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Lattice Boltzmann model of a square natural circulation loop with small inner diameter: working fluid effects

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Abstract. Natural circulation loops are systems used to transport heat by the free convection of a working fluid in a closed thermo-hydraulic circuit. Many examples of the Lattice Boltzmann method applied to free convection can be found in the literature, but most of them are limited to model simple enclosures. This work is one of the first approaches to an engineering system as the Natural Circulation Loops using this numerical method. This study describes the implementation and validation of a numerical model of a rectangular loop characterized by a small inner diameter. This research is focused on the thermohydraulic response of the NCL varying the working fluid. We have obtained satisfactory results demonstrating that accepted analytical correlations for the steady-state behavior are reproduced by the thermal Lattice Boltzmann Method (double distribution function). Overall, these results suggest that the temperature and velocity oscillations during the transient increase directly with the fluid Prandtl number; instead, the temperature difference between the vertical legs is inversely correlated and decreases.

1. Introduction

Natural circulation loops (NCL) are thermal systems that transport heat from a heat source to a heat sink by the movement of a working fluid into a closed pipes system. The fluid flow is induced by natural convection determined by thermal expansion and gravity [1]. These engineering systems are very interesting in geothermic, solar energy, nuclear plants, or electronic cooling systems, mainly by the absence of an active pump system [2]. The common shape of an NCL is rectangular and oriented vertically. Some analytical relationships can predict the flow characteristics of the loops under selected operational parameters such as geometric dimension, fluid properties, source, and sink characteristics for laminar regime [3,4] and transition or turbulent regime [5]. Those relationships have been validated by comparison with experimental data from laboratories worldwide. In recent years experimental works validated the applicability of the analytical model to NCL with a small inner diameter connected in parallel [7], [8].

Previous works evaluate the performance of rectangular-shaped single-phase NCL with heat end exchangers mainly by developing analytical models, simulations, or experiments. Early computational works use a one-dimensional model [9] solved using finite differences [10]. Yadav et al. in 2014 [11] performed a simulation with different tilt angles and found that the tilt angle increases the mass flow rate and decreases the heat exchange. Moreover, they also found that higher operating pressure reduces the time to reach a steady state. They corroborated the Swapnalee and Vijayan empirical correlation for the turbulent regime [5]. Cheng et al. 2018 [12], using a 3D CFD model, simulate the transient response of a single-phase NCL evaluating mass flow rate and energy generation. They use

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Vijayan's correlation [5] for the laminar regime (originally proposed for imposed heat flux at the heater) with a good fitting for the tested Reynolds numbers (lower than 100). Recently a study on the jump of heat transfer coefficient by tilting the square NCL (single and coupled) was developed using 2D and 3D numerical models [13].

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In the above papers, the numerical simulation employed the classic techniques of CFD. The Lattice Boltzmann Method (LBM) was adopted in the present work. LBM is a numerical method characterized by a mesoscopic approach based on the solution of the discretized Boltzmann transport equation [14,15]. The LBM differs from the macroscopic approach adopted in the Finite Element Methods, even if, in LBM, some numerical schemes are designed to solve the macroscopic Navier-Stokes equations. Additionally, the LBM is linked to statistical mechanics but differs from the microscopic approach, and no information can be traced back to Molecular Dynamics. This method is highly parallelizable by its local algorithmic rules. It can handle multi-physics by considering different lattices simultaneously, i.e., one lattice for the fluid density and momentum, a second one for the temperature field (thermal double distribution function or DDF), and even additional lattices if particle or chemical species transport are of interest [16]. Different upgrades of the LBM have been developed to account for thermal effects [17]. Examples of studies using LBM to model natural convection show the interest and applicability of the method in this topic: Rayleigh-Bernard [18], rectangular cavities [19], 2D channel [20], nanofluids into a curved boundaries cavity [21], ferrofluids in a linear heated cavity [22], channel heated by active blocks [23], turbulent Rayleigh-Bernard in a channel [24], or a cavity with low Prandtl number fluid [25]. If even the method was successfully applied to natural circulation in cavities and channels, applications to NCL are scarce: our previous work shows the effect of the heater-cooler orientation, and we found an influence on the time to start the natural circulation and on the steady-state converge time [26,27]. This study explores, for the first time, the application of the LBM to NCL under a fixed heater-cooler orientation and different parameter configurations (this is the first approach using LBM to study the effects of changing the working fluid in simple NCL circuits and varying the modified Grashof numbers).

This work aims to present a single-phase NCL characterized by a small diameter, simulated by LBM, and study the thermo-hydrodynamic behavior operating with different working fluids (characterized by different Prandtl numbers). The model was validated by comparison with the analytical model proposed by Cheng et al. [4] for the temperature distribution along the loop and the relationship between the Reynolds number at steady-state and the modified Grashof number. We found a significative effect of the Prandtl number in the thermal oscillations during the transient and on the steady-state Reynolds number. This study provides important insights into the validity of a 2D LBM model to study the steady-state thermal flow in the laminar regime of an NCL.

2. Methods

A two-dimensional model of a squared NCL was developed [26,27]. The loop is characterized by two horizontal heat end exchangers (modeled as fixed hot and cold temperatures at the tube walls) and two vertical legs that connect the heater and the sink (adiabatic), see figure 1. Fluids characterized by different Prandtl numbers (Pr = 0.1, 1.0, 7.0) were tested. Thermophysical properties of the working fluid were fixed during the simulations, and a single-phase condition was assumed.

The model was implemented using C++ and PALABOS (Parallel Lattice Boltzmann Solver library), [28]. The LBM double distribution function (DDF) approach was used, the first distribution function was used to solve the fluid dynamic field, and the second one was used to simulate the thermal field. Each distribution function is implemented in a separate lattice; D2Q9 for the fluid dynamic field and D2Q5 for the thermal field, see figure 2. The two lattices are overlapped and coupled through the buoyancy force term. Pr = 1.0 in DDF-LBM means that both lattices (D2Q5 & D2Q9) have the same relaxation time (physically have the same diffusivity ratio, i.e., viscosity and thermal conductivity).

horizontal

 c_1

cooler

 $x + \Delta x$

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Figure 2. Thermal LBM model using two lattices, every single node has some vectors representing the two discretized probability density functions. (a) D2Q9 hydrodynamic lattice, (b) D2Q5 thermal lattice.

2.1. Stability and convergence

The convergence of the system to the steady-state was determined by calculating the relative standard deviation of the Nusselt number, and if it reaches a given threshold (10⁻¹⁶), convergence is assumed, and the simulation is finished. Additionally, the convergence of the temperature difference between the vertical legs (ΔT_{avg}) and the Reynolds number was studied. In the laminar regime, both quantities converge. The simulations do not present computational instabilities or divergencies in the tested Rayleigh number range (input parameter). The lattice spatial resolution effect on flow conditions was investigated by calculating the Reynolds number at steady-state, changing the number of nodes per unit length. The following spatial resolution values were tested: 500(diverge), 1000, 2000, 4000, 8000, and 10000 grid points per unit length. Results are presented in figure 3. It was noted that the Reynolds number converges for a resolution up to 4000; thus, 40 mesh points per pipe diameter were used in the simulations, i.e., 1000x1000 lattice.





Figure 3. Grid convergence study in laminar regime, Re_{ss} vs. resolution. Pr=1.0.

3. Results

3.1. Steady-state behavior

The one-dimensional model proposed in the literature [3–5] was used to validate the LBM simulation. The effects of the input thermal energy (modified Grashof number, Gr_m , Eq. 1) on the mass flow rate (Reynolds number at steady-state, Re_{ss}) were studied. The analytical model is resumed in the Eq. 2. It is possible to show that this model (used for imposed temperature conditions at the heater and heat sink) is equivalent to the model proposed in [3,5] for the laminar and turbulent region in an NCL (with a heat flux boundary condition at the heater).

$$Gr_m = \frac{g\beta\Delta T_{avg}D^2H}{v^2} \tag{1}$$

$$Re_{ss} = \sqrt{\frac{Gr_m}{N_G}} \tag{2}$$

The geometrical parameter, N_G , described by Eq. 3, accounts for local and concentrated friction losses, considering the frictional coefficient, f, and the local resistance coefficient, K.

$$N_G = \frac{1}{2} \sum_i (f \frac{L_i}{D} + K) \tag{3}$$

The analytical correlation (Eq. 2) between Re_{ss} and Gr_m/N_G was verified regardless of the fluid properties, as presented in figure 4. When the value of the Prandtl number was changed to a higher value, lower values of the modified Grashof number were reached with the same initial setup (global Rayleigh number), and subsequently, lower values of the *steady-state Reynolds number* were obtained. However, all the points fall in the same trend described in Eq. 2, see figure 4. The LBM results for Pr = 7.0 show a small deviation for the points corresponding to high Ra numbers even when the flow regime remains laminar.



Figure 4. Thermo-hydraulic behavior of the NCL described by the Eq. 2, [3–5].

A change in the slope in this graphic is noticed over $Re_{ss} = 320$. The velocity field, over this transition limit, shows vortex formation near the heater and heat sink walls, see figure 5.



Resuming, two flow regimes were found, i.e., a laminar regime and a transient regime. The *laminar regime* is characterized by a parabolic velocity distribution in the pipes. The *transition regime* is characterized by traveling eddies near the walls of the heater and cooler (during this regime, the Nusselt number increases).

The temperature distribution predicted by the one-dimensional model is simple and regular because it does not consider the cross-sectional distribution of thermal flow and predicts only the behavior of the *laminar regime*. The vorticity in the transition regime highly influences the temperature distribution along the circuit near the heater and heat sink walls and in the first section of the vertical legs, figure 6(a). The oscillations in the average temperature profile decrease with a lower Prandtl number, as shown in Figure 6(b). The shape of the temperature profile in Figure 6(a) (predicted by the one-dimensional model) has a poor similarity to the LBM results. The difference in the predictions could be linked to resolution and average errors; the average over the tube cross-section shows more variations in the case of higher *Pr*. In the *transition regime*, the timescale of the flow field variations could be under-resolved in the high *Ra* number zone, depending on the *Pr* value (e.g., lower *Pr* values show more regular cross-sectional profiles).



Figure 6. Dimensionless temperature distribution (average over the cross-sections) along the NCL. (a) $Re_{ss} = 510$, Pr = 1.0. (b) $Re_{ss} = 660$, Pr = 0.1.

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3.2. Transient behavior

Differences in the transient response can be noted; lower Pr fluid presents more dampened oscillations and faster convergence to the steady-state, figure 7(a). A higher temperature difference between the adiabatic legs is noted for the lower Pr fluid (at the same Re_{ss}). This trend is also visible in the velocity oscillations presented in the phase diagrams, figure 7(b). The increment of the Pr implies a dominance of momentum transport over thermal conduction, which means that the fluid transports the heat mainly by convection. The fluid increase or decreases (locally) its temperature with more difficulty, and of course, this difficult the convection because the body force term is considered linear and dependent on this temperature change. In contrast, a fluid with a low Pr is heated easily; therefore, the density changes are quickly induced with a subsequent higher flow rate.



Figure 7. Transient response of the NCL simulated by LBM for different Reynolds numbers and Prandtl numbers. (a) ΔT_{ava} vs. time, (b) phase diagram: normalized velocity vs. normalized ΔT_r .

The main limitation of this work is the scalability of the results to a 3D model. Although the results must be taken with care regarding the limit between the *laminar* and *transition regime* and the complex flow pattern presented in the *transition regime*, our results support further research implementing a full 3D LBM model of an NCL, with relatively small modifications of the tested 2D LBM model. The present results support the applicability of the 2D model to low Re_{ss} , thanks to the positive validation with the analytical model of Eq. 2, this analytical model used in the validation has been verified experimentally in diverse NCL circuits and is a reference correlation in the NCL field.

4. Conclusions

This study shows that a numerical model using the thermal (double distribution function) Lattice Boltzmann Method can reproduce the transient and steady-state behavior of a square single-phase NCL. The results of this study underline that the numerical model reproduces accepted analytical correlations for steady-state behavior.

The main effects of the working fluid were studied by changing the Prandtl number. The observed effects of increasing the Prandtl number are incrementing the temperature and velocity oscillations during the transient response and decreasing the temperature difference between the adiabatic legs at a steady state.

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