \frac{1}{4} (1 + \tilde{\delta}_{l_p}) (1 + \tilde{\delta}_{l_q}).$$
(3.27)

The Equations (3.25) to (3.27) depend exclusively on geometrical parameters given by the definition of the boundary, as well as the diagonal moments. Analogously, the two other non-diagonal moments can be determined based on symmetry arguments, written as:

$$m_{x_{1}x_{3},I}^{(2)} = \rho(Q_{13}^{(1)} + u_{x_{1}}Q_{13}^{(u)} + u_{x_{3}}Q_{31}^{(u)}) + \rho m_{x_{1}x_{1}}^{(2)} \frac{1}{12}l_{1}l_{3} + \rho m_{x_{3}x_{3}}^{(2)} \frac{1}{12}l_{1}l_{3} - \rho m_{x_{2}x_{2}}^{(2)} \frac{1}{24}l_{1}l_{3} + \rho m_{x_{1}x_{3}}^{(2)}Q_{13}^{(m)},$$
(3.28)

$$m_{x_{2}x_{3},I}^{(2)} = \rho(Q_{23}^{(1)} + u_{x_{2}}Q_{23}^{(u)} + u_{x_{3}}Q_{32}^{(u)}) + \rho m_{x_{2}x_{2}}^{(2)} \frac{1}{12}l_{2}l_{3} + \rho m_{x_{3}x_{3}}^{(2)} \frac{1}{12}l_{2}l_{3} - \rho m_{x_{1}x_{1}}^{(2)} \frac{1}{24}l_{2}l_{3} + \rho m_{x_{2}x_{3}}^{(2)}Q_{23}^{(m)}.$$
(3.29)

Last, the regularized \hat{f}_i and equilibrium $f_i^{(eq)}$ particle functions, with mass conservation, are expanded and summed up in the outgoing set index O_s , obtaining:

$$\rho_{I} = \rho \left(R_{123}^{(1)} + u_{x_{1}} R_{123}^{(1)} + u_{x_{2}} R_{231}^{(u)} + u_{x_{3}} R_{312}^{(u)} \right) + \rho \omega \left(u_{x_{1}}^{2} \frac{a_{s}^{4}}{2} P_{123}^{(1)} + u_{x_{2}}^{2} \frac{a_{s}^{4}}{2} P_{231}^{(1)} \right) \\
+ u_{x_{3}}^{2} \frac{a_{s}^{4}}{2} P_{312}^{(1)} \right) + u_{x_{1}} u_{x_{2}} a_{s}^{4} Q_{12}^{(1)} + u_{x_{1}} u_{x_{3}} a_{s}^{4} Q_{13}^{(1)} + u_{x_{2}} u_{x_{3}} a_{s}^{4} Q_{23}^{(1)} + (1 - \omega) \\
\left(\rho m_{x_{1}x_{1}}^{(2)} \frac{a_{s}^{4}}{2} P_{123}^{(1)} + \rho m_{x_{2}x_{2}}^{(2)} \frac{a_{s}^{4}}{2} P_{231}^{(1)} + \rho m_{x_{3}x_{3}}^{(2)} \frac{a_{s}^{4}}{2} P_{312}^{(1)} + \rho m_{x_{1}x_{2}}^{(2)} \frac{a_{s}^{4}}{2} Q_{12}^{(1)} \\
+ \rho m_{x_{1}x_{3}}^{(2)} \frac{a_{s}^{4}}{2} Q_{13}^{(1)} + \rho m_{x_{2}x_{3}}^{(2)} \frac{a_{s}^{4}}{2} Q_{23}^{(1)} \right),$$
(3.30)

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$$R_{pqr}^{(1)} = \frac{7}{12} + \frac{1}{9} (\widetilde{\delta}_{l_p} + \widetilde{\delta}_{l_q} + \widetilde{\delta}_{l_r}) + \frac{1}{36} (\widetilde{\delta}_{l_p} \widetilde{\delta}_{l_q} + \widetilde{\delta}_{l_p} \widetilde{\delta}_{l_r} + \widetilde{\delta}_{l_q} \widetilde{\delta}_{l_r}),$$
(3.31)

$$R_{pqr}^{(u)} = -\frac{1}{3}l_p(1 + \frac{1}{4}(l_q + l_r)).$$
(3.32)

3.1.5 Explicit Solution for the Boundary Conditions

To make it clear, in this subsection, the boundary conditions are presented explicitly, especially considering the corners, edges, and faces, which are given in the following sub-subsections.

3.1.5.1 Corners

The corners can be represented by the signs of l_1 , l_2 and l_3 . Therefore, as a function of the modified Kronecker delta, $\tilde{\delta}_{l_1} = \tilde{\delta}_{l_2} = \tilde{\delta}_{l_3} = 0$. For zeroth-order moments, the corner solutions are:

$$\rho = \rho_I \frac{b_C}{d_C},\tag{3.33}$$

where

$$b_{C} = \frac{1}{24} (1 - \omega) \left(m_{x_{1}x_{1},I}^{(2)} + m_{x_{2}x_{2},I}^{(2)} + m_{x_{3}x_{3},I}^{(2)} - 2l_{1}l_{2}m_{x_{1}x_{2},I}^{(2)} - 2l_{1}l_{3}m_{x_{1}x_{3},I}^{(2)} - 2l_{2}l_{3}m_{x_{2}x_{3},I}^{(2)} \right),$$

$$(3.34)$$

and

$$d_{C} = 4 + 10\omega + (4\omega - 12) \left(l_{1}u_{x_{1}} + l_{2}u_{x_{2}} + l_{3}u_{x_{3}} \right) - 9\omega \left(u_{x_{1}}^{2} + u_{x_{2}}^{2} + u_{x_{3}}^{2} \right) + 6\omega \left(l_{1}l_{2}u_{x_{1}}u_{x_{2}} + l_{1}l_{3}u_{x_{1}}u_{x_{3}} + l_{2}l_{3}u_{x_{2}}u_{x_{3}} \right).$$
(3.35)

For the second-order moments, we have:

$$\rho m_{x_1 x_1, I}^{(2)} = \frac{1}{3} \rho_I \left(10 m_{x_1 x_1, I}^{(2)} - 2 m_{x_2 x_2, I}^{(2)} - 2 m_{x_3 x_3, I}^{(2)} - 6 l_1 l_2 m_{x_1 x_2, I}^{(2)} - 6 l_1 l_3 m_{x_1 x_3, I}^{(2)} - 6 l_2 l_3 m_{x_2 x_3, I}^{(2)} \right) + \frac{2}{3} \rho (1 - 2 l_1 u_{x_1} + l_2 u_{x_2} + l_3 u_{x_3}).$$

$$(3.36)$$

By symmetry and in analogous way, it is possible to express the terms for $\rho m_{x_2x_2,I}^{(2)}$ and $\rho m_{x_3x_3,I}^{(2)}$. Taking, for example, $\rho m_{x_2x_2,I}^{(2)}$, and swapping indices 1 and 2, but leaving index 3 alone.

For the cross terms,

$$\rho m_{x_1 x_2, I}^{(2)} = \frac{1}{3} \rho_I \left(-3l_1 l_2 m_{x_1 x_1, I}^{(2)} - 3l_1 l_2 m_{x_2 x_2, I}^{(2)} + 3l_1 l_2 m_{x_3 x_3, I}^{(2)} + 17 m_{x_1 x_2, I}^{(2)} - l_2 l_3 m_{x_1 x_3, I}^{(2)} - l_1 l_3 m_{x_2 x_3, I}^{(2)} \right) - \frac{2}{9} \rho (l_1 l_2 + l_1 u_{x_2} + l_2 u_{x_1} + l_1 l_2 l_3 u_{x_3}).$$

$$(3.37)$$

Also by symmetry and in analogous way, it is possible to express the terms for $\rho m_{x_1x_3,I}^{(2)}$ and $\rho m_{x_2x_3,I}^{(2)}$. It can be done by taking, for example, $\rho m_{x_1x_3,I}^{(2)}$, and swapping indices 1 and 3, but leaving apart index 2.

3.1.5.2 Edges

The edges can be represented by the orientations l_1 and l_2 . Thus, as a function of the modified Kronecker delta, $\tilde{\delta}_{l_1} = \tilde{\delta}_{l_2} = 0$ and $\tilde{\delta}_{l_3} = 1$ with $l_3 = 0$. For zeroth-order moments, the edges solutions are:

$$\rho = \rho_I \frac{b_E}{d_E},\tag{3.38}$$

where

$$b_E = 1656 - 216(\omega - 1) \left[8m_{x_1x_1,I}^{(2)} + 8m_{x_2x_2,I}^{(2)} - 2m_{x_3x_3,I}^{(2)} - 19l_1l_2m_{x_1x_2,I}^{(2)} \right]$$
(3.39)

and

$$b_E = 720 - 660(l_1u_{x_1} + l_2u_{x_2}) + \omega(430 - 30(l_1u_{x_1} + l_2u_{x_2}) + 414l_1l_2u_{x_1}u_{x_2} - 690(u_{x_1}^2 + u_{x_2}^2) - 69u_{x_3}^2).$$
(3.40)

And then, for the second-order moments, the expressions are:

$$\rho m_{x_1 x_1, I}^{(2)} = \frac{1}{23} \rho_I \left(47 m_{x_1 x_1, I}^{(2)} + m_{x_2 x_2, I}^{(2)} - 6 m_{x_3 x_3, I}^{(2)} - 34 l_1 l_2 m_{x_1 x_2, I}^{(2)} \right) - \frac{2}{69} \rho (-8 + 15 l_1 u_{x_1} + 8 l_2 u_{x_2}),$$
(3.41)

and

$$\rho m_{x_3 x_3, I}^{(2)} = \frac{2}{69} \rho_I \left(-9 m_{x_1 x_1, I}^{(2)} - 9 m_{x_2 x_2, I}^{(2)} + 54 m_{x_3 x_3, I}^{(2)} + 30 l_1 l_2 m_{x_1 x_2, I}^{(2)} \right) - \frac{4}{69} \rho (1 + l_1 u_{x_1} + l_2 u_{x_2}).$$
(3.42)

By the symmetry, the relation for $\rho m_{x_2x_2,I}^{(2)}$ comes from Equation 3.41 exchanging indices 1 and 2.

The cross-terms are given by:

$$\rho m_{x_1 x_2, I}^{(2)} = \frac{1}{23} \rho_I \left(l_1 l_2 \left(-17 m_{x_1 x_1, I}^{(2)} - 17 m_{x_2 x_2, I}^{(2)} + 10 m_{x_3 x_3, I}^{(2)} \right) + 118 m_{x_1 x_2, I}^{(2)} \right) - \frac{19}{69} \rho (l_1 l_2 + l_1 u_{x_2} + l_2 u_{x_1}),$$
(3.43)

and

$$\rho m_{x_1 x_3, I}^{(2)} = 2\rho_I m_{x_1 x_3, I}^{(2)} - \frac{1}{3} l_1 \rho u_{x_3}.$$
(3.44)

By the symmetry, the relation for $\rho m_{x_2x_3,I}^{(2)}$ comes from Equation 3.43 exchanging indices 1 and 2.

3.1.5.3 Faces

The faces can be represented by $l_1 \neq 0$ (the orientation of the face is defined by its sign) only, then $l_2 = l_3 = 0$. Thus, as a function of the modified Kronecker delta, $\tilde{\delta}_{l_2} = \tilde{\delta}_{l_3} = 1$ and $\tilde{\delta}_{l_1} = 0$. For zeroth-order moments, the faces solutions are:

$$\rho = \rho_I \frac{9(1-\omega)m_{x_1x_1,I}^{(2)} + 12}{\omega(1-6u_{x_1}^2) - 3l_1u_{x_1}(1+\omega) + 9}.$$
(3.45)

Finally, for the second-order moments, the expressions are given by:

$$\rho m_{x_1 x_1, I}^{(2)} = \frac{3}{2} \rho_I m_{x_1 x_1, I}^{(2)} - \frac{1}{2} l_1 \rho u_{x_1} + \frac{1}{6} \rho, \qquad (3.46)$$

$$\rho m_{x_2 x_2, I}^{(2)} = \frac{4}{33} \rho_I (10 m_{x_2 x_2, I}^{(2)} - m_{x_3 x_3, I}^{(2)}), \qquad (3.47)$$

and

$$\rho m_{x_3 x_3, I}^{(2)} = \frac{4}{33} \rho_I (10 m_{x_3 x_3, I}^{(2)} - m_{x_2 x_2, I}^{(2)}).$$
(3.48)

It can be noted that the second-order moments of Equation 3.47 and Equation 3.48 are similar, due to symmetry.

At last, for the cross-terms,

$$\rho m_{x_1 x_2, I}^{(2)} = 2\rho_I m_{x_1 x_2, I}^{(2)} - \frac{1}{3} l_1 \rho u_{x_2}, \qquad (3.49)$$

$$\rho m_{x_1 x_3, I}^{(2)} = 2\rho_I m_{x_1 x_3, I}^{(2)} - \frac{1}{3} l_1 \rho u_{x_3}, \qquad (3.50)$$

$$\rho m_{x_2 x_3, I}^{(2)} = \rho_I m_{x_2 x_3, I}^{(2)}. \tag{3.51}$$

It can be seen that the second-order moments of Equation 3.49 and Equation 3.50 are similar, due to symmetry.

To clarify the difference between this work from the Hegele et al. (2018) one, we are going to explain how do we have calculated the new 256 different boundary sites in the following subsection.

3.1.6 New Boundary Sites

As we showed above, Hegele et al. (2018) presented 12 edges, 8 corners and 6 faces, which give 26 different boundaries. But, in order to improve their work and define boundary sites that could deal with more general cases, we found 256 different boundaries. The lattices take role as fluid or solid, and our velocity sets are established from 8 normal vectors: {(-1, -1, -1), (-1, -1, 1), (-1, 1, 1), (1, -1, -1), (1, -1, 1), (1, 1, -1), (1, 1, 1)}. By that, we go for $2^8 = 256$.

To determine the new boundary sites, initially, the zeroth- and first-order moments were established. After calculating the Hermite polynomials, it was consequently possible to found the non- and regularized second-order moments.

Further, to observe which of these velocities sites were belonging to a certain boundary, it was necessary to associate each cubic normal vector, as showed above, to direction sets (direction list). For example, the (-1, -1, -1) relates every associated direction that evolves both numbers -1 and 0, but not the number 1.

With this, it was possible to value the velocity sites attached to the new boundary sites, where 7 velocity sites were present in 8 boundaries, 10 velocity sites in 12 boundary sites, 12 velocity sites in 12 boundary sites, 13 velocity sites in 28 boundary sites, 14 velocity sites in 6 boundary sites, 15 velocity sites in 24 boundary sites, 16 velocity sites in 40 boundary sites, 17 velocity sites in 54 boundary sites, 18 velocity sites in 36 boundary sites, and the massive 19 velocity sites were present in 35 boundary sites. These determinations give a complex of 255 boundary sites, but of course, we have the totally solid one (which is boundary number 0) and improve to a total of 256 boundary sites. The boundary number 255 corresponds to the total fluid one.

To elucidate, if we get, for example, cubic $\{(-1, -1, -1), (-1, 1, -1), (1, -1, -1)\}$, following the order presented in the beginning of this subsection, we have $2^0 + 2^2 + 2^4 = 21$, which is corresponding to the boundary site number 21, as we see in Figure 12.

Figure 12 – Region plot of the boundary site number 21. Yellow corresponds to the fluid, and white to the solid.



Source: Elaborated by the author (2021).

The determination of these 256 boundary sites is a decisive improvement on the work of Hegele et al. (2018). This is because the authors only deal with faces, edges, and corners, which are also took into account in the present work.

Still, taking cubic $\{(-1, -1, -1), (-1, -1, 1), (-1, 1, -1), (1, 1, -1)\}$, we have $2^0 + 2^1 + 2^2 + 2^6 = 71$, corresponding to the boundary site number 71, as follows Figure 13.

On the other hand, with cubic $\{(-1, -1, 1), (1, 1, 1)\}$, we have $2^1 + 2^7 = 130$, corresponding to the boundary site number 130. Figure 14 illustrates this boundary.



Figure 13 – Region plot of the boundary site number 71. Yellow corresponds to the fluid, and white to the solid.

Source: Elaborated by the author (2021).

Figure 14 – Region plot of the boundary site number 130. Yellow corresponds to the fluid, and white to the solid.



Source: Elaborated by the author (2021).

Finally, with cubic {(-1, -1, -1), (-1, -1, 1), (1, -1, 1), (1, 1, -1), (1, 1, 1)}, the expression $2^0 + 2^1 + 2^5 + 2^6 + 2^7 = 227$ leads to the boundary site number 227, as shows Figure 15.

Figure 15 – Region plot of the boundary site number 227. Yellow corresponds to the fluid, and white to the solid.



Source: Elaborated by the author (2021).

Expressing these new boundary sites in general and explicit equations is tough and complex work, especially because there are too many different terms and boundaries themselves. So, for objectivity, we chose to do not to write them here.

3.2 BOUNDARY AND INITIAL CONDITIONS

As well as other CFD methods, LBM calls for proper boundary and initial conditions to be specified to solve the considering problem, determining the existence and uniqueness of the solution. On the other hand, from a physical standpoint, although a general theoretical framework to model fluid flows relies on the same set of the equation, i.e., the NSEs, the formulation of the physical problem remains incomplete as the NSEs by themselves have no information about the particular flow one. This information is contained in the boundary and initial conditions (KRÜGER et al., 2017).

We can see a typical cycle of the LBM algorithm in Figure 16, which expresses the importance of boundaries consideration in the implementation, even though they are applied to a small portion of the fluid domain. Compared to other traditional numerical methods, LBM presents a difficult task to define the correct boundaries because the degrees of freedom in the system of mesoscopic variables (more populations f_i) are higher than the macroscopic ones (moments).

Figure 16 – Overview of a typical cycle of the LBM algorithm, where the initial conditions are intrinsically considered in the initialization.



Source: Krüger et al. (2017).

Krüger et al. (2017) bring that LBM presents two groups which the discretizations of the boundary conditions belong, despite having considerable methods to define boundaries:

- Link-wise: boundary lies on *lattice links;*
- Wet-node: boundary is located on *lattice nodes*.

The link-wise shifts the boundary nodes from a physical boundary approximately midway between the solid and the boundary nodes (the exact boundary location is not fixed). It has the advantage that having the lattice nodes located at the center of the computational cells, its surface will coincide with the borders of the physical domain. By contrast, wet-node lies on the physical boundary, having the vertices set in the computational cells to ensure it will coincide with the borders of the physical domain (KRÜGER et al., 2017). Figure 17 shows these two different schemes at the same domain. But, in this work, we consider the regularization process for the boundaries, as explained in subsection 3.1.2.

Nonetheless, the complexity of boundary conditions in a 3D simulation consists specifically in the numerical implementation rather than the mathematical concept. This is because the 3D lattice contains lots of discrete velocity vectors more than 2D ones (more unknown population). We can observe these differences more clearly in the Table 4:

Table 4 – U	4 – Unknown populations in different lattices and boundary configurations.							
	Configuration	D2Q9	D3Q15	D3Q19	D3Q27			
	Face	-	5	5	9			
	Edge (concave)	3	8	9	15			
	Corner (concave)	5	10	12	17			

Source: Adapted from Krüger et al. (2017).

According to Krüger et al. (2017), the two techniques presented above are not equally simple to extend to 3D:





Source: Krüger et al. (2017).

- Link-wise: specify the missing populations based on simple reflection rules (naturally extend to 3D);
- Wet-node: based on specific rules incorporating the consistency with bulk dynamics, and also often modify just the unknown boundary populations (non-trivial extension to 3D). Formulations that replace all populations are simpler to implement in 3D.

Finally, dealing with initial conditions requires a general step, called initialization (as we can see in Figure 16). The initial conditions are set by the physics of the problems (time-dependent), and the initialization is required even in steady problems (part of the numerical procedure, regardless of the time-dependence). No matter what about the simulation using LBM is, we have the following categories which it occurs (KRÜGER et al., 2017):

- **Steady flows:** LBM is generally not well suited for a steady problem, taking a larger number of iteration steps compared to methods tailored for steady problems. All unphysical transients caused by the initial state decay after some time;
- Unsteady flows after long times: LBM deals very well in unsteady problems like suspension flows, flow instabilities, or fluid mixing. The statistical long-time behavior of such systems is usually independent of the initial state;
- **Time-periodic flows:** Fully converged time-periodic flows do not depend on the details of initialization, but it can take a long time until undesired transients have decayed. Womersley flow is an example of time-periodic flow;
- **Initialization-sensitive flows:** In some situations, the entire simulation depends on the initial state, where any error in this one can propagate in time and detrimentally affect the accuracy of the entire simulation.

Last, the implementation of the algorithm consists of starting the simulation with the initialization followed by collision, as the way the Boltzmann equation is discretized. The equilibrium distribution, which is used for collision, is calculated using the known velocity and pressure fields, then the streaming is performed. Still, the equilibrium and non-equilibrium parts of the populations after initialization assume a state compatible with the state after streaming, but before the collision.

3.3 FORCES

Forces are an important factor in many hydrodynamic problems, which comprehends mostly as force density instead of forces. They can be obtained with the integral operator at surface stresses or bulk force densities. Gravitational acceleration g, for example, can be related into a force density F_g , such as $F_g = \rho g$. When two fluids with different densities are mixed or the temperature in a fluid is non-homogeneous, density gradients in the gravitational field lead to buoyancy effects and phenomena like the Rayleigh-Bénard instability (convection patterns develop when warmed fluid rises from a hot surface and falls after cooling) or Rayleigh-Taylor instability (layer of denser fluid descends as lower-density fluid below it rises) (KRÜGER et al., 2017).

We can also evaluate forces in a rotating fluid, charged or magnetic particles immersed in a fluid, driving mechanisms of the pressure gradient field (in incompressible fluids). Especially working with LBM, forces are treated, in general, as presents Figure 18. With a BGK collision operator, we determine the force density F for the time step; compute the fluid density and velocity as:

$$\rho = \sum_{i} f_{i}, \boldsymbol{u} = \frac{1}{\rho} \sum_{i} f_{i} \boldsymbol{c}_{i} + \frac{\boldsymbol{F} \Delta t}{2\rho}; \qquad (3.52)$$

and posteriorly the equilibrium populations to obtain the collision operator:

$$\Omega_i = \frac{1}{\tau} \left(f_i - f_i^{eq} \right); \tag{3.53}$$

iterate the source term:

$$S_{i} = \left(1 - \frac{\Delta t}{2\tau}\right) w_{i} \left(\frac{c_{i\alpha}}{c_{s}^{2}} + \frac{(c_{i\alpha}c_{i\beta} - c_{s}^{2}\delta_{\alpha\beta})u_{\beta}}{c_{s}^{4}}\right) F_{\alpha}, \qquad (3.54)$$

where source S_i and forcing F_i terms are related as $S_i = \left(1 - \frac{1}{2\tau}\right)F_i$; apply collision and source to get the post-collision particle distribution:

$$f^{\star} = f_i + (\Omega_i + S_i)\Delta t; \qquad (3.55)$$

propagate them; and place a new time step.

It is important to point that F depends on the physics and is not given by the LB algorithm itself. Still, the velocity u enters the equilibrium distributions and is also the macroscopic fluid

Figure 18 – Overview of a typical cycle of the LBM algorithm, considering forces but not boundary conditions.



Source: Krüger et al. (2017).

velocity (can be interpreted as average velocity in the time step). For this relation, we explore the discretization in velocity space and space and time one, respectively, in the following subsections, considering the force schemes as Guo, Zheng, and Shi (2002) proposed above (also Hermite expansion). They analyzed the lattice effects attached to the presence of a force, especially pointing that the considerations they had in their study removed undesired derivatives in the continuity and momentum equation due to time discretization artifacts.

3.3.1 Forcing terms representation

As we apply the forcing term to the LBE, we get the new modified particle distribution function $\overline{f}_i(\mathbf{r}, t)$ as:

$$\overline{f}_{i}(\boldsymbol{r}+\boldsymbol{c}_{i},t+1) = \overline{f}_{i}(\boldsymbol{r},t) + \omega_{LB} \left(f_{i}^{(eq)}(\boldsymbol{r},t) - \overline{f}_{i}(\boldsymbol{r},t) \right) + \left(1 - \frac{\omega_{LB}}{2} \right) F_{i}(\boldsymbol{r},t), \quad (3.56)$$

where $\omega_{LB} = 1/\overline{\tau}$ is the modified collision frequency, and $\overline{\tau} = \tau + A$ is the modified relaxation time (A = 0.5 is a model dependent parameter).

Also, we can express the F_i term as:

$$F_{i} = w_{i} \left(a_{s}^{2} F_{\alpha} c_{i\alpha} + a_{s}^{4} F_{\alpha} u_{\beta} \mathcal{H}_{\alpha\beta,i}^{(2)} \right), \qquad (3.57)$$

where we can rewrite $F_{\alpha}u_{\beta}$ as sum of its symmetric and anti-symmetric counterparts since it contracts with the symmetric tensor $\mathscr{H}^{(2)}_{\alpha\beta,i}$:

$$F_{\alpha}u_{\beta}\mathcal{H}^{(2)}_{\alpha\beta,i} = \left(\frac{1}{2}(F_{\alpha}u_{\beta} + F_{\beta}u_{\alpha}) + \frac{1}{2}(F_{\alpha}u_{\beta} - F_{\beta}u_{\alpha})\right)\mathcal{H}^{(2)}_{\alpha\beta,i} = \frac{1}{2}(F_{\alpha}u_{\beta} + F_{\beta}u_{\alpha})\mathcal{H}^{(2)}_{\alpha\beta,i}, \quad (3.58)$$

then F_i goes by:

$$F_{i} = w_{i} \left(a_{s}^{2} F_{\alpha} c_{i\alpha} + \frac{1}{2} a_{s}^{4} (F_{\alpha} u_{\beta} + F_{\beta} u_{\alpha}) \mathscr{H}_{\alpha\beta,i}^{(2)} \right).$$
(3.59)

Consequently, we have new moments for the \overline{f}_i parameter, which are:

$$\rho(\mathbf{r},t) = \sum_{i} \overline{f}_{i} \rho(\mathbf{r},t), \qquad (3.60)$$

$$\rho(\mathbf{r},t)\overline{u}_{\alpha}(\mathbf{r},t) = \sum_{i} \overline{f}_{i}(\mathbf{r},t)c_{i\alpha},$$
(3.61)

and

$$\rho(\mathbf{r},t)\overline{m}_{\alpha\beta}^{(2)}(\mathbf{r},t) = \sum_{i} \overline{f}_{i}(\mathbf{r},t)\mathscr{H}_{\alpha\beta,i}^{(2)}.$$
(3.62)

To make it clear, we must show that the hydrodynamical velocity is expressed as:

$$u_{\alpha} = \overline{u}_{\alpha} + \frac{1}{2\rho} F_{\alpha}. \tag{3.63}$$

After this, we can also apply the regularization procedure to the modified distribution function with the forcing term, denoted as $\hat{f}_i(\mathbf{r}, t)$. So:

$$\widehat{\overline{f}}_{i}(\boldsymbol{r},t) = \rho w_{i} \left(1 + a_{s}^{2} \overline{u}_{\alpha} c_{i\alpha} + \frac{1}{2} a_{s}^{4} \overline{m}_{\alpha\beta}^{(2)} \mathscr{H}_{\alpha\beta,i}^{(2)} \right),$$
(3.64)

and Equation 3.56 goes by:

$$\overline{f}_{i}(\boldsymbol{r}+\boldsymbol{c}_{i},t+1) = (1-\omega_{LB})\widehat{\overline{f}}_{i}(\boldsymbol{r},t) + \omega_{LB}f_{i}^{(eq)}(\boldsymbol{r},t) + \left(1-\frac{\omega_{LB}}{2}\right)F_{i}(\boldsymbol{r},t), \quad (3.65)$$

or

$$\overline{f}_{i}^{\prime} = (1 - \omega_{LB})\widehat{\overline{f}}_{i} + \omega_{LB}f_{i}^{(eq)} + \left(1 - \frac{\omega_{LB}}{2}\right)F_{i}.$$
(3.66)

Following the short form in Equation 3.66, we explicitly write the three moments. The zeroth-order moment is:

$$\rho' = \sum_{i} \overline{f}'_{i} = \rho, \qquad (3.67)$$

the first-order moment:

$$\rho' u'_{\alpha} = \sum_{i} \overline{f}'_{i} c_{i\alpha} = (1 - \omega_{LB}) \rho \overline{u}_{\alpha} + \omega_{LB} \rho u_{\alpha} + \left(1 - \frac{\omega_{LB}}{2}\right) F_{\alpha}, \qquad (3.68)$$

where:

$$\rho \overline{u}_{\alpha} = \rho u_{\alpha} - \frac{F_{\alpha}}{2}, \qquad (3.69)$$

also, ρu_{α} is the hydrodynamical used for the equilibrium distribution, and the one used for streaming:

$$\rho' u'_{\alpha} = \rho u_{\alpha} + \frac{F_{\alpha}}{2}, \qquad (3.70)$$

then

$$\rho' u'_{\alpha} = \rho \overline{u}_{\alpha} + F_{\alpha}, \qquad (3.71)$$

and for the second-order moment:

$$\rho'\overline{m}_{\alpha\beta}^{(2)'} = \sum_{i} \overline{f}_{i}'(\boldsymbol{r},t) \mathscr{H}_{\alpha\beta,i}^{(2)} = (1-\omega_{LB})\rho\overline{m}_{\alpha\beta}^{(2)} + \omega_{LB}\rho u_{\alpha}u_{\beta} + \left(1-\frac{\omega_{LB}}{2}\right)(F_{\alpha}u_{\beta} + F_{\beta}u_{\alpha}). \quad (3.72)$$

3.3.2 General Observations

In a general form, based on second-order velocity and space-time discretizations, we can express LBE as:

$$f_i(\boldsymbol{x} + \boldsymbol{c}_i \Delta t, t + \Delta t) - f_i(\boldsymbol{x}, t) = [\Omega_i(\boldsymbol{x}, t) + S_i(\boldsymbol{x}, t)]\Delta t, \qquad (3.73)$$

often called Guo forcing. The fluid velocity in the presence of a force must be redefined to guarantee the second-order space-time accuracy:

$$\boldsymbol{u} = \frac{1}{\rho} \sum_{i} f_i \boldsymbol{c}_i + \frac{\boldsymbol{F} \Delta t}{2t}.$$
(3.74)

As the Equation (3.74) enters the equilibrium distribution $f_i^{eq} = f_i^{eq}(\rho, \boldsymbol{u})$ and therefore the BGK collision operator $\Omega_i = -(f_i - f_i^{eq})/\tau$, we can say that the fluid velocity in and the equilibrium velocity \boldsymbol{u}^{eq} are equivalent to Guo forcing. It is possible to generalise the forcing method as:

$$\boldsymbol{u}^{eq} = \frac{1}{\rho} \sum_{i} f_i \boldsymbol{c}_i + A \frac{\boldsymbol{F} \Delta t}{\rho}.$$
(3.75)

If *A* value is deviated, the collision operator is modified, so to maintain the sum $\Omega_i + S_i$ unchanged, S_i also must be modified. In particular, A = 0 would lead to a term $\propto \nabla \cdot F$ in the continuity equation and another term $\propto \nabla \cdot (\boldsymbol{uF} + F\boldsymbol{u})$ in the momentum equation.

3.4 QUANTIFYING ACCURACY FOR THE NUMERICAL SOLUTION

Statistically speaking, a simple procedure to quantify the error of a numerical simulation consists in comparing it with a know analytical solution or even other simulation that is dealing with the same problem, in a different mesh, for example. One of this procedures is the L_2 error norm, that consists on comparing the analytically (or other simulation) known quantity $q_a(\mathbf{x}, t)$, which is generally a function of space and time, and the numerical simulation you implemented $q_n(\mathbf{x}, t)$, given as:

$$\epsilon_q(t) = \sqrt{\frac{\sum_x (q_n(\boldsymbol{x}, t) - q_a(\boldsymbol{x}, t))^2}{\sum_x q_a^2(\boldsymbol{x}, t)}}.$$
(3.76)

The sum runs over the entire spatial domain where q is defined, and L_2 error is sensitive to any deviation from q_a . It can also be used as a criterion for convergence to steady flows. As close as the L_2 error is to zero, means that both qs are accurate.

4 RESULTS AND DISCUSSIONS

In this chapter, we present the results of the simulations to evaluate and discuss the flow inside an annulus using the LBM. We focused on validating our boundary conditions to the proposed domain and compared them with some early works that also studied the problem.

We start discussing our results with forces. So, we have implemented it in a flow between parallel plates with a pure Poiseuille flow to compare results to the analytical solutions of velocity and volume rate of flow, according to Equation 2.11 and Equation 2.13 (WHITE, 2006), respectively. We have fixed both $F_{g_z} = 1 \times 10^{-7}$ and $\tau = 0.8$. Also, we define 2h = D. The stopping criteria for all the simulations are always based on the observation of kinetic energy behavior. In the first comparison, we noted that at the time step 250,000 with D = 200, the simulation had already reached the steady-state, as follows Figure 19.



Figure 19 – The kinetic energy of a flow between parallel plates with D = 200.

Source: Elaborated by the author (2021).

The velocity plot is illustrated in Figure 20, where the numerical solution presents to be a little smaller than the analytical one. Still, the chosen F_{g_z} is considerably lower than the one set by Krüger et al. (2017, p. 255), this because the select parameter was the best fit in this problem simulations. The calculated total volume rate of the numerical solution is $Q_{num} = 0.6567$ and analytical $Q_{ana} = 0.6667$.



Figure 20 – Velocity flow between parallel plates with D = 200.

Source: Elaborated by the author (2021).

The second geometry have reached the steady state at time step 1,000,000, which can be observed in Figure 21.

Figure 21 – The kinetic energy of a flow between parallel plates with D = 400.



In Figure 22, on the other hand, numerical velocity is closer to the analytical one. It

is possible to note that the maximum velocity is four times higher than the one shown with the D = 200 grid, doubling the mesh. The numerical total volume rate is $Q_{num} = 5.2943$ and analytical $Q_{ana} = 5.3333$.



Figure 22 – Velocity flow between parallel plates with D = 400.

Figure 23 – The kinetic energy of a flow between parallel plates with D = 800.



Source: Elaborated by the author (2021).

The kinetic energy with D = 800, can be seen in Figure 23. The steady state is reached at time step 4,000,000.

Following the earlier idea, Figure 24 indicates an increased velocity, four times higher than the one with D = 400, doubling again, the mesh grid. The valued total volume rate to this numerical solution is $Q_{num} = 42.5348$ and analytical $Q_{ana} = 42.6667$.



Figure 24 – Velocity flow between parallel plates with D = 800.

Source: Elaborated by the author (2021).

With Equation 3.76 we might evaluate the L_2 norm to quantify the error of the numerical simulation. It consists of comparing results with the analytical solution of the flow between parallel plates simulations, where Table 5 presents that with D = 200, $\epsilon_{q_{U_z}}$ is a high result, despite Figure 20 seems to not express such big difference between numerical and analytical solutions, and the ϵ_{q_Q} , on the other hand, explicit a low value. With D = 400, $\epsilon_{q_{U_z}}$ decreases but yet still a high value, and ϵ_{q_Q} also decreases presenting a good parameter. Finally, with D = 800, $\epsilon_{q_{U_z}}$ decreases that the velocity presents reasonable results and the total volume rate seems a better resultant.

2 -			··· • • • • • • • • • • • • • • • •	
	D	$\epsilon_{q_{U_z}}$	ϵ_{q_Q}	
	200	0.1283	0.0149	
	400	0.0880	0.0073	
	800	0.0475	0.0031	
Sou	rce: Elabo	orated by th	e author (2021).	

Table $5 - L_2$ error norm of a flow between parallel plates.

White (2006) have also determined analytical solution of a flow between concentric cylinders, which the velocity is expressed in Equation 2.14 and the volume rate of flow in

Equation 2.15. Using same terms as in the flow between parallel plates, both $F_{g_z} = 1 \times 10^{-7}$ and $\tau = 0.8$ were fixed. To a first comparison, kinetic energy is presented in Figure 25, which have reached the steady state near the time step 4,000 with D = 25.



Figure 25 – Annulus flow: kinetic energy with D = 25.

Source: Elaborated by the author (2021).



Figure 26 – Annulus flow: velocity with D = 25.

Source: Elaborated by the author (2021).

The numerical solution presented a lower velocity than the analytical one, as we can see in Figure 26. The narrow geometry is our first consideration to justify that results are away

between both solutions. Once LBM works with Cartesian coordinates, the velocity faces lattice corners impediment to enabling the fluid flow with the streaming and collision of particles. The total volume rate of the numerical solution is $Q_{num} = 0.2501$ and analytical $Q_{ana} = 0.2769$.





Source: Elaborated by the author (2021).



Figure 28 - Annulus flow: velocity with D = 50.

Source: Elaborated by the author (2021).

Doubling the mesh, another grid was implemented. The kinetic energy with a gap D = 50 is plotted in Figure 27. The steady-state is reached about the 16,000 time step. Numerical

solution with D = 50 presented to be closer to the analytical one, when compared with D = 25, but still with reasonable results. Figure 28 The valued total volume rate of the numerical solution is $Q_{num} = 4.4675$ and analytical $Q_{ana} = 4.6854$.

The last simulation, which we have implemented using forces, takes a gap with D = 100, where the kinetic energy is observed in Figure 29 reaching state steady near of time step 65,000.



Figure 29 – Annulus flow: kinetic energy with D = 100.

Source: Elaborated by the author (2021).



Figure 30 - Annulus flow: velocity with D = 100.

Source: Elaborated by the author (2021).

The velocity is now better placed and closer in the numerical solution to the analytical one. As a consequence, the total volume rate of the numerical solution is $Q_{num} = 75.2504$ and analytical $Q_{ana} = 77.0462$.

To measure how close the numerical solution is to the analytical one, Table 6 shows the L_2 norm. With D = 25, it is clear that the geometry was too tight, leading to a high value of error. ϵ_{q_Q} presented better results, but still greater than expected. As the mesh doubled, little improvement was observed for the velocity and total volume rate, where $\epsilon_{q_{U_z}}$ and ϵ_{q_Q} to the gap with D = 50 seems lower. Last, with D = 100, the L_2 norm of velocity and total volume rate still decreasing when compared to the first two simulations.

Table $6 - L_2$ error norm of a flow in an annulus, using forces.

	D	$\epsilon_{q_{U_z}}$	ϵ_{q_Q}				
-	25	0.1861	0.0971				
	50	0.1466	0.0465				
	100	0.1037	0.0233				
ura Eleborated by the author (20)							

Source: Elaborated by the author (2021).

After presenting and discussing the results using forces in the modeling, we are now going to evaluate the flow between concentric cylinders, with the inner pipe rotating. At first, a bi-dimensional annulus flow with fixed Re = 10 for a constant $\eta = \frac{5}{7}$ was implemented. The first analysis consists on comparing the numerical solution with the analytical one, following Equation 2.9 and Equation 2.10 presented by Mohammadipour, Succi, and Niazmand (2018).

Figure 31 – Kinetic energy of a bi-dimensional annulus flow at Re = 10.



Source: Elaborated by the author (2021).

To start the comparison, we can check Figure 31 to observe the kinetic energy behavior. We have implemented four different geometries varying the gap D but maintaining η fixed. For all four simulations, the kinetic energy behaves with close results. Close to the time step 20,000, all four simulations have already reached a steady state.

As we are especially interested in the *Re* number, a good parameter to evaluate is the tangential velocity u_{θ} . In Figure 32, the normalized tangential velocity for both numerical and analytical solutions *versus* the dimensionless radial distance R^* are plotted. In general, they kept a very close and straight profile all along the annulus grid, which seems to be an assertive implementation. And of course, it is getting better and accurate as *D* increases, with D = 200 not so easily discern for both solutions, presenting to be a good match.



Figure 32 – Normalized tangential velocity at Re = 10.

Source: Elaborated by the author (2021).

It is possible to remark a grid view of the tangential velocity for different *D*, as follow Figure 33. For all the four simulations, the maximum velocity is different from each other, where we believe that the geometry impacts significantly on the implementations. Another point is that, just with D = 25 we obtained the expected velocity pipe imposed at R_1 , which is $u_{pipe} = \text{Ma} * c_s$. So, possibly an option that might be considered to improve the results is to implement tangential tensor derivatives equal to zero at the inner cylinder.



Figure 33 – Grids of a bi-dimensional annulus flow at Re = 10.

Source: Elaborated by the author (2021).

Nevertheless, pressure is also an important parameter to be evaluated, once the drilling mud and the wellbore are directly affected by it. For the pressure, we can observe the comparison between numerical and analytical solutions in Figure 34.

With D = 25, the numerical solution presents five points that are discrepant from the whole profile of the analytical one. Once more the tangential tensor derivatives equal to zero at the inner cylinder would bring better results. Another point is that the pressure depends on ρ , as presented in Equation 3.3. Despite that ρ is constant, the pressure is not, but it varies just a little bit. Following this idea and because of that, the pressure accumulates for some points in the annulus.

As *D* increases, fewer discrepant points appear, as D = 50 shows three of them, D = 100 presents two, and with D = 200 geometry, we do not observe this situation. We obtain better results for the numerical solution once it gets very close to the analytical one.

In addition, in order to compare L_2 error norm, Table 7 potentially presents particularities for the tangential velocity and pressure. For the tangential velocity, lower L_2 norm results appear, as the gap *D* increases. Although the values with D = 25 and D = 50 are high, with D = 100 and D = 200 the $\epsilon_{q_{u_a}}$ values are good results.

On the other hand, the L_2 norm of pressure ϵ_{q_p} behaves with distinct results, despite some discrepant points presented before. As mentioned, even with pressure depending on ρ , it varies a little bit, so ϵ_{q_p} for all the four gaps were perfectly low, decreasing significantly, as *D* increases. Notwithstanding that some results were a step aside from accurate, in a general view, we assume that boundary conditions worked perfectly.



Figure 34 - Pressure at Re = 10.

Source: Elaborated by the author (2021).

D	$\epsilon_{q_{u_{ heta}}}$	ϵ_{q_p}
25	0.0365	1.0218×10^{-4}
50	0.0326	4.6202×10^{-5}
100	6.8010×10^{-3}	3.1985×10^{-5}
200	5.2552×10^{-3}	1.2961×10^{-5}

Table 7 – L_2 error norm of different gaps at Re = 10.

Source: Elaborated by the author (2021).

As discussed in Chapter 2, Taylor-Couette presents particularities that can lead us to understand and take essential considerations to the flow of the drilling mud inside an annulus. As we see that the new fluid conditions are dealing well with the problem, we have implemented simulations to compare it with Ostilla et al. (2013).

To evaluate velocity, we define $\langle \overline{\omega} \rangle_z = \frac{u_{\theta}}{r}$ as the *z*-averaged angular velocity where u_{θ} is the tangential velocity and *r* the radial coordinate. $\widetilde{r} = \frac{(r-R_1)}{(R_2-R_1)}$ is the normalized radius.

For the simulations, we have considered the same parameters as Ostilla et al. (2013), where the aspect ratio is $\Gamma = 2\pi$, radius ratio $\eta = 5/7$ and gap D = 20. The bottom and top of the cylinder is closed in our implementations, instead of Ostilla et al. (2013) apply periodic boundary conditions. It is crucial to say that we sought for comparing more Ta numbers, but the two lower ones did not present rolls, and the other three greater were too turbulent for the geometry used, so we have not taken consistent results. Another point is that, at first moments, we have simulated both cylinders with periodic boundary conditions to different Ta numbers but all of them would not present any rolls, justifying our chosen closed cylinders implementations.

In Figure 35, kinetic energy is plotted in order to establish stopping criteria at a $Ta = 2.44 \times 10^5$ simulation. It looks like at time step 80,000 had reached the steady state.



Figure 35 – Kinetic energy at $Ta = 2.44 \times 10^5$.

Source: Elaborated by the author (2021).

With a flow at $Ta = 2.44 \times 10^5$, Figure 36 shows that data presents a profile different than the Ostilla et al. (2013). Near both R_1 and R_2 , $\langle \overline{\omega} \rangle_z$ vary less as increases \tilde{r} , while Ostilla et al. (2013) with periodic boundary conditions vary a lot in a descending way for the $\langle \overline{\omega} \rangle_z$ as \tilde{r} increases. On the other hand, in the middle of the flow in the current gap, $\langle \overline{\omega} \rangle_z$ presents a profile similar to the one in Ostilla et al. (2013).



Figure 36 - z-averaged angular velocity at $Ta = 2.44 \times 10^5$.

Source: Elaborated by the author (2021).

We can assure that Taylor-Couette flow governs this implementation, checking Figure 37. It is possible to observe that three rolls (pairs of toroidal vortices) comprehended this respective simulation. This way, we confirm what was explained in section 2.2.1 especially by Di Prima and Swinney (1985), Wereley and Lueptow (1998) and Lueptow (2009).



Figure 37 – Streamlines at time step 100,000 at $Ta = 2.44 \times 10^5$.

Source: Elaborated by the author (2021).

The second comparison, with kinetic energy plotted, is shown in Figure 38, where also near time step 80,000, steady-state has been reached. Figure 39 contrast the z-averaged angular

z x y velocity following the same behavior to what was presented in Figure 36. But, even though it can be seen that is this respective $Ta = 7.04 \times 10^5$, this work presents results farther than the Ostilla et al. (2013), clearly because of Ta number is greater than the first simulation.



Figure 38 – Kinetic energy at $Ta = 7.04 \times 10^5$.

Source: Elaborated by the author (2021).

Figure 39 - z-averaged angular velocity at $Ta = 7.04 \times 10^5$.



Source: Elaborated by the author (2021).

Streamlines at the $Ta = 7.04 \times 10^5$ simulation can be seen in Figure 40. Again, three rolls are illustrated, maintaining coherence with theoretical and experimental previous studies. We must also highlight the velocity magnitude, which is greater in this respective Ta number, once the flow is expected to be more unstable, whereas the gap is fixed.



Figure 40 – Streamlines at time step 100,000 at $Ta = 7.04 \times 10^5$.

Source: Elaborated by the author (2021).

In Table 2, it is possible to be noted that the critical Ta number for this implemented η is a little less than $Ta_{crit} \approx 2.7 \times 10^3$. So, theoretically, the simulations with periodic boundary conditions would present rolls. But, in our simulations, we did not reach it. To complement, it is important to say that we have simulated combined rotating inner cylinder and use of forces in many different study cases but in all of them, the modeling did not present stable results of the Taylor-Couette flow.

From what was showed in Figure 37 and Figure 40, it is possible to calculate the wavelength λ , since we have the critical wavenumber k_{crit} from Table 2. Once our $\eta = 5/7 = 0.71$, we took $\eta = 0.70$ as an approximation. Table 8 exhibits the values of λ , remembering that, as Lueptow (2009) states, it assumes $\lambda \approx 2D$, matching values as planned.

Table 6 Wavelengur / for the respective 7 a numbers.							
Ta	Calculated	Lueptow (2009)	This Work				
2.44×10^{5}	40.05	42	42				
7.04×10^{5}	40.05	42	42				
Source: Elaborated by the author (2021)							

Table 8 – Wavelength λ for the respective Ta numbers.

Source: Elaborated by the author (2021).

It is possible to remark in Figure 41 a longitudinal slice comparison between the two Ta number implementations, reinforcing what we discussed above, where rolls have resulted for both simulations. Figure 41 **a**) shows that the three rolls, and more specifically the pair of toroidal vortices, are well distinct from each other. Figure 41 **b**) also present well distinct rolls, but near the two closed lids, the toroidal profiles are more unstable than in the first case.



Figure 41 – Longitudinal slices of Taylor-Couette flow for different *Ta* numbers.

Source: Elaborated by the author (2021).

5 CONCLUSIONS

Even with years of studies about the flow between concentric cylinders, it was possible to understand and verify the complex modeling necessary to implement and simulate this type of flow. Further, once the lattice Boltzmann method does not work directly with the cylindrical coordinates, this adds a new difficulty to one already complex problem. one more difficult step to deal with. But, the results obtained in this proposed work were good, using the referenced methodology as a computational solution method to implement the flow inside an annulus to observe its behavior.

The first and principal objective proposed to this work was reached, once results and extensive discussions about the flow between concentric annulus were presented. Also, a literature review and theoretical foundation helped to understand what we were modeling and would face.

Based on Hegele et al. (2018), we successfully have determined new 256 boundary sites, improving coverage to general and complex cases in which the previous study could not implement robust modeling. The use of 8 cubic normal vectors facilitates understanding how the boundary conditions could be determined, and some examples of them were presented in the respective subsection.

The forcing terms simulations were resolved to a pure Poiseuille flow between parallel plates and an annulus, and compared to the analytical solutions by White (2006), fixing for both cases $F_{g_z} = 1 \times 10^{-7}$ and $\tau = 0.8$. The flow between parallel plates was implemented in large gaps, once did not require much computational resource. L_2 norms for $\epsilon_{q_{U_z}}$ decreased for the velocity while *D* increased, as well as ϵ_{q_Q} showed good results for the total volume rate.

Conversely, the modeling with forces for the comparison of an annulus flow required more computational resources, so we had to implement thinner meshes than the one used in the parallel plates. But, L_2 norm $\epsilon_{q_{U_z}}$ decreased as expected for the velocity while *D* increased, as well as ϵ_{q_Q} for the total volume rate.

Comparisons with the analytical solution of Mohammadipour, Succi, and Niazmand (2018) for a bi-dimensional flow at Re = 10 with the inner cylinder rotating, clarify the application of boundaries, with tangential velocity reaching close profile for numerical and analytical solutions. It can be noted that, while the gap was getting higher, the tangential velocity decreased as expected. The pressure parameter evidences that implementing tangential tensors derivatives equal to zero at the inner cylinder would bring better results.

As introduced and discussed by Di Prima and Swinney (1985), Wereley and Lueptow (1998) and Lueptow (2009), instability begins to appear as the rotational speed of the inner cylinder increases. Results at $Ta = 2.44 \times 10^5$ and $Ta = 7.04 \times 10^5$ show rolls formation in our work, having agreement with the previous works. Also, *z*-averaged angular velocity near both R_1 and R_2 , vary less as increases \tilde{r} , while Ostilla et al. (2013) with periodic boundary conditions vary a lot in a descending way as \tilde{r} increases for the two implemented Ta numbers. But, in the middle of the flow, *z*-averaged angular velocity presents a profile similar to the Ostilla et al.

(2013) one.

It was not possible to evaluate the transitional flow, as firstly desired. This because, as we already discussed, computational limitations and modeling improvement were required. So, this is a suggestion for future works. Also, another crucial parameter to be evaluated is the temperature, once it is a fundamental part of understanding the behavior of the flow inside the annulus.

Another suggestion for future works is to implement the modeling considering the presence of cuttings mixed with the drilling mud. As explained at the beginning of this study, despite it is robust and complex, that is how Drilling Engineering faces daily in exploration and production of the petroleum industry.
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