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# An enthalpy-based lattice Boltzmann formulation for unsteady convection-diffusion heat transfer problems in heterogeneous media

Auteurs : Rihab Hamila[1], Moudhaffar Nouri[1], Sassi Ben Nasrallah[1], Patrick Perré[2]
*[1]Laboratoire d'Études des Systèmes Thermiques et Énergétiques,*
*École Nationale d'Ingénieurs de Monastir, Université de Monastir*
*Avenue Ibn El Jazzar, 5019 Monastir, Tunisia*
*[2]Laboratoire de Génie des Procédés et Matériaux, CentraleSupélec,*
*Université de Paris-Saclay*
*Grande Voie des Vignes 92295 Châtenay-Malabry Cedex, France*

*Email des auteurs : Rihab Hamila:* **hamilara7@gmail.com**,
*Moudhaffar Nouri: nouri.mdafer@gmail.com,*
*Sassi Ben Nasrallah: sassi.bennasrallah@yahoo.fr,*
*Patrick Perré: patrick.perre@ecp.fr*

**Abstract:** In this paper, we propose an enthalpy-based lattice Boltzmann formulation for solving conduction and/or convection heat transfer problems in heterogeneous media. The main idea of this formulation is to introduce an extra source term to the collision step, avoiding any additional treatment on the distribution functions at the interface between two or more different phases with various thermo-physical properties. This approach is independent of the choice of lattice scheme. The simplicity in implementing this method allows an easy solution of heat transfer problem in heterogeneous media with complex and time dependent interfaces. The performance of the present method is successfully validated by comparison with Control Volume Methods solutions of several heat transfer problems in heterogeneous media

**Keywords**:

Enthalpic Formulation; Lattice Boltzmann Method; Heterogeneous media; Convection-diffusion heat transfer.

## 1. Introduction

Heat transfer in heterogeneous media is widely encountered in many fields such as energy engineering, cooling electronics or mechanical equipment, food engineering, and environmental control. Due to its major significance, many researchers have investigated this field [1-6]. Over the last decade, the Lattice Boltzmann method (LBM) [7] became a popular numerical method for many different configurations. Its main asset is its simple algebraic manipulation, its easy solution procedure and implementation of boundary conditions, together with its ability of dealing with complex fluids [8]. This explains why LBM is a very promising and competitive numerical tool in solving heat transfer process [9-11], turbulent flows [12,13], micro-flows [14,15], porous media [16-18] and multiphase flow [19-21]. However, this apparent simplicity still has some limitations. When trying to simulate conjugate heat transfer, one has to take into account the discontinuities existing at the interface between two components with different thermo-physical properties. This imposes extra conditions at the interfaces to ensure continuity of temperature and normal heat flux, which are often considered as a conjugate condition. The problem becomes more complex when interfaces are curved and move or evolve over time, in response to phase change, fluid flow or chemical reactions.

In this paper, we propose an enthalpic Lattice Boltzmann formulation for heat transfer through diffusion and/or convection in heterogeneous media. This formulation gives rise to a source term, which ensures heat flux and temperature continuity at the interface. It does not require any specific treatment dependent on interface topology. It is also independent on the choice of lattice. This approach is validated by comparison with analytical and numerical results of several heat conduction and/or convection problems for flat and curved interfaces.

The paper is organized as follows; Section 2 presents the enthalpic formulation of the lattice Boltzmann Method. Section 3 provides the validation of the proposed method through comparisons with Control Volume Method solutions of several heat convection-diffusion problems for flat and curved interfaces. Section 4 concludes the paper.

## 2. Enthalpic formulation

The single relaxation time (BGK) lattice Boltzmann equation for an advection-diffusion problem is [22]:

$$f_k(\boldsymbol{r}+\boldsymbol{e}_k\Delta t, t+\Delta t) = f_k(\boldsymbol{r},t) - \frac{\Delta t}{\tau}\left[f_k(\boldsymbol{r},t) - f_k^{eq}(\boldsymbol{r},t)\right] \quad \textbf{(1)}$$

where, $f_k$ is the distribution function, $\tau$ is the relaxation time, $f_k^{eq}$ is the equilibrium distribution function and $\Delta t$ is the time step.

For the $D2Q9$ lattice arrangement, $\tau$ and $f_k^{eq}$ are given by the following expressions [22]:

$$\tau = \frac{3\alpha}{|\boldsymbol{e}_k|^2} + \frac{\Delta t}{2} \quad \textbf{(2)}$$

$$f_k^{eq}(\boldsymbol{r},t) = w_k T(\boldsymbol{r},t)\left[1 + \frac{\boldsymbol{e}_k \boldsymbol{U}}{c_s^2}\right] \quad \textbf{(3)}$$

where $\alpha = k/\rho C_p$ is the thermal diffusivity, $\boldsymbol{U}$ is the velocity vector, $k$ the thermal conductivity $\rho$ the density and $C_p$ the heat capacity. The nine velocities $\boldsymbol{e}_k$ and their corresponding weights $w_k$ in the $D2Q9$ lattice read as [22]:

$$e_0 = (0,0), e_1 = (\pm 1,0).c, e_{2,4} = (0,\pm 1).c, e_{5,6,7,8} = (\pm 1,\pm 1).c \quad \textbf{(4)}$$

$$w_0 = \frac{4}{9}, w_{1,2,3,4} = \frac{1}{9}, w_{5,6,7,8} = \frac{1}{36} \quad \textbf{(5)}$$

where $= \frac{\Delta x}{\Delta t}$ ; $c_s$ is the speed of sound and $\Delta x$ is the grid size.

At each node, the temperature $T$ is calculated from the values of $f_k$ over all directions [22]:

$$T(\boldsymbol{r},t) = \sum_{k=0}^{8} f_k(\boldsymbol{r},t) \quad \textbf{(6)}$$

By using a Chapmann-Enskog expansion, the lattice Boltzmann model (Eq.1) retrieves the following heat diffusion-convection equation:

$$\frac{\partial T}{\partial t} + \nabla.(\boldsymbol{U}T) = \nabla.(\alpha\nabla.T) \quad \textbf{(7)}$$

However, in general, the heat diffusion-convection equation takes the following form:

$$\frac{\partial(\rho C_p T)}{\partial t} + \nabla.(\rho C_p \boldsymbol{U} T) = \nabla.(\mathrm{k}\nabla.T) \quad \textbf{(8)}$$

For multi-domain problems, additional conditions should be applied at the interface between domains to ensure continuity of temperature and normal heat flux:

$$T_+ = T_- \quad \textbf{(9)}$$

$$\boldsymbol{n}.\left[k\nabla T - \rho C_p \boldsymbol{U}T\right]_+ = \boldsymbol{n}.\left[k\nabla T - \rho C_p \boldsymbol{U}T\right]_- \quad \textbf{(10)}$$

$\boldsymbol{n}$ is the normal to the interface, **+** and **–** denote parameter on either side of the interface.

The conventional LBM formulation (Eq.1) solves Eq. (7), which allows Eq. (8) to be solved only in two simplified configurations: uniform heat capacitance $\rho C_p$ in all domains or steady-state heat diffusion-convection transfer configurations. This is the reason why, a few LBM studies using the conventional formulation are limited to steady conjugate heat conduction transfer problems. Indeed, once steady-state heat conduction is achieved, only the thermal conductivity plays a role in the solution for temperature distribution. The heat capacitance is not relevant anymore and one can, for simplicity, assume $\rho C_p$to be identical in all components.

In other way, a jump balance at the interface applied to equation (7) leads to:

$$T_+ = T_- \quad \textbf{(11)}$$

$$\boldsymbol{n}.[\alpha\nabla T - \boldsymbol{U}T]_+ = \boldsymbol{n}.[\alpha\nabla T - \boldsymbol{U}T]_- \quad \textbf{(12)}$$

This leads to:

$$T_{+} = T_{-} \quad \textbf{(13)}$$

$$\boldsymbol{n}.\frac{1}{\rho C_{p+}}\left[k\nabla T - \rho C_p \boldsymbol{U}T\right]_{+} = \boldsymbol{n}.\frac{1}{\rho C_{p-}}\left[k\nabla T - \rho C_p \boldsymbol{U}T\right]_{-} \quad \textbf{(14)}$$

The Eq. (12) leads to Eq. (14) only when the heat capacity is the same:

$$\rho C_{p-} = \rho C_{p+} \quad \textbf{(15)}$$

Therefore, the conventional LBM formulation (Eq.1) ensures the normal heat flux continuity only when the heat capacity is the same on either side of the interface.

In order to solve Eq. (8) using Lattice Boltzmann method, we scale it by a constant heat capacity value (the one of layer "n" in this case) to obtain the same form as Eq. (7) and ensure temperature and normal heat flux continuity at the interface. We start from Eq. (8) written for $p$ layers with different thermo physical properties:

$$\frac{\partial\left(\rho C_{pl}T\right)}{\partial t} + \nabla.\left(\rho C_{pl}\boldsymbol{U}T\right) = \nabla.\left(k_l \nabla.T\right) \qquad for\ \ l = 1, \dots, p \quad \textbf{(16)}$$

By using the enthalpy $h = \rho C_{pn}T$ as a new variable, Eq. (8) becomes:

$$\frac{\partial(h)}{\partial t} + \nabla.(h\boldsymbol{U}) = \nabla.(\alpha_l \nabla.h) + S_l \qquad for\ \ l = 1, \dots, p \quad \textbf{(17)}$$

where

$$S_l = \left[1 - \frac{\rho C_{pl}}{\rho C_{pn}}\right]\left[\frac{\partial h}{\partial t} + \nabla.(h\boldsymbol{U})\right] \qquad for\ l = 1, \dots, p \quad \textbf{(18)}$$

and

$$\alpha_l = \frac{k_l}{\rho C_{pn}} \qquad for\ \ l = 1, \dots, p \quad \textbf{(19)}$$

where $\rho C_{pn}$ is the heat capacitance of layer n.

A jump balance at the interface between two layers ( $l\ and\ l-1$) using equation (12) leads to:

$$\boldsymbol{n}.\left(\alpha_l \nabla h - \frac{\rho C_{pl}}{\rho C_{pn}} h\boldsymbol{U}\right)_{+} = \boldsymbol{n}.\left(\alpha_{l-1}\nabla h - \frac{\rho C_{pl-1}}{\rho C_{pn}} h\boldsymbol{U}\right)_{-} \qquad for\ \ l = 1, \dots, p \quad \textbf{(20)}$$

$$h_{+} = h_{-} \quad \textbf{(21)}$$

Which leads to continuity of normal heat flux and temperature:

$$\boldsymbol{n}.\left(k_l \nabla T - \rho C_{pl} T\boldsymbol{U}\right)_{+} = \boldsymbol{n}.\left(k_l \nabla \mathrm{T} - \rho C_{pl-1} T\boldsymbol{U}\right)_{-} \qquad for\ \ l = 1, \dots, p \quad \textbf{(22)}$$

$$T_{+} = T_{-} \quad \textbf{(23)}$$

Equation (16) is of the same form as Eq. (8) and the normal heat flux continuity at the interface is ensured. Consequently, equation (17) can be solved using the lattice Boltzmann equation (Eq. 1) with an extra source term $F_k = w_k S_l$

$$f_k(\boldsymbol{r} + \boldsymbol{e}_k \Delta t, t + \Delta t) = f_k(\boldsymbol{r}, t) - \frac{\Delta t}{\tau}\left[f_k(\boldsymbol{r}, t) - f_k^{eq}(\boldsymbol{r}, t)\right] + \Delta t.F_k \quad \textbf{(24)}$$

$f_k^{eq}$ is now given by:

$$f_k^{eq}(\boldsymbol{r}, t) = w_k h(\boldsymbol{r}, t)\left[1 + \frac{\boldsymbol{e}_k \boldsymbol{U}}{c_s^2}\right] \quad \textbf{(25)}$$

In the case of two-dimensional transfers, the source term is approximated using a Control Volume Method (CVM) on a rectangular grid:

$$S_l = \left[1 - \frac{\rho C_{pl}}{\rho C_{pn}}\right]\left[\frac{1}{\Delta t}\left(h_{i,j,t} - h_{i,j,t-\Delta t}\right) + \frac{1}{\Delta x}\left((hu)_{i+1/2,j,t} - (hu)_{i-1/2,j,t}\right) + \frac{1}{\Delta y}\left((hv)_{i,j+1/2,t} - (hv)_{i,j-1/2,t}\right)\right] \qquad for\ \ l = 1, \dots, p \quad \textbf{(26)}$$

where $u$ and $v$ are the x-component and the y-component of the velocity vector $\boldsymbol{U}$ respectively. $i$ and $j$ are the grid nodes indices along x- and y-axis, respectively.

An upwind scheme is used to evaluate the convective terms:

$$(hu)_{i+1/2,j,t} = h_{i+1,j,t} max\llbracket u_{i+1/2,j,t}, 0\rrbracket - h_{i+1,j,t} max\llbracket -u_{i+1/2,j,t}, 0\rrbracket \quad \textbf{(27)}$$

$$(hu)_{i-1/2,j,t} = h_{i-1,j,t} max\llbracket u_{i-1/2,j,t}, 0\rrbracket - h_{i,j,t} max\llbracket -u_{i-1/2,j,t}, 0\rrbracket \quad \textbf{(28)}$$

$$(hv)_{i,j+1/2,t} = h_{i,j+1,t} max\llbracket v_{i,j+1/2,t}, 0\rrbracket - h_{i,j,t} max\llbracket -v_{i,j+1/2,t}, 0\rrbracket \quad \textbf{(29)}$$

$$(hv)_{i,j-1/2,t} = h_{i,j-1,t} max\llbracket v_{i,j-1/2,t}, 0\rrbracket - h_{i,j-1,t} max\llbracket -v_{i,j-1/2,t}, 0\rrbracket \quad \textbf{(30)}$$

The $\boldsymbol{r}$ components along x- and y-axis are respectively $i \times \Delta x$ and $j \times \Delta y$, ( $i = 0,1 \dots N_x$; $j = 0,1 \dots N_y$) $N_x$ and $N_y$ are the grid mesh size along x- and y-axis, respectively.

Once the $f_k$ are determined the temperature $T$ can be deduced:

$$T(\boldsymbol{r},t) = \frac{1}{\rho C_{pn}} \sum_{k=0}^{8} f_k(\boldsymbol{r},t) \quad \textbf{(31)}$$

## 3. Numerical results

### 3.1. Transient heat conduction in two layered medium with vertical interface

The first benchmark problem is 2D heat conduction in a two layered stratified medium. Initially the entire medium is at $T_0 = 0$. At time $(t > 0)$, Dirichlet boundary conditions are imposed at the left and right walls, while the horizontal ones are insulated (Fig. 1).

The results presented in Fig. 2, are for transient temperature distribution at the mid-length of the square enclosure. The thermophysical properties used in calculations are $k_1 = 2.0$, $k_2 = 0.5$, $\rho C_{p1} = 2.0$ and $\rho C_{p2} = 1.0$. Comparisons of obtained results with those of the finite volume method, shows excellent agreements, at transient period and also at the steady-state

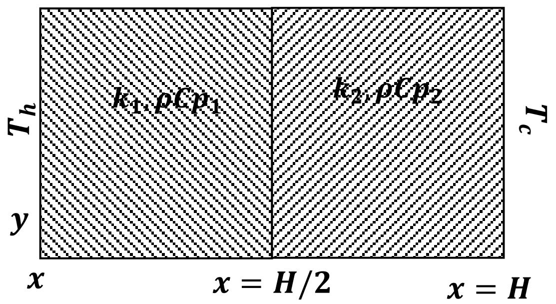


Fig. 1: Two layered medium

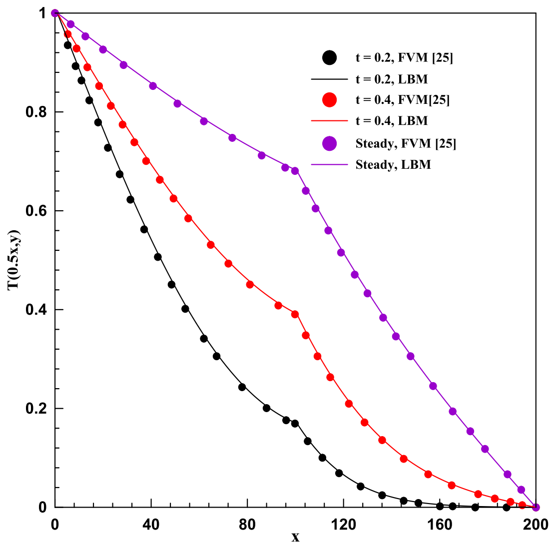


Fig. 2: Comparison of CVM with the present LBM formulation solutions for heat conduction in two layered medium.

### 3.2. Transient heat conduction in a square medium containing discrete circular media Transient heat conduction in two layered medium with vertical interface

To further demonstrate the capacity of the proposed method in simulating conjugate heat transfer in more complex geometry, we chose to solve transient heat conduction in a square medium containing discrete circular intrusions (Fig. 3) with different thermal properties.

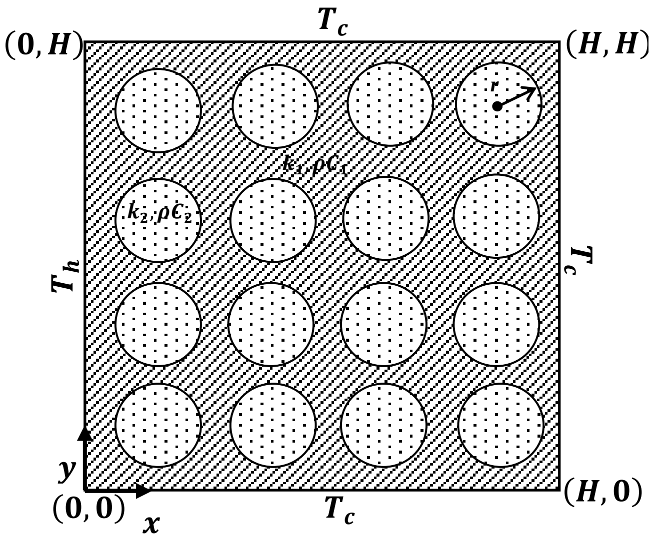


Fig. 3: Square medium containing discrete circular intrusions

We imposed a cold temperature, $T = 0.0$, at three walls (namely the north, south and east walls), the west side is raised to hot temperature equal to unity. The whole medium is initially at a uniform temperature $T_0 = 0$. The radius of each circular media is $r = 0.08$. The thermophysical properties used in the calculations are $k_1 = 1$, $k_2 = 10$, $\rho C_1 = 40$ and $\rho C_2 = 20$.

Fig. 4 shows comparisons of isotherms prediction obtained by the present LBM source formulation and CVM respectively at transient period and at a steady state. In both time $t$, excellent agreements are found.

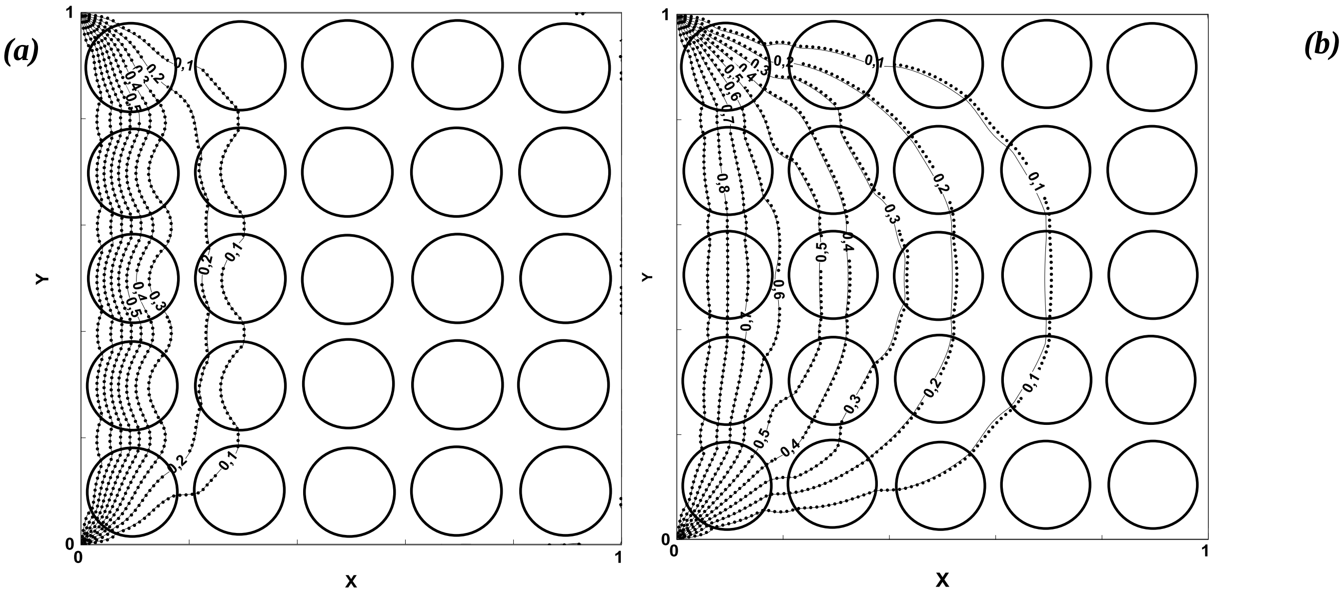


Fig. 4: Comparisons between present LBM source formulation (solid line) and CVM (symbol) prediction of isotherms at (a) $t = 0.1$ and (b) steady-state in a square medium containing multiple discrete intrusions of circular shape.

In this last test problem solved, we approach a porous media with different thermophysical properties and demonstrate the potential of the presented source term formulation to deal with more complexes heterogeneous media approaching more real applications.

### 3.3. Planar Taylor-Couette flow

The fourth test problem investigated is a planar Taylor-Couette in a 2D square medium as shown in Fig. 5. In this case, we further assess the ability of the proposed LBM formulation to solve a more complex convection-diffusion heat transfer problem involving a cylinder rotating at constant angular velocity $\omega_a$.

Initially, the entire domain is at the cold temperature $T_c$. Then, for any time ($t > 0$), the bottom face is set at the hot temperature $T_h$.

One crucial criterion fulfilled in this simulation is a Reynolds number that ensures a laminar flow between the two cylinders. The Reynolds number is given by

$$Re_c = U_0 \frac{(r_b - r_a)}{\nu} \quad \textbf{(32)}$$

where $U_0$, $r_a$, and $r_b$ are the viscosity of the fluid rotating between the cylinders, velocity of the fluid flow, radius of the inner cylinder and radius of the outer cylinder, respectively .

The value of the critical Reynolds number is [23] $Re_c = 156.7$

For $Re < Re_c$, the analytical velocity profile between two co-axial cylinders is given by [24]:

$$u(r) = \frac{a}{r} + br \quad \textbf{(33)}$$

where constants $a$ and $b$ have the following form [24]:

$$a = \frac{r_a^2 r_b^2}{(r_b^2 - r_a^2)} \omega_a \quad \textbf{(34)}$$

$$b = -\frac{r_a^2}{(r_b^2 - r_a^2)} \omega_a \quad \textbf{(35)}$$

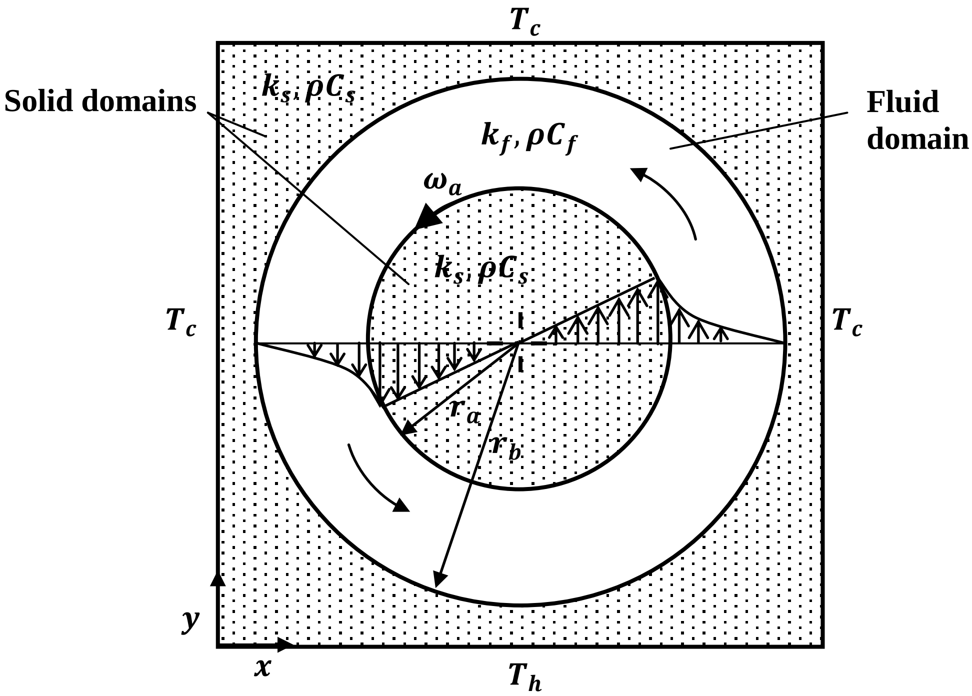


Fig. 5: Schematic of planar Taylor-Couette flow

Fig. 5 shows the computational domain, the boundary conditions and the velocity profile in the inner rotating cylinder and between the two cylinders. Initially the entire medium is set at a cold temperature $T = 0$.

The thermo-physical properties used to compute the solutions are: $k_s = 0.3$, $k_f = 0.5$, $\rho C_{ps} = 4$ and $\rho C_{pf} = \frac{10}{3}$ (Fig. 6) and $k_s = 0.3$ and $k_f = 0.5$, $\rho C_{ps} = 4$, and $\rho C_{pf} = 2$ (Fig. 7). The velocity value is $U_0 = 10^{-2} (m/s)$ . The radius of inner cylinder and outer cylinder are $r_a = 0.25$ and $r_b = 0.4$, respectively. Simulation was carried out with a $400 \times 400$ mesh.

Adopting a planar Couette-Taylor heat transfer problem brings us to implement the full source term expression (Eq. 26). A solid enthalpy based formulation is chosen for this test problem and when detailing calculation of the source term in the whole geometry, we have for the fixed solid domain, $S_l = 0$.

For the rotating cylinder and for the fluid between the two cylinders, $S_l$ takes the expression given in Eq. (26). In this case, both x-and y-components of the velocity are taken into consideration and have impacts on the obtained results. With this particular test problem, we also show the potential of the proposed LBM formulation to deal efficiently with curved interfaces.

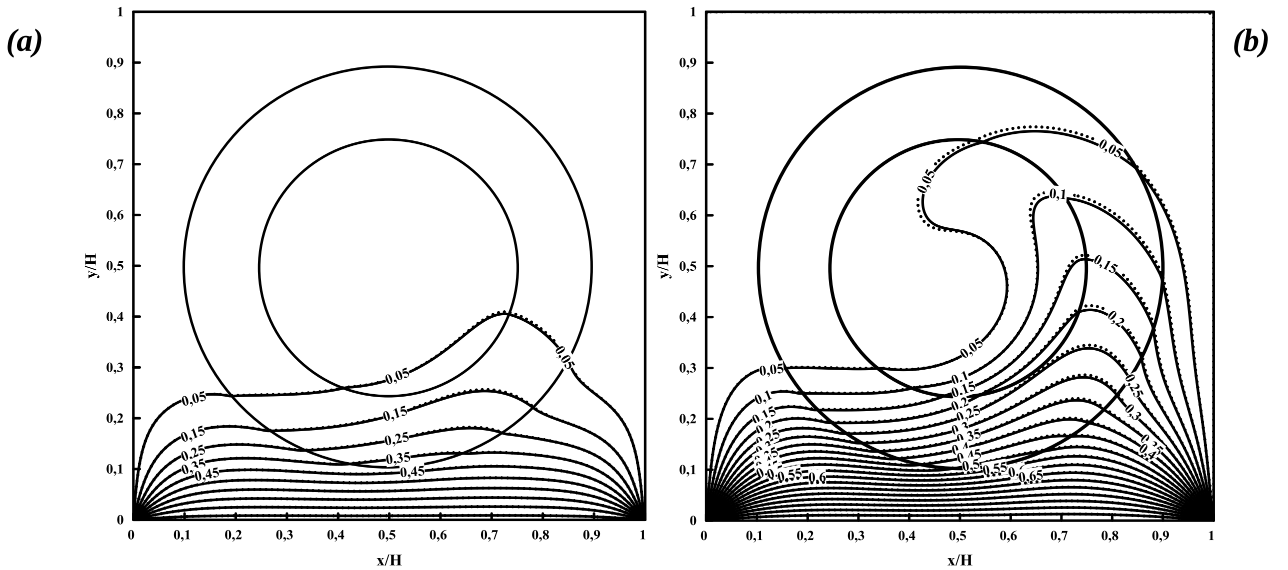


Fig. 6: Comparisons between present LBM formulation (symbol) and CVM (solid line) prediction of isotherms at *(a)*$t = 2$ and (b) $t = 5.0$ for planar Taylor-Couette flow $k_s = 0.3$ and $k_f = 0.5$, $\rho C_{ps} = 4$, and $\rho C_{pf} = 10/3$

We provide comparison of isotherms obtained by the present LBM formulation and Control Volume Method at various time steps (Fig. 6-7). All the comparisons are in very good agreement.
As time evolves, the temperature gradient develops with a clear effect of the direction of the fluid flow, together with the movement of the inner cylinder, which keeps the memory of its heating while in the bottom zone. In Fig. 7(b), the asymmetry is illustrated between the right and left side of the enclosure. This asymmetry is mainly the result of rotation, which produces a convective transport, both in the fluid and in the rotating cylinder

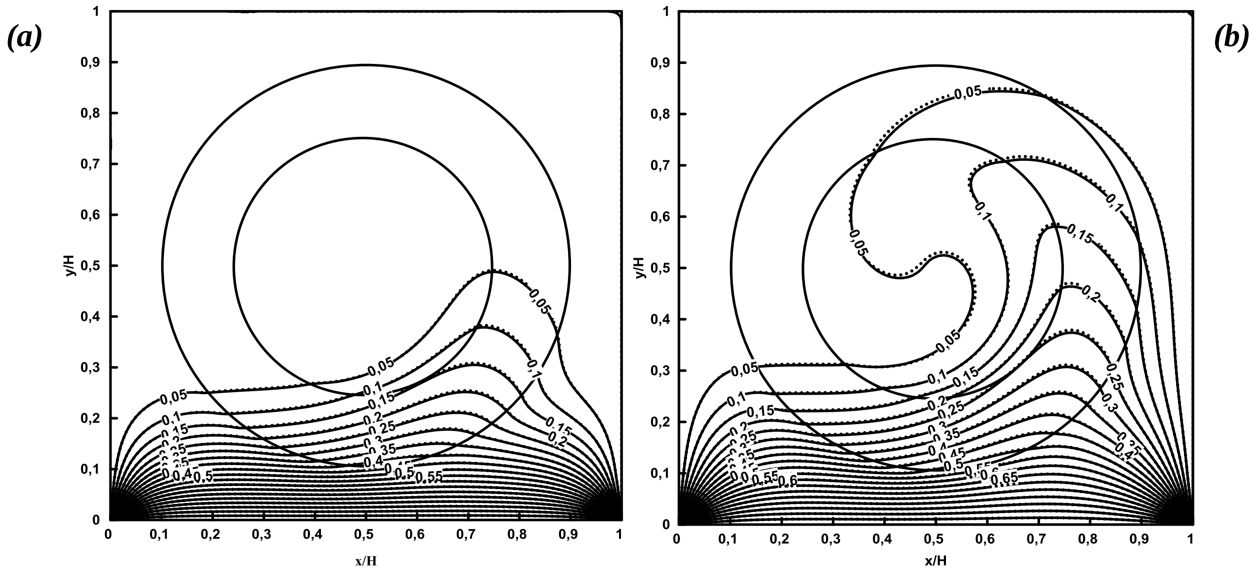


Fig. 7: Comparisons between present LBM formulation (symbol) and CVM (solid line) prediction of isotherms at, *(a)*$t = 2$ and (b) $t = 5.0$ for planar Taylor-Couette flow, $k_s = 0.3$ and $k_f = 0.5$, $\rho C_{ps} = 4$, and $\rho C_{pf} = 2$

## 4. Conclusion

An enthalpic lattice Boltzmann Method formulation to deal with convection-diffusion heat transfer problems in heterogeneous media is presented in this study. By using this new source formulation, relatively simple and easy to implement, two benchmarks of conjugate heat diffusion problems, and one conjugate convection-diffusion problem have been successfully investigated. In all cases, excellent agreement was found with the Control Volume Method solutions. This approach does not require any specific treatment and/or constraint on the distribution functions at the interfaces. It is also independent on the choice of Lattice scheme( $D2Q9, D2Q4, D3Q15, \dots$). Therefore it possesses a great potential to solve any heat convection-diffusion problem with irregular and evolving interface in multiphase and multi-component media. It can naturally be extended to multiple relaxation time lattice Boltzmann models

## Nomenclature

| | |
|---|---|
| $a, b$ | constants in analytical velocity profile |
| $c$ | lattice streaming speed $\left(c = \frac{\Delta x}{\Delta t}\right)$ |
| $C_p$ | heat capacity $(J/KgK)$ |
| $c_s$ | speed of sound |
| $\boldsymbol{e}_k$ | propagation velocity in the $k^{t\square}$ direction in a lattice |
| $f_k$ | particle distribution function in the $k$ direction |
| $f_k^{eq}$ | equilibrium particle distribution function in the $k$ direction |
| $F_k$ | source term in the $k^{t\square}$ direction in a lattice |
| □ | enthalpy |
| $H$ | characteristic height $(m)$ |
| $\boldsymbol{n}$ | normal to the interface |
| $N_x, N_y$ | grid mesh size |
| $r_a$ | radius of inner cylinder |
| $r_b$ | radius of outer cylinder |
| $R_e$ | Reynolds number |
| $R_{ec}$ | critical Reynolds number |
| $S$ | source term |
| $t$ | time |
| $T$ | temperature |
| $\boldsymbol{U}$ | velocity vector |
| $u, v$ | velocity components |
| $w_k$ | weight factor in the $k$ direction |
| $\Delta t$ | time step |
| $\Delta x$ | lattice size |
| $x, y$ | axial coordinates |

**Greek symbols**

| | |
|---|---|
| $\alpha$ | thermal diffusivity $(m^2/s)$ |
| $\lambda$ | thermal conductivity $(W/mK)$ |
| $\nu$ | viscosity of the fluid $(m^2/s)$ |
| $\rho$ | density $(Kg/m^3)$ |
| $\tau$ | relaxation time |
| $\omega_a$ | angular velocity |

**Superscripts**

| | |
|---|---|
| $eq$ | equilibrium |

**Subscripts**

| | |
|---|---|
| $f$ | fluid |
| $i, j$ | grid nodes indices |
| $k$ | direction $k$ in a lattice |
| $l$ | layer suffix |
| $s$ | solid |

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