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LATTICE BOLTZMANN METHOD IN NON-INERTIAL REFERENCE FRAME

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Abstract. *This works aims at studying the fluid flow motion in non-inertial reference frames. That is comparable to the study of flows inside Lab-on-a-CD microfluidic devices. The numerical analysis is performed through the use of the lattice Boltzmann method. Since non-inertial effects can be accounted for by including a body force term in the dynamical evolution equations, the first part of this works aims at finding a correct expression for such body force model so that the macroscopic equations are correctly reproduced in the asymptotic limit. This was performed by using the Chapman-Enskog analysis. The theoretical results obtained showed that: First, the body force model typically accepted as the correct one in the lattice Boltzmann method is in fact inaccurate when steady-state hydrodynamic problems are solved, and; Second, there is no body force model that correctly models steady and unsteady-state flow phenomena. The body force model in the lattice Boltzmann equations must always consider the time-dependency of the hydrodynamic equations to be solved. Based on this result the lattice Boltzmann equations are written in a non-inertial reference frame and solved for two constructed flow examples: a steady fully developed centrifugal flow and a steady periodic Coriolis flow. In both cases the results obtained were physically meaningful, revealing the applicability of using the lattice Boltzmann method to simulate non-inertial hydrodynamic problems. Furthermore, it was verified that, even for low Reynolds number, the use of a rotational microfluidic platform can be advantageous as the Coriolis acceleration term induces transverse convection streams that allow for the increase of the, typically, slow flow mixing rates*

1 INTRODUCTION

There is currently a great interest in combining into small, integrated units the functional components that are necessary for performing complex chemical and biochemical analyses. These integrated units have been described as microscale total analysis systems (µTAS) or laboratories-on-a-chip [1,2]. According to [2] these systems have the potential to be of great importance in genomics, drug screening and clinical applications. Microfluidics, i.e. the control of flow of small volumes (from fL to mL) of liquids in microscopic (1-1000 µm) channels is the central technology in this field. Microfluidic systems require the design, fabrication and implementation of the appropriate pumps, valves and mixing elements needed to carry out generic manipulations of fluids. There are various technologies for moving small quantities of fluids or suspended particles from reservoirs to mixing and reaction sites, to detectors and eventually to waste or to the next instrument. Methods to accomplish this include syringe and peristaltic pumps, electrochemical bubble generation, acoustics, magnetics, DC and AC electrokinetics, centrifuge, etc. All carry advantages and disadvantages that place them, presently, at an approximately equal footing in terms of their research and development. Nevertheless, the use of a centrifuge approach to create and control the microfluidic flow movement has been advocated as one of the most promising technologies among the others (see [1,2] and the references therein for a thorough discussion on this subject). Platforms that take advantage of a centrifuge pumping mechanism to perform the common microfluidic functions are generally named as a Lab-on-a-CD or a BioCD [1,2]. One of the distinct differences between a Lab-on-a-CD and conventional Lab-on-a-Chips is the non-inertial frame of the spinning disk that causes non-inertial forces such as Coriolis and centrifugal (centripetal) forces. Thus, in order to correctly design the fluidic components in these spinning platforms one needs to have a thorough understanding of the fluid dynamics taking place there.

The continuity and Navier-Stokes equations in a non-inertial reference of frame read as follows:

$$\frac{\partial}{\partial x_\alpha}(u_\alpha) = 0 \tag{1a}$$

$$\frac{\partial}{\partial t}(u_\beta) + u_\alpha \frac{\partial}{\partial x_\alpha}(u_\beta) = -\frac{1}{\rho}\frac{\partial}{\partial x_\beta}(p) + \nu \frac{\partial^2}{\partial x_\alpha \partial x_\alpha}(u_\beta) \underbrace{-\left(e_{\kappa\gamma\beta} 2\Omega_\kappa u_\gamma + e_{\kappa\gamma\beta}\Omega_\kappa e_{\delta\eta\gamma}\Omega_\delta (x_\eta - x_{0\eta})\right)}_{=a_\beta} \tag{1b}$$

where in eq. (1b) $e_{\kappa\gamma\beta}$ represents the Levi-Civita symbol, Ω_κ represents the angular velocity [s^{-1}], $x_\eta - x_{0\eta}$ represents the position of the control volume at x_η relatively to the origin $x_{0\eta}$ [m].

The effect of the non-inertial reference frame in the hydrodynamic equations can be viewed as that of a body force, a_β, added to the momentum balance equations. In particular this non-inertial effect is represented by two distinctive body force terms (per unit mass): a centrifugal term, $(a_\beta)_\omega = -e_{\kappa\gamma\beta}\Omega_\kappa e_{\delta\eta\gamma}\Omega_\delta (x_\eta - x_{0\eta})$, and a Coriolis term, $(a_\beta)_c = -e_{\kappa\gamma\beta} 2\Omega_\kappa u_\gamma$.

In this work the hydrodynamic equations in a non-inertial reference frame, i.e. eqs. (1) and (2), will be solved through lattice Boltzmann (LB) method. The main question that has to be answered before going any further is: How to represent the inclusion of the, previously discussed, body force term in the LB equations?

The LB method is presently a well established numerical technique for fluid mechanics problems [3-12]. In opposition to traditional computational fluid dynamics (CFD) approaches, based on the numerical solution of continuum macroscopic equations, the LB method aims at describing the fluid flow physics from a mesoscopic point of view. This new approach exhibits several advantages making the physical and numerical formulations of the flow modelling a much more straightforward task [3-5]. One of the most referred advantages is the method's ability to simulate quite diverse phenomena by simply including appropriate body force modelling terms into the LB equation. Hence several authors have proposed distinctive general expressions to represent the body force in order to asymptotically recover the hydrodynamic equations [12-29]. A major breakthrough on the study of body force models in LB, with the BGK collision operator, was obtained in the seminal work of Guo et al. [21]. These authors demonstrated that there is only one body force model that unequivocally recovers the macroscopic isothermal and incompressible continuity and Navier-Stokes equations as the asymptotic solution of the lattice Boltzmann BGK equation with a forcing term. Although their analysis is correct, the body force expression derived in their work is limited to time dependent solutions. In fact, to the authors' knowledge, all literature studies have never considered the time-dependency of the hydrodynamic solution as a relevant parameter when expressing the body force term in LB. To clarify this problem the present work aims at showing how the LB body force model should be expressed at both time regimes, allowing thus for the non-inertial effects in eq. (1b) to be correctly reproduced.

This manuscript starts with a brief description of the LB equation with emphasis on D2Q9 model, section 2. Section 3 focuses on the use of the incompressible BGK collision operator and section 4 discusses the main difficulties associated with the inclusion of a body force term in the LB equations. Moreover, the methodology used to express the body force model in this work is also introduced in section 4. In section 5 the different forms the LB body force model must have, depending on the steady or unsteady dependency of the hydrodynamic problem, are derived, through Chapman-Enskog analysis. Based on that result section 6 solves two simplified benchmark flow problems aiming at examining the isolated effect of the centrifugal and the Coriolis acceleration terms in the fluid motion. Finally, in section 7 the conclusions of the present work are withdrawn.

1 THE LATTICE BOLTZMANN EQUATION

Historically, the lattice Boltzmann model was developed from earlier work on lattice-gas (LG) models [3-5]. More recently it was demonstrated that the LB equation can also be formulated from a discrete representation of the continuous Boltzmann equation, [19,20,26]. Using the BGK collision operator [40], the lattice Boltzmann equation with a forcing term can be written as:

$$f_i\left(x_\alpha + e_{i\alpha}\Delta t, t+\Delta t\right) - f_i\left(x_\alpha, t\right) = -\frac{1}{\tau}\left(f_i\left(x_\alpha, t\right) - f_i^{(eq)}\left(x_\alpha, t\right)\right) + \Delta t\, F_i\left(x_\alpha, t\right). \tag{2}$$

It must be stressed that such equation is a particular, but not unique, form of discretising the continuous Boltzmann BGK equation, [30]. The term f_i^{eq} in eq. (2) is the equilibrium single particle distribution function and is obtained from constant temperature and small velocity (up to second order) approximation of the Maxwell-Boltzmann equilibrium distribution function, which is expressed by the following equation:

$$f_i^{(eq)} = w_i \rho \left(1 + \frac{e_{i\alpha} u_\alpha}{c_s^2} + \frac{\left(e_{i\alpha} e_{i\beta} - c_s^2 \delta_{\alpha\beta} \right)}{2 c_s^4} u_\alpha u_\beta \right). \tag{3}$$

In the above equation w_i is a weighting factor with values depending on the chosen lattice geometry so that specific symmetry conditions are respected [3-7] and c_s is the lattice sound speed. For the D2Q9 model employed in this study $w_0 = 4/9$, $w_i = 1/9$ for i = 1, 2, 3, 4 and $w_i = 1/36$ for i = 5, 6, 7, 8. The lattice sound speed is $c_s = \left(1/\sqrt{3}\right) c$ and the particle velocities are defined as $e_{0\alpha} = (0,0)$, $e_{i\alpha} = (\cos[\pi(i-1)/2], \sin[\pi(i-1)/2])\, c$ for i=1, 2, 3, 4 and $e_{i\alpha} = \sqrt{2}(\cos[\pi(i-9/2)/2], \sin[\pi(i-9/2)/2])\, c$ i=5, 6, 7, 8, where $c = \Delta x/\Delta t$. The fluid density, ρ, and velocity, u_α, can be found from the single particle distribution moments as:

$$\rho = \sum_i f_i\,, \tag{4a}$$

$$\rho u_\alpha = \sum_i f_i\, e_{i\alpha} + a F_\alpha \Delta t\,. \tag{4b}$$

The first order moment of the single particle distribution function, eq. (4b), also accounts for the body force presence as first proposed in the works of Ginzburg and Alder [14] and Ladd [15]. This modification over the traditional definition of the first order moment of the single particle distribution function will later be demonstrated to be an important requisite so that the correct hydrodynamic equations with a body force are reproduced. The weighting parameter a is a constant to be determined [21,22].

2 LATTICE BOLTZMANN BGK INCOMPRESSIBLE MODEL

The standard LB model is a pseudo-compressible method used for simulating isothermal incompressible flows, [6,7]. A drawback of this approach is that the recovered macroscopic hydrodynamic equations are not exactly the isothermal and incompressible continuity and Navier-Stokes equations as additional terms referring to density spatial derivatives are also present. It can be demonstrated that these terms scale with the third power of the Mach number, i.e. $O\left(M^3\right)$, and thus can be made negligibly small by simply decreasing the simulation Mach number. However, for a fixed Reynolds number, decreasing the Mach number goes together with the increase in the number of simulation nodes, $N_{\Delta x}$, since $M \propto \tau \,\mathrm{Re}/N_{\Delta x}$. As a result the computational effort of the numerical simulation has to be enlarged in order to reduce the influence of erroneous compressibility terms. To overcome this disadvantage, Zou et al. [31], and later He and Luo [32], proposed the use of a lattice BGK scheme with slightly changes, which allowed for the recovering of the steady-state hydrodynamic equations with no compressibility errors. In this study the incompressible lattice BGK model of He and Luo [32] will be used, which, in practice, comprises the following two changes in the standard lattice BGK model:

$$f_i^{(eq)} = w_i \left(\rho + \rho_0 \left[\frac{e_{i\alpha} u_\alpha}{c_s^2} + \frac{\left(e_{i\alpha} e_{i\beta} - c_s^2 \delta_{\alpha\beta} \right)}{2 c_s^4} u_\alpha u_\beta \right] \right), \tag{5a}$$

$$\rho_0 \, u_\alpha = \sum_i f_i \, e_{i\alpha} + a F_\alpha \Delta t \, . \tag{5b}$$

It must be stressed that due to the small velocity approximation in $f_i^{(eq)}$ the incompressible lattice BGK model is still limited to small Mach numbers. Moreover, for the unsteady-state case it can be demonstrated that the incompressible lattice BGK model does not remove all compressibility errors. In fact, errors of the same order of those present in the standard model are preserved when the macroscopic fields to be solved are time dependent, [33,34].

3 INTRODUCTION OF A BODY FORCE TERM IN THE LATTICE BOLTZMANN EQUATION

Comparing eq. (2) with the continuous BGK Boltzmann equation, i.e. $\left(\partial/\partial t + e_\alpha \, \partial/\partial x_\alpha + F_\alpha \, \partial/\partial p_\alpha\right) f\left(x_\alpha, p_\alpha, t\right) = -1/\tau \left(f\left(x_\alpha, p_\alpha, t\right) - f^{\,eq}\left(x_\alpha, p_\alpha, t\right)\right)$, and considering the fact that the LB formulation takes into account only a small set of constant velocities it is immediate to conclude that the term representing the rate of change of the single particle distribution function along momentum space, i.e. $\partial f / \partial p_\alpha$, cannot be discretised using a formal procedure. Thus, the introduction of the body force term, F_i , in the LB model, eq. (2), requires a different approach. Since the long wavelength limit of the LB equation is sought as solution of the isothermal and incompressible continuity and Navier-Stokes equations, the inclusion of a body force term in the LB equation must comply with this requisite. Moreover, the order of accuracy of the body force term must be consistent with that of the overall numerical scheme. To fulfil these two requirements Ladd and Verberg [11] suggested obtaining the structure of the forcing term by expressing it as a power series expansion in velocity space:

$$F_i = w_i \left[A + \frac{e_{i\alpha} B_\alpha}{c_s^2} + \frac{\left(e_{i\alpha} e_{i\beta} - c_s^2 \delta_{\alpha\beta} \right)}{2 c_s^4} C_{\alpha\beta} \right]. \tag{6}$$

Taking into account the lattice symmetry structure it is straightforward to demonstrate that the first three moments of F_i yield eqs. (7), e.g. [11,21]. The coefficients A, B_α and $C_{\alpha\beta}$ appearing in those equations are functions of the macroscopic body force term F_α and their values are chosen so that the inclusion of eq. (6) into eq. (2) yields correct macroscopic hydrodynamic equations in the asymptotic limit, e.g. [11,21].

$$\sum_i F_i = A \, , \; \sum_i e_{i\alpha} F_i = B_\alpha \text{ and } \sum_i e_{i\alpha} e_{i\beta} F_i = A c_s^2 \, \delta_{\alpha\beta} + \frac{1}{2}\left(C_{\alpha\beta} + C_{\beta\alpha} \right). \tag{7}$$

4 RECOVERY OF THE HYDRODYNAMIC EQUATIONS WITH A FORCING TERM THROUGH CHAPMAN-ENSKOG EXPANSION APPLIED TO THE LBGK INCOMPRESSIBLE MODEL

There are several numerical perturbation techniques that can recover the continuity and Navier-Stokes equations as the asymptotic solution of the Boltzmann equation [3-5]. In this work the Chapman-Enskog expansion procedure is adopted, as previously done by others in works related to the present one, e.g. [11,21,22].

Since the fundamental objective of this work is to show how the LB body force model expression can be sensitive to the fact that a time-dependent or time-independent hydrodynamic equations are sought it is convenient to first clearly define the meaning of a time-independent hydrodynamic solution in the LB framework. An hydrodynamic problem is said to be steady when the macroscopic variables of interest have the following form: $p = p(\mathbf{x})$, $u_\alpha = u_\alpha(\mathbf{x})$. Given that in the LB method these two quantities are determined by the zeroth and the first order moments of the single particle distribution function, eqs. (4), that is a function that evolves both in space and time, i.e. $f_i = f_i(\mathbf{x},t)$, the method, during its pathway towards the steady-state solution, will provide us solutions of the form $p = p(\mathbf{x},t)$ and $u_\alpha = u_\alpha(\mathbf{x},t)$. However, since the problem is time independent these intermediate results are not physically significant. In fact, when using the LB method to solve time independent problems the parameter t should be comprehended simply as a measure of the number of iterations of the numerical algorithm, which implies that when the following conditions are achieved $\rho(\mathbf{x}) = \sum f_i(\mathbf{x},t)$ and $\rho(\mathbf{x})u_\alpha(\mathbf{x}) - aF_\alpha(\mathbf{x})\Delta t = \sum f_i(\mathbf{x},t)e_{i\alpha}$ our solution is converged. Nevertheless, apart from this theoretical aspect, when recovering the steady-state hydrodynamic equations, the Chapman-Enskog analysis follows the same philosophy as that traditionally employed in the time-dependent case.

The Chapman-Enskog expansion starts by Taylor expanding the first term on the left-hand side of eq. (2) in terms of the increment Δt, so that it can be expressed at location (x_α, t).

$$f_i(x_\alpha + e_{i\alpha}\Delta t, t + \Delta t) = \sum_{n=0}^{\infty} \frac{\Delta t^n}{n!}\left[\frac{\partial}{\partial t} + e_{i\alpha}\frac{\partial}{\partial x_\alpha}\right]^n f_i(x_\alpha, t). \tag{8}$$

Retaining terms up to $O(\Delta t^2)$ in eq. (8) and introducing them into eq. (2), this equation can be rewritten as:

$$f_i + \Delta t\left[\frac{\partial}{\partial t} + e_{i\alpha}\frac{\partial}{\partial x_\alpha}\right] f_i + \frac{\Delta t^2}{2}\left[\frac{\partial}{\partial t} + e_{i\alpha}\frac{\partial}{\partial x_\alpha}\right]^2 f_i = f_i - \frac{1}{\tau}\left(f_i - f_i^{(eq)}\right) + \Delta t F_i. \tag{9}$$

Introducing the parameter ε, which is proportional to the ratio of the lattice spacing to a characteristic macroscopic length scale, i.e. ε can be considered as a lattice Knudsen number, and using it as an expansion parameter, the formal expansion of f_i about $f_i^{(0)}$ yields:

$$f_i = \sum_{n=0}^{\infty} \varepsilon^n f_i^{(n)} = f_i^{(0)} + \varepsilon f_i^{(1)} + \varepsilon^2 f_i^{(2)} + O(\varepsilon^3). \tag{10}$$

In a similar fashion, this procedure can be applied to F_i. As it was mathematically demonstrated by Buick and Greated [22], in order to recover correct hydrodynamics the zeroth order term of the F_i expansion, $F_i^{(0)}$, must be nil. Hence the F_i expansion up to $O(\varepsilon^2)$ yields:

$$F_i = \varepsilon F_i^{(1)} + O\left(\varepsilon^2\right). \tag{11}$$

Due to eq. (11) the coefficients of the body force model, eqs. (6) and (7), are expressed as:

$$A = \varepsilon\, A^{(1)} + O\left(\varepsilon^2\right),\ B_\alpha = \varepsilon\, B_\alpha^{(1)} + O\left(\varepsilon^2\right) \text{ and } C_{\alpha\beta} = \varepsilon\, C_{\alpha\beta}^{(1)} + O\left(\varepsilon^2\right). \tag{12}$$

Introducing eqs. (10) and (11) into eq. (9) one obtains:

$$\begin{aligned} &\Delta t\left[\frac{\partial}{\partial t} + e_{i\alpha}\,\frac{\partial}{\partial x_\alpha}\right]\left(f_i^{(0)} + \varepsilon\, f_i^{(1)} + \varepsilon^2\ f_i^{(2)}\right) \\ &+\frac{\Delta t^2}{2}\left[\frac{\partial}{\partial t} + e_{i\alpha}\,\frac{\partial}{\partial x_\alpha}\right]^2\left(f_i^{(0)} + \varepsilon\, f_i^{(1)} + \varepsilon^2\ f_i^{(2)}\right) \\ &= -\frac{1}{\tau}\left(f_i^{(0)} + \varepsilon\, f_i^{(1)} + \varepsilon^2\ f_i^{(2)} - f_i^{(eq)}\right) + \Delta t \varepsilon F_i^{(1)} \end{aligned} \tag{13}$$

In order to remove discrete lattice artifacts from the macroscopic equations, a macroscopic space scale $x_{1\alpha} = \varepsilon\, x_\alpha$ is defined, together with two macroscopic time scales $t_1 = \varepsilon\, t$ and $t_2 = \varepsilon^2\, t$. Physically, the introduction of two time scales is justified by the fact that macroscopically the two fundamental momentum transfer mechanisms occur at two distinctive time scales: vorticity diffusion that takes place at time scale t_2 is much slower than the propagation of sound waves that occurs at the convective time scale t_1. Neglecting the influence of higher order terms, which have no influence on the isothermal incompressible hydrodynamic equations, the chain rule applied to spatial and temporal derivative operators yield:

$$\frac{\partial}{\partial x_\alpha} = \varepsilon\,\frac{\partial}{\partial x_{1\alpha}} + O\left(\varepsilon^2\right), \tag{14a}$$

$$\frac{\partial}{\partial t} = \varepsilon\,\frac{\partial}{\partial t_1} + \varepsilon^2\,\frac{\partial}{\partial t_2} + O\left(\varepsilon^3\right). \tag{14b}$$

Introducing these new scales into eq. (13) and grouping this last equation in terms of powers of ε one obtains:

- ε^0: $$0 = -\frac{1}{\tau}\left(f_i^{(0)} - f_i^{(eq)}\right). \tag{15a}$$

- ε^1: $$\frac{\partial f_i^{(0)}}{\partial t_1} + e_{i\alpha}\,\frac{\partial f_i^{(0)}}{\partial x_{1\alpha}} = -\frac{1}{\Delta t\,\tau}\, f_i^{(1)} + F_i^{(1)}\,. \tag{15b}$$

- ε^2: $$\frac{\partial f_i^{(0)}}{\partial t_2} + \left(1 - \frac{1}{2\tau}\right)\left(\frac{\partial f_i^{(1)}}{\partial t_1} + e_{i\alpha}\,\frac{\partial f_i^{(1)}}{\partial x_{1\alpha}}\right) = -\frac{1}{\Delta t\,\tau}\, f_i^{(2)} - \frac{\Delta t}{2}\left(\frac{\partial F_i^{(1)}}{\partial t_1} + e_{i\alpha}\,\frac{\partial F_i^{(1)}}{\partial x_{1\alpha}}\right). \tag{15c}$$

Taking the zeroth, $\sum_i(\cdot)$, and first, $\sum_i(\cdot)\, e_{i\beta}$, order moments of eq. (15b) one recovers the following macroscopic equations at t_1 time scale:

$$\frac{\partial(\rho)}{\partial t_1} + \frac{\partial}{\partial x_{1\alpha}}\left(\rho_0\, u_\alpha\right) = A^{(1)}, \tag{16a}$$

$$\frac{\partial}{\partial t_1}\left(\rho_0\, u_\beta\right)+\frac{\partial}{\partial x_{1\alpha}}\left(\Pi^{(0)}_{\alpha\beta}\right)=\left(\frac{a}{\tau}+b\right)F^{(1)}_\beta . \tag{16b}$$

It should be noted that in eq. (16b) the following identities are defined: $\Pi^{(0)}_{\alpha\beta}=\sum_i e_{i\alpha}e_{i\beta}\, f_i^{(0)}$ and $B^{(1)}_\alpha = bF^{(1)}_\alpha$. It is a simple task to demonstrate that the first expression, named as equilibrium momentum flux tensor, is $\Pi^{(0)}_{\alpha\beta}=\rho\, c_s^2\,\delta_{\alpha\beta}+\rho_0\, u_\alpha u_\beta$.

In order to recover the correct inviscid hydrodynamic equations:

$$\frac{1}{\rho_0}\frac{\partial(\rho)}{\partial t}+\frac{\partial}{\partial x_\alpha}\left(u_\alpha\right)=0\,, \tag{17a}$$

$$\frac{\partial}{\partial t}\left(u_\beta\right)+\frac{\partial}{\partial x_\alpha}\left(u_\alpha u_\beta\right)=-\frac{1}{\rho_0}\frac{\partial}{\partial x_\beta}\left(\rho\, c_s^2\right)+\frac{F_\beta}{\rho_0}\,, \tag{17b}$$

the following constraints in eqs. (16) have to be satisfied:

$$A^{(1)}=0\,, \tag{18a}$$

$$\left(\frac{a}{\tau}+b\right)=1\,. \tag{18b}$$

As it is verified, provided that the external forcing term fulfils the requisites expressed by eqs. (18), the time-independent hydrodynamic regime, at the inviscid time scale, can be regarded as the asymptotic limit of the time-dependent solution when $\partial(\cdot)/\partial t\to 0$. In other words, when the hydrodynamic variables take the form: $\rho=\rho(\mathbf{x})$ and $u_\alpha=u_\alpha(\mathbf{x})$ eqs. (18a-b) will still correctly describe the inviscid hydrodynamic behaviour of a flow field at steady-state without non-hydrodynamic terms arising from the fact that $\partial(\cdot)/\partial t = 0$. The same, however, does not happen at the viscous time scale as it will be shown next.

Taking the zeroth, $\sum_i(\cdot)$, and first, $\sum_i(\cdot)\, e_{i\beta}$, order moments of eq. (15c), the macroscopic equations at t_2 time scale are expressed as:

$$\frac{\partial}{\partial t_2}(\rho)=\Delta t\left(a-\frac{1}{2}\right)\frac{\partial}{\partial x_{1\alpha}}\left(F^{(1)}_\alpha\right), \tag{19a}$$

$$\begin{aligned}&\frac{\partial}{\partial t_2}\left(\rho_0\, u_\beta\right)+\left(1-\frac{1}{2\tau}\right)\left(\frac{\partial}{\partial t_1}\left(-aF^{(1)}_\beta\Delta t\right)+\frac{\partial}{\partial x_{1\alpha}}\left(\Pi^{(1)}_{\alpha\beta}\right)\right)\\&=-\frac{\Delta t}{2}\left(\frac{\partial}{\partial t_1}\left(bF^{(1)}_\beta\right)+\frac{\partial}{\partial x_{1\alpha}}\left(\frac{1}{2}\left(C^{(1)}_{\alpha\beta}+C^{(1)}_{\beta\alpha}\right)\right)\right)\end{aligned}\;. \tag{19b}$$

In the last equation the non-equilibrium momentum flux tensor is defined as $\Pi^{(1)}_{\alpha\beta}=\sum_i e_{i\alpha}e_{i\beta}\, f_i^{(1)}$. This parameter can be computed taking into account eq. (15b), the form of the equilibrium distribution function, using the incompressible LBGK model, eq. (7a), and the fact that $A^{(1)}=0$, eq. (18a), yielding:

$$\Pi_{\alpha\beta}^{(1)} = -\Delta t\,\tau \begin{bmatrix} \frac{\partial}{\partial t_1}\left(\Pi_{\alpha\beta}^{(0)}\right) + \frac{\partial}{\partial x_{1\gamma}}\left(\rho_0\, c_s^2\, u_\gamma \delta_{\alpha\beta} + \rho_0\, c_s^2\, u_\beta \delta_{\alpha\gamma} + \rho_0\, c_s^2\, u_\alpha \delta_{\beta\gamma}\right) \\ -\frac{1}{2}\left(C_{\alpha\beta}^{(1)} + C_{\beta\alpha}^{(1)}\right) \end{bmatrix}. \tag{20}$$

Introducing eq. (20) into eq. (19b), and taking into account the condition expressed by eq. (18b) one obtains the following momentum balance equation at the viscous time scale:

$$\begin{aligned} &\frac{\partial}{\partial t_2}\left(\rho_0\, u_\beta\right) - \Delta t\left(\tau - \frac{1}{2}\right)\frac{\partial}{\partial x_{1\alpha}}\left(\frac{\partial}{\partial x_{1\gamma}}\left(\rho_0\, c_s^2\, u_\gamma \delta_{\alpha\beta} + \rho_0\, c_s^2\, u_\beta \delta_{\alpha\gamma} + \rho_0\, c_s^2\, u_\alpha \delta_{\beta\gamma}\right)\right) \\ &= \frac{\Delta t}{2}(2a-1)\frac{\partial}{\partial t_1}\left(F_\beta^{(1)}\right) + \Delta t\left(\tau - \frac{1}{2}\right)\frac{\partial}{\partial x_{1\alpha}}\left(\frac{\partial}{\partial t_1}\left(\rho\, c_s^2\, \delta_{\alpha\beta} + \rho_0\, u_\alpha u_\beta\right)\right) \\ &- \tau\frac{\Delta t}{2}\frac{\partial}{\partial x_{1\alpha}}\left(C_{\alpha\beta}^{(1)} + C_{\beta\alpha}^{(1)}\right) \end{aligned} . \tag{21}$$

In order to obtain correct hydrodynamics the parameters a and $C_{\alpha\beta}^{(1)}$ have to be defined carefully so that the right-hand side of both eqs. (19a) and (21) become nil.

It is easy to verify that the value of the a parameter must be that given by eq. (22) in order to nullify the non-hydrodynamic terms where it appears in eqs. (19a) and (21).

$$a = \frac{1}{2}. \tag{22}$$

This value of a implies that the first order moment of the single particle distribution function, eq. (5b), has to be expressed as:

$$\sum_i f_i\, e_{i\alpha} = \rho_0\, u_\alpha - \frac{\Delta t}{2} F_\alpha . \tag{23}$$

The conclusion that the mass flux computation is not exclusively determined by the first order moment of the single particle distribution function, but it is also affected by half the body force magnitude, is not new. In fact one can find similar deductions in the early works of Ginzburg and Alder [14] and Ladd [15]. However, apart from a few exceptions, e.g. Guo et al. [21] and Buick and Greated [22], more recent studies have ignored this result, e.g. [3,4,5,12,17,18,19,20,25,26,27,28].

Concerning the $C_{\alpha\beta}^{(1)}$ parameter, which comes from the second order moment of the LB body force model, eq. (7), its definition is way more problematical. From eq. (21) one verifies that in order to obtain the correct hydrodynamic equations the spatial derivative term containing $C_{\alpha\beta}^{(1)}$ must exactly balance the other term containing a space/time cross derivate. However, in opposition to the space/time cross derivate term, the $C_{\alpha\beta}^{(1)}$ term is not affected by time-dependencies. Hence one cannot find a unique value of $C_{\alpha\beta}^{(1)}$ that simultaneously satisfies the correct momentum balance between the body force and the viscous stress terms at both steady and unsteady-state regimes.

If a time-independent solution is sought, i.e. a solution of the form $\rho = \rho(\mathbf{x})$ and $u_\alpha = u_\alpha(\mathbf{x})$, then because the space/time cross derivative containing these terms is nil the parameter $C_{\alpha\beta}^{(1)}$ has to be constant in all the solution domain:

$$C_{\alpha\beta} = C \qquad ,C \in \Re\,, \tag{24}$$

which implies that the correct body force model must have the following form:

$$F_i = \left(1 - \frac{1}{2\tau}\right)\frac{w_i e_{i\alpha} F_\alpha}{c_s^2} + C\,. \tag{25}$$

As a result, using eqs. (22) and (24) the steady hydrodynamic equation at the viscous time scale takes the following form[1]:

$$\rho_0\, c_s^2 \left(\tau - \frac{1}{2}\right)\Delta t \frac{\partial}{\partial x_{1\alpha}}\left(\frac{\partial}{\partial x_{1\gamma}}\left(u_\gamma \delta_{\alpha\beta} + u_\beta \delta_{\alpha\gamma} + u_\alpha \delta_{\beta\gamma}\right)\right) = 0\,. \tag{26}$$

Combining the time-independent mass and momentum conservation equations obtained at the inviscid and the viscous time scales, eqs. (17a-b) and (26), one finds the correct steady-state incompressible continuity and Navier-Stokes equations:

$$\frac{\partial}{\partial x_\alpha}\left(u_\alpha \right) = 0 + O\left(\varepsilon^2\right), \tag{27a}$$

$$\frac{\partial}{\partial x_\alpha}\left(u_\alpha u_\beta\right) = -\frac{1}{\rho_0}\frac{\partial}{\partial x_\beta}(p) + g_\beta + \nu \frac{\partial}{\partial x_{1\alpha}}\left(\frac{\partial}{\partial x_{1\beta}}(u_\alpha) + \frac{\partial}{\partial x_{1\alpha}}\left(u_\beta\right)\right) + O\left(\varepsilon^2\right). \tag{27b}$$

The first term on the right-hand side of eq. (26b) represents the normalized pressure, considering the equation of state $p = \rho c_s^2$, the second term represents the diffusion of momentum with the kinematic viscosity defined as $\nu = c_s^2\left(\tau - 1/2\right)\Delta t$ and the third term is the acceleration resulting from the body force, i.e. $g_\beta = F_\beta / \rho_0$. The last term is each equation $O\left(\varepsilon^2\right)$ indicates the discretisation error of second order.

If, alternatively, a time-dependent solution is sought, i.e. a solution of the form $\rho = \rho(\mathbf{x},t)$ and $u_\alpha = u_\alpha(\mathbf{x},t)$, then the value of $C_{\alpha\beta}^{(1)}$ must be set as:

$$C_{\alpha\beta} = \left(1 - \frac{1}{2\tau}\right)\left(u_\alpha F_\beta + u_\beta F_\alpha\right) + C \qquad ,C \in \Re \tag{28}$$

where again C is an arbitrary constant, which implies a body force model of the form:

$$F_i = \left(1 - \frac{1}{2\tau}\right)\left[\frac{\left(e_{i\alpha} - u_\alpha\right)}{c_s^2} + \frac{\left(e_{i\beta} u_\beta\right)}{c_s^4} e_{i\alpha}\right] F_\alpha + C\,. \tag{29}$$

Using eqs. (22) and (28) the unsteady hydrodynamic equations obtained at the viscous time scale are:

$$\frac{\partial}{\partial t_2}(\rho) = 0\,, \tag{30a}$$

$$\frac{\partial}{\partial t_2}\left(\rho_0\, u_\beta\right) - \rho_0\, c_s^2\left(\tau - \frac{1}{2}\right)\Delta t \frac{\partial}{\partial x_{1\alpha}}\left(\frac{\partial}{\partial x_{1\gamma}}\left(u_\gamma \delta_{\alpha\beta} + u_\beta \delta_{\alpha\gamma} + u_\alpha \delta_{\beta\gamma}\right)\right) = 0\,. \tag{30b}$$

Combining the unsteady mass and momentum equations obtained at the inviscid and the viscous time scales, eqs. (17a-b) and (30a-b), one finds the following time-

[1] Note that the zeroth order moment equation, accounting for the mass balance, at the viscous time scale is not shown here as it yields the trivial solution 0=0.

dependent incompressible continuity and Navier-Stokes equations, expressed in an artificial compressibility form, [32,33]:

$$\frac{1}{\rho_0 c_s^2}\frac{\partial}{\partial t}(p)+\frac{\partial}{\partial x_\alpha}(u_\alpha)=0+O(\varepsilon^2), \quad (31a)$$

$$\begin{aligned}&\frac{\partial}{\partial t}(u_\beta)+\frac{\partial}{\partial x_\alpha}(u_\alpha u_\beta)=-\frac{1}{\rho_0}\frac{\partial}{\partial x_\beta}(p)+g_\beta\\&+\nu\frac{\partial}{\partial x_{1\alpha}}\left(\frac{\partial}{\partial x_{1\beta}}(u_\alpha)+\frac{\partial}{\partial x_{1\alpha}}(u_\beta)+\frac{\partial}{\partial x_\gamma}(u_\gamma\delta_{\alpha\beta})\right)+O(\varepsilon^2)+O(\varepsilon M^3)\end{aligned}. \quad (31b)$$

As demonstrated by [33, 34] when using the incompressible BGK model the time-dependent hydrodynamic equations recovered are still affected by compressibility errors as the $O(\varepsilon M^3)$ term indicates.

Based on eq. (20) and on the fact that the shear stress tensor $\sigma_{\alpha\beta}$ and the non-equilibrium momentum flux tensor are related through $\sigma_{\alpha\beta}=-\left(1-\frac{1}{2\tau}\right)\Pi_{\alpha\beta}^{(1)}$ (the reader is referred to [22] for a thorough discussion on this subject), it is easy to verify that the dependency of $\Pi_{\alpha\beta}^{(1)}$ on $C_{\alpha\beta}$ makes the correct shear stress expression also influenced by the time-dependency of the macroscopic solution.

Concerning the body force models derived in this work, at both steady and unsteady-state regimes, i.e. eqs. (25) and (29) respectively, it must be stressed that their expressions have already been presented in the literature.

In fact, taking into account that C is an arbitrary constant and, without any loss of generality, if the constant takes the value zero then eq. (24) becomes similar to the body force model proposed by Buick and Greated [22]. Similarly, the body force model expressed by eq. (28), which was shown to be the correct one when time-dependent hydrodynamics are sought, was originally proposed by Guo et al. [21]. However, in both works the time-dependency of the hydrodynamic solution was never considered as a relevant constraint in the body model formulation. This fact is revealed by the numerical tests of the referred works where their body force models were benchmarked for both steady and unsteady flow regimes without any further concerns.

5 LATTICE BOLTZMANN EQUATION IN A NON-INERTIAL REFERENCE FRAME: SOME NUMERICAL TESTS

Several numerical tests were performed corroborating the previous theoretical analysis. Such results are presented in [35] and consist of a steady periodic vortex flow and an extended Poiseuille flow. They both showed that the body force model proposed by Guo et al. [21] and generally accepted as the correct one is in fact inaccurate at steady-state flow regimes whereas the body force model previously derived as the correct one for time-independent hydrodynamics is the one providing the most accurate solutions.

In the following numerical tests the LB parameters and initialization routines used are identical to those discussed in the up mentioned reference [35].

Furthermore, based on the previous analysis, which focused on the correct modelling of the LB body force term, it is straightforward to write the LB equations in a non-inertial reference frame. This is done by simply introducing in eqs. (25) or (29), depending on the time regime, the term

$F_\alpha = -\rho\left(e_{\kappa\gamma\alpha}\, 2\,\Omega_\kappa\, u_\gamma + e_{\kappa\gamma\alpha}\,\Omega_\kappa\, e_{\delta\eta\gamma}\,\Omega_\delta\left(x_\eta - x_{0\eta}\right)\right)$. As a result, the hydrodynamic equations, eqs. (1), are recovered as the long-wavelength and high-frequency asymptotic limit of the LB equation.

6.1. Steady fully developed centrifugal flow

In this first test we will study the LB solution of a steady fully developed flow in a pure centrifugal field. Assuming an angular velocity of the form $\Omega_\kappa = (0, \Omega, 0)$ the hydrodynamic equations in this case read as:

$$\frac{d}{dy}\left(\mu \frac{d}{dy} u_x(y,z)\right) + \frac{d}{dz}\left(\mu \frac{d}{dz} u_x(y,z)\right) = \frac{dp}{dx} - \rho\,\Omega^2 \left|x - x_0\right|. \tag{32}$$

This equation as the following analytical solution:

$$\begin{aligned} u_x(y,z) &= -\frac{1}{2\mu}\left\{\left(\frac{dp}{dx}\right) - \rho\,\Omega^2\left|x - x_0\right|\right\} \\ &\times\left[z(H-z) - \frac{8H^2}{\pi^3}\sum_{m=1}^{\text{odd}} \frac{1}{m^3}\frac{\cosh\left[m\pi\left(y - W/2\right)/H\right]}{\cosh\left(m\pi W/2H\right)} \sin\left(\frac{m\pi}{H} z\right)\right] \end{aligned} \tag{33}$$

where H and W are the cross-section channel height and weight, respectively.

Defining the flow Reynolds as: $\mathrm{Re} = \hat{u}_x W/\nu$ where $\hat{u}_x$ is the centreline (maximum) velocity, it can be shown that the terms in right-hand side of eq. (32) may be expressed as:

$$\left(\frac{dp}{dx}\right) - \rho\,\Omega^2\left|x - x_0\right| = -\frac{2\,\mathrm{Re}\,\rho\,\nu^2}{\left(\dfrac{H^2}{4} - \dfrac{8H^2}{\pi^3}\displaystyle\sum_{m=1}^{\text{odd}}\frac{1}{m^3}\frac{\sin\left(m\pi/2\right)}{\cosh\left(m\pi W/2H\right)}\right)}. \tag{34}$$

For a two dimensional situation, *i.e.* assuming $z = \infty$, the steady fully developed centrifugal solution yields the well known parabolic velocity profile solution:

$$u_x(y) = -\frac{1}{2\mu}\left\{\left(\frac{dp}{dx}\right) - \rho\,\Omega^2\left|x - x_0\right|\right\} y\left(y - W\right), \tag{35}$$

with:

$$\left(\frac{dp}{dx}\right) - \rho\,\Omega^2\left|x - x_0\right| = -\frac{8\,\mathrm{Re}\,\rho\,\nu^2}{W^3}. \tag{36}$$

Solving the two-dimensional case, eq. (35), with the D2Q9 model one important result, from the theoretical view point, is obtained. It is observed that if the body force previously derived, eq. (25), is used then the solution obtained belongs to the restrict family of LB analytical solutions. In other words, machine accurate results are always obtained, regardless the mesh size, when the centrifugal term is modelled with eq. (25). This result indicates that the only body force model that is simultaneously second order accurate and does not bring numerical artifacts into the hydrodynamic equations is the one derived herein, eq. (25). In this numerical test in particular one obtains (up to the truncation error) the exact classical parabolic velocity profile solution and also the exact streamwise parabolic pressure profile typical of fully developed centrifugal flows as depicted in fig. 1.

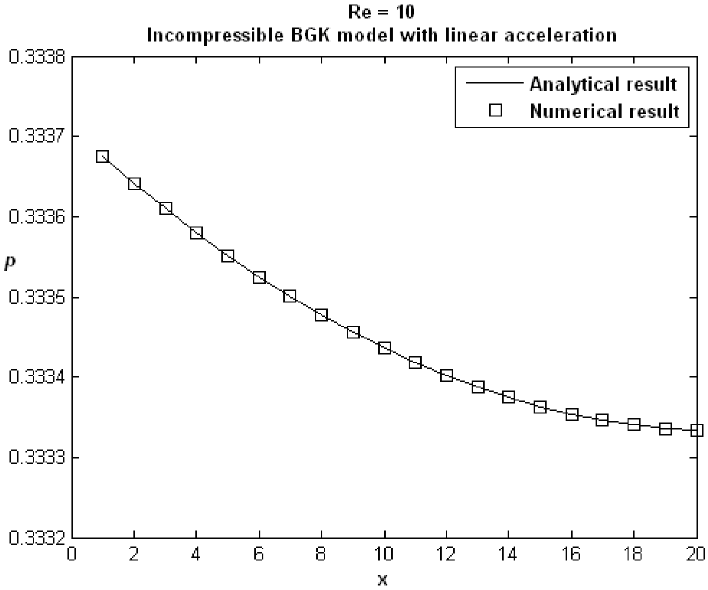

Figure 1: Analytical and numerical pressure profiles in lattice units obtained from the solution of the D2Q9 LB equations for Re=10 with a linear (centrifugal) acceleration.

The solution of the three-dimensional problem, using the D3Q19 LB model, shows that results are no longer machine accurate. In effect the numerical data converges towards the analytical solution, eq. (33), with a second order rate, fig. 2. Nevertheless, the higher accuracy of the body force model derived herein in comparison to that proposed by Guo et al. [21] is clearly verified. This conclusion is depicted in fig. 2, where the common $\|L_2\|_\infty$ error for the velocity field is displayed as function of the grid size. Concerning the pressure field, as it happened in the two-dimensional case, it presents a parabolic variation along the streamwise direction.

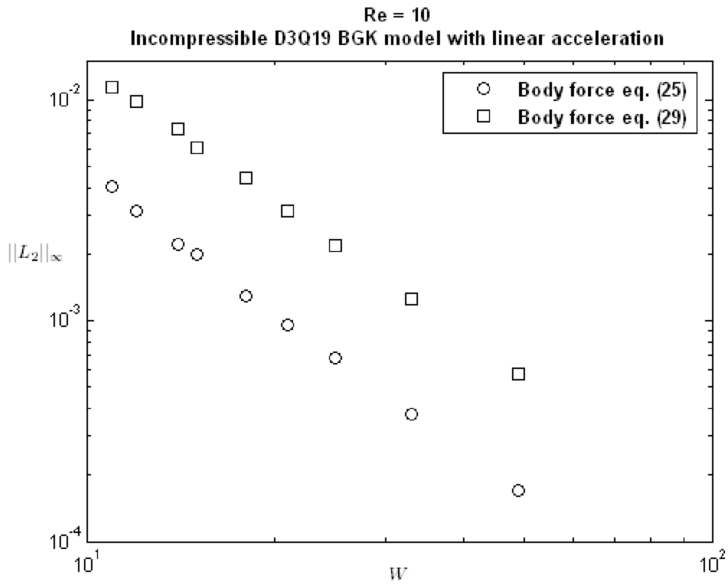

Figure 2: Convergence plot of the $\|L_2\|_\infty$ error for the velocity field as function of the grid size solution obtained from the D3Q19 LB equations for Re=10 with a linear (centrifugal) acceleration. The both body models studied were those expressed by eq. (25) – correct for steady-state hydrodynamics; and eq. (29) – correct for unsteady-state hydrodynamics. The convergence rate is 1.92 for body force eq. (25) and 1.83 for body force eq. (29).

6.2. Steady periodic Coriolis flow

In the second test we will focus on the LB solution of a steady periodic Coriolis flow. The main objective of this study is to observe the isolated effect of the Coriolis acceleration field on the fluid flow motion at low Reynolds number. For that reason we have constructed here a simplified flow model based on several assumptions. First, the flow is considered time-independent and the fluid incompressible. Moreover, we have also assumed that the flow is periodic in the flow streamwise direction, i.e. $x=\infty$, and that the flow streamwise velocity is much higher than the other two velocity components, i.e. $u_x >> u_y, u_z$. This last hypothesis allow us to neglect the Coriolis acceleration term in the momentum flow streamwise component, i.e. $2\Omega u_z << \Omega^2 |x - x_0|$, which makes the flow main component to be produced solely by a known constant body force value. Note that since the flow is periodic in the x direction the centrifugal acceleration has a constant value. This allow us to estimate the error of the numerical model through the comparison of the flow streamwise velocity component against the analytical Poiseuille solution, given by eq. (33). Since the effects of using an incorrect body force model appear, in the recovered hydrodynamic equations, as body force gradients [Ref], in this case all body force models yield identical accuracies. The main differences occur in the other two velocity components. As fig 3 depicts these are no longer zero but have a vortex like behaviour.

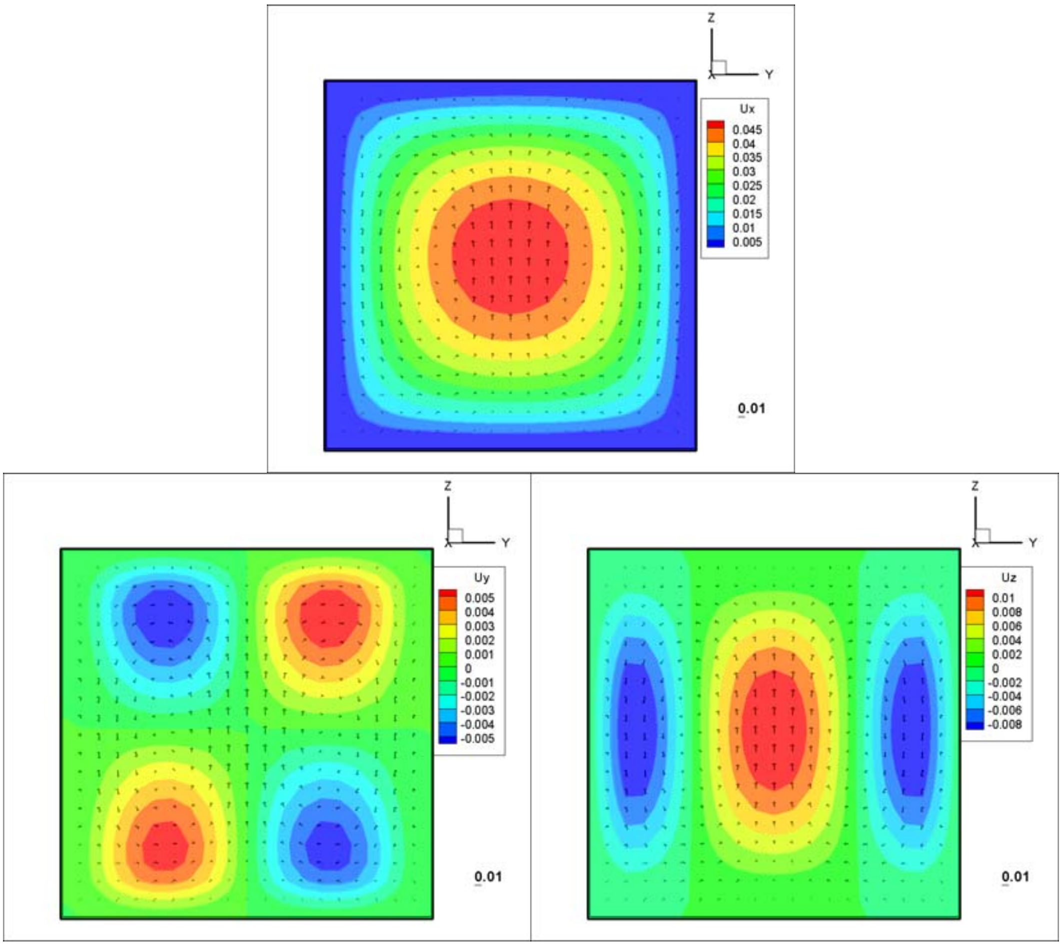

Figure 2: Velocity contour plots of steady periodic Coriolis flow obtained with the D3Q19 LB model for a grid size of 3×21×21 nodes, Ma=0.05 and Re=10. It should be noted that the results here depicted present similar behaviour for more refined grids; hence mesh convergence is considered to be verified.

In fact the transverse motion induced by the Coriolis force in this flow resembles that observed in the duct flow in bends. In that case, although no body force is present, it is the dynamic balance between the radial pressure gradient and the centrifugal force due to the wall curvature that produces the vortex structures known as Dean vortices.

Since, in microfluidic applications flows are generally laminar the mixing rates are generally quite slow due to the fact that mixing is controlled by the molecular diffusion. Therefore, the use of a rotating platform allows on to use the Coriolis force to promote convection streams that will allow for the decrease of mixing time scales.

6 CONCLUSIONS

In this work it was demonstrated that when a body force term is included in LB equations the time-dependency of the hydrodynamic problem to be solved becomes a constraint of crucial importance in the formulation of the correct expression for the LB body force model. This means that one cannot employ the same body force model expression to recover correct hydrodynamic equations at both steady and unsteady-state flow regimes. This happens because it is not possible to find a single LB body force expression whose second order moment exactly balances the viscous stress tensor at the two time regimes, since this last term has two different forms depending on whether the hydrodynamic problem to be solved is steady or unsteady. The Chapman-Enskog analysis demonstrates that the body force model generally accepted as being the correct one for isothermal incompressible hydrodynamic problems, i.e. eq. (29), introduces non-hydrodynamic error terms when a time-independent solution is sought. For recovering correct steady-state macroscopic equations the LB body force model should have a constant second order moment value as indicated by eq. (25).

Based on this result the LB equations were written in a non-inertial reference frame and two constructed benchmark flow tests were studied: (1) a steady centrifugal flow and (2) a steady Coriolis flow. With these two examples two important conclusions were observed. First, in the steady fully developed centrifugal flow it was verified that the LB body force model derived herein yields, as the theoretical analysis predicted, the most accurate results. Second, it was verified that, even for low Reynolds number, the use of a microfluidic device in a rotational reference frame can be advantageous as the Coriolis acceleration term will induce transverse convection streams that will allow for the promotion and increase of the, typically, slow flow mixing rates.

Further studies on this subject are still required. For instance studies focusing on: (1) the implement of more general outflow boundary conditions, which account for the body force presence; (2) the influence of different rotational speeds in the fluid flow behaviour, in particular in the flow vortex structures; and also (3) the extension of this study into more complex geometries as those typically found in Lab-on-a-CD prototype devices; will surely bring a deeper insight into this field.

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