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A three-dimensional enthalpic Lattice Boltzmann formulation for convection-diffusion heat transfer problems in heterogeneous media

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Abstract : In this paper, an enthalpic Lattice Boltzmann method formulation for 3-D unsteady convection-diffusion heat transfer problems, is used to overcome discontinuity issues in heterogeneous media. The new formulation is based on the appearance of a source term added to the collision step. The major achievement of the proposed enthalpic LB formulation is avoiding any interface treatments or geometry considerations even when dealing with complex geometries. The performance of the present method is tested for several three-dimensional convection-diffusion problems. Comparisons are made with the Control Volume Method and numerical results show excellent agreements.

Keywords: Lattice Boltzmann Methods, Enthalpic formulation, 3-D simulation, unsteady convection-diffusion, heterogeneous media.

1. Introduction

Due to its substantial significance, heat transfer in heterogeneous media is investigated by many researchers[1-6]. This field is widely encountered in many domains such as energy engineering, cooling electronics or mechanical equipments, food engineering, and environmental control. Indeed, in a wide range of academic or engineering applications, media can be heterogeneous or compose, fluid flow and heat transfer are coupled. As an example of conjugate heat transfer problems, fluid flows occurring within ducts. One of the most common multiphase flows, where energy exchange occurs at interface between component is observed in evaporation process. In this specific thermal phenomena, thermo-physical properties can change sharply between components like liquid and it's vapor phase, or solid and fluid phases.

Lattice Boltzmann Methods (LBM) is widely used to simulate successfully industrial and real life fluid flow problems in many specific topics like multiphase flows [7, 8], turbulent flows [9, 10], micro-fluidics [11,12], or deformable boundary [13]. Although it has many advantages, namely it's simple algebraic manipulation, it's easy

solution procedure and implementation of boundary conditions, the lattice Boltzmann method still have 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. Some researchers narrow studies on steady-state condition to avoid such constraints [14-16]. 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 that heat capacitance is the same in all components. This strategy was presented for traditional CFD methods to simplifies computation[17]. Wang et al. [18] and Tarokh et al. [19] engage successful studies on this particular case. Unfortunately, those approaches lack of maturity against other CFD methods like Control Volume Method, among others, where discontinuities are easily overcome. For this reason improvements in the conventional LBM become a mandatory task. Up until recently, the common idea of most proposed researches was based on introducing conjugate boundary conditions at interfaces to take into account the balance of energy in those particular regions (interfaces). Meng et al. [20] used double-spaces lattice Boltzmann model based on internal energy to resolve temperature scalar fields. The interface in this case close to the wall and fluid node in each internal direction and unknown distribution function, are treated by internal energy counter-slip boundary condition assuming that they are at equilibrium. Seddiq et al. [21] resolved distribution function at row node interface assuming that the ratio of their gradient is proportional to thermal conductivities ratio, this yields to an explicit expression for non tangential distribution function at interface using the solid-fluid relaxation parameter, where formulation of tangential one is obtained by supposing that their difference is proportional to the difference of their post-streaming distribution function. Li et al. [22] proposed to treat interface using Dirichlet and Neumann boundary based bounce back. The approach considers that boundary interface thickness is zero, this means that the interface nodes are common for the solid and fluid media. The formulation of distribution function of first interior node in each medium was derived, taking into account local geometry. Moreover, the spatial interpolation help to describe boundary shape, and the formulation is appropriate for curved boundary. Mohamad et al. [23] used finite difference scheme to calculate iteratively temperature at interface. Two approaches were proposed: considering the working medium whether as two separated medium or as a single medium. In the first one, the two media are treated independently and the value of unknown distribution function can be calculated using temperature at surface. In the second approach the two medium are treated as a single one. The technique is inspired from multi-grid technique, largely used in fluid flow simulation, the non equilibrium part is rescaled at interface whereas the relaxation time is the average of the relaxation time of two working media. The equilibrium part is calculated directly with temperature value.

In the above mentioned studies, solutions proposed needs to localize exactly the interface boundary which predict complication of those techniques for the case of deformable boundary or multiphase flow where interface section can change position and shape during simulation. The procedure will be, obviously, computationally demanding. Moreover, most of the above cited studies take in consideration only the conservation of normal conductive heat flux. This restricts studies for fixed boundary whereas moving ones cannot be handled. Recently, some research studies begin to propose another approach by introducing an LBM formulation independent of boundary shape, and without interface treatment. Karani and Huber [24] introduced a source term for LBM formulation. The expression of the proposed source term is defined as the product of the gradient of volumetric heat capacity calculated by finite difference methods, and the total heat flux calculated locally. However, Hu et al. [25] assume that previous formulation suffer from mathematical rigor in differentiating a piecewise constant

function, and proposed an adaptation of the technique in [24], by replacing the heat capacity of the solid phase of that of the fluid phase and provided proofs that by doing so, continuity of the normal heat flux is ensured even for the cases of curved interfaces.

Nearly, a new lattice Boltzmann formulation based on enthalpic diffusion equation was proposed by Hamila et al. [26] to solve conduction in heterogeneous medium. A source term formulation was applied and the continuity of temperature and normal conductive heat flux was satisfied across components. Moreover no extra treatments were needed at interfaces. The method is greatly simple and can be easily implemented.

In this paper the same approach is adopted and developed to perform three dimensional transient convection-diffusion heat transfer problems for three dimensional problems. The performance of the present method is successfully validated by several three dimensional heat convection-diffusion problems in heterogeneous media.

The remainder of the present paper is organized as follows; Section II presents the proposed three-dimensional enthalpic lattice Boltzmann formulation for unsteady convection-diffusion. Section III provides the validation of the proposed method through comparisons with Control Volume Method solutions of several test problems. Section IV concludes the paper.

2. ENTHALPIC LATTICE BOLTZMANNFORMULATION

The macroscopic heat transfer diffusion-convection equation takes the following form [27]:

$$\frac{\partial T}{\partial t} + \nabla.(\boldsymbol{U}T) = \nabla.(\alpha\nabla.T) \tag{1}$$

where $\alpha = k/\rho C_p$ is the thermal diffusivity , ρ is the density, C_p is the volumetric heat capacity, and k is the thermal conductivity.

The macroscopic diffusion-convection equation is recovered with Chapmann-Enskog expansion from the following BGK lattice Boltzmann equation [27]:

$$f_k(\boldsymbol{r} + \boldsymbol{e}_k\Delta t, t + \Delta t) = f_k(\boldsymbol{r}, t) - \frac{\delta t}{\tau}\left[f_k(\boldsymbol{r}, t) - f_k^{eq}(\boldsymbol{r}, t)\right] \tag{2}$$

where δt denotes lattice time step, $\boldsymbol{e}_k$ is the discrete lattice velocity. τ denotes the lattice relaxation parameter, f_k is the distribution function and f_k^{eq} denotes the equilibrium distribution function.

The relaxation parameter and equilibrium function are defined as following:

$$\tau = \frac{3\alpha}{|\boldsymbol{e}_k|^2} + \frac{\Delta t}{2} \tag{3}$$

$$f_k^{eq}(\boldsymbol{r}, t) = w_k T(\boldsymbol{r}, t)\left[1 + \frac{\boldsymbol{e}_k \boldsymbol{U}}{c_s^2}\right] \tag{4}$$

$\boldsymbol{U}$ is the velocity vector, e_k and w_k represent respectively the discretized velocities and their corresponding weight.

For the D3Q19 scheme, the value of the discretized velocities are [27]:

$$e_k = \begin{cases} (0,0,0)c, & k = 0 \\ (\mp 1,0,0)c, (0,\mp 1,0)c, & k = 1,2,\dots,6 \\ (\mp 1,\mp 1,0)c, (\mp 1,0,\mp 1)c, (0,\mp 1,\mp 1)c, & k = 7,8,\dots,18 \end{cases} \tag{5}$$

$$w_0 = \frac{1}{3}, w_{1,\dots,6} = \frac{1}{18}, w_{7,\dots,18} = \frac{1}{36} \tag{6}$$

where c_s represent the speed of sound on lattice, and $c = \Delta x/\Delta t$ with Δx is the grid size.

In general, the heat diffusion convection equation takes the following form:

$$\frac{\partial(\rho C_p T)}{\partial t} + \nabla.(\rho C_p \boldsymbol{U} T) = \nabla.(\mathrm{k}\nabla.T) \tag{7}$$

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

$$T_+ = T_- \tag{8}$$

$$\boldsymbol{n}.\left[k\nabla T - \rho C_p \boldsymbol{U} T\right]_+ = \boldsymbol{n}.\left[k\nabla T - \rho C_p \boldsymbol{U} T\right]_- \tag{9}$$

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

The conventional LBM formulation given by Eq.(2) solves Eq.(1) which allow Eq.(7) to be solved only in two simplified configurations: uniform heat capacitance ρC_p and steady-state heat diffusion-convection transfer configurations. This restriction on conventional LBM can be demonstrated by writing a jump balance at interface to Eq.(1)

$$T_+ = T_- \tag{10}$$

$$\boldsymbol{n}.[\alpha\nabla T - \boldsymbol{U} T]_+ = \boldsymbol{n}.[\alpha\nabla T - \boldsymbol{U} T]_- \tag{11}$$

This leads to:

$$T_+ = T_- \tag{12}$$

$$\boldsymbol{n}.\frac{1}{\rho C_{p+}}\left[k\nabla T - \rho C_p \boldsymbol{U} T\right]_+ = \boldsymbol{n}.\frac{1}{\rho C_{p-}}\left[k\nabla T - \rho C_p \boldsymbol{U} T\right]_- \tag{13}$$

The Eq. (11) leads to Eq. (13) only when the heat capacity is the same:

$$\rho C_{p-} = \rho C_{p+} \tag{14}$$

In order to extend the LBM to solve general diffusion-convection equation [Eq.(7)], we begin by write the macroscopic convection-diffusion equation for an heterogeneous media composed by p layers:

$$\frac{\partial(\rho C_{pl} T)}{\partial t} + \nabla.(\rho C_{pl} \boldsymbol{U} T) = \nabla.(k_l \nabla.T) \qquad for\ \ l = 1, \dots, p \tag{15}$$

In the above Eq.(15), we define a new enthalpic variable $h = C_{pn}T$ to get Eq. (16)

$$\frac{\partial(h)}{\partial t} + \nabla.(h\boldsymbol{U}) = \nabla.(\alpha_l \nabla.h) + S_l \qquad for\ \ l = 1, \dots, p \tag{16}$$

where

$$S_l = \left[1 - \frac{\rho C_{pl}}{\rho C_{pn}}\right]\left[\frac{\partial h}{\partial t} + \nabla.(h\boldsymbol{U})\right] \qquad for\ l = 1, \dots, p \tag{17}$$

and

$$\alpha_l = \frac{k_l}{\rho C_{pn}} \qquad for\ \ l = 1, \dots, p \tag{18}$$

where ρC_{pn} is the heat capacitance of layer *n*.

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

$$\boldsymbol{n}.\left(\alpha_l \nabla h - \frac{\rho C_{pl}}{\rho C_{pn}} h\boldsymbol{U}\right)_+ = \boldsymbol{n}.\left(\alpha_{l-1} \nabla h - \frac{\rho C_{pl-1}}{\rho C_{pn}} h\boldsymbol{U}\right)_- \qquad for\ l = 1, \dots, p \tag{19}$$

$$h_+ = h_- \tag{20}$$

The two above equations (19) and (20) leads to continuity interface equation for temperature and its normal heat flux:

$$\boldsymbol{n}.\left(k_l \nabla T - \rho C_{pl} T\boldsymbol{U}\right)_+ = \boldsymbol{n}.\left(k_l \nabla \mathrm{T} - \rho C_{pl-1} T\boldsymbol{U}\right)_- \qquad for\ l = 1, \dots, p \tag{21}$$

$$T_+ = T_- \tag{22}$$

With the enthalpic formulation the jump interface conditions is satisfied for total heat flux and numerically the problem can be seen as a single medium. Moreover, the Eq.(16) can be solved directly with BGK-lattice Boltzmann equation (Eq.(2)) and S_l is taken as an extra source term. This source term is discretized with Control Volume Methods (CVM) on a rectangular grid. For a three-dimensional case its expression is as below:

$$\begin{aligned} S_l = \left[1 - \frac{\rho C_{pl}}{\rho C_{pn}}\right]\Big[&\frac{1}{\Delta t}\left(h_{i,j,m,t} - h_{i,j,m,t-\Delta t}\right) + \frac{1}{\Delta x}\left((hu)_{i+1/2,j,m,t} - (hu)_{i-1/2,j,m,t}\right) \\ &+ \frac{1}{\Delta y}\left((hv)_{i,j+1/2,m,t} - (hv)_{i,j-1/2,m,t}\right) \\ &+ \frac{1}{\Delta z}\left((hw)_{i,j,m+1/2,t} - (hw)_{i,j,m-1/2,t}\right)\Big] \qquad for\ l = 1, \dots, p \end{aligned} \tag{23}$$

where $u;\ v; w$ denote respectively x-component, y-component and z-component of U velocity vector and i, j, m denotes indices of lattice in x, y, z direction

For the convective terms appeared in the source term expression (Eq.(23)), an upwind scheme is used for their evaluations. Once f_k are determined, the temperature can be deduced:

$$T(\boldsymbol{r}, t) = \frac{1}{\rho C_{pn}} \sum\nolimits_k f_k(\boldsymbol{r}, t) \tag{24}$$

The present method can be naturally extended to multiple relaxation time lattice Boltzmann models.

3. NUMERICAL RESULTS

In this section three dimensional conjugate heat transfer problems are solved through three benchmarks configurations, namely a diffusion-convection heat transfer problem inside a cubic duct and a 3-D Couette-Taylor inside a cubic medium. All numerical simulation tests are performed with D3Q19 lattice scheme. Results obtained by the proposed enthalpic lattice Boltzmann formulation are compared with Control Volume solutions.

3.1. 3-D diffusion-convection heat transfer inside square duct

To demonstrate the validity and accuracy of the proposed enthalpic formulation, we start by solving a three dimensional heat transfer inside a square duct. In such case, the discontinuities at the interface appear between duct walls and fluid domains. The wall duct is taken with a non null thickness as show in Fig. 1. The velocity profile of flow flowing inside the square duct is given by [28]. For a rectangular section of height b and width a, and for $-a \le y \le a$ and $-b \le z \le b$, we have [28]:

$$u(y,z) = \frac{16a^2}{\mu\pi^3}\left(-\frac{d\hat{p}}{dx}\right) \sum_{i=1,2,\dots}^{\infty} (-1)^{\left(\frac{i-1}{2}\right)} \left[1 - \frac{cosh\left(\frac{i\pi z}{2a}\right)}{cosh\left(\frac{i\pi b}{2a}\right)}\right] \frac{cos\left(\frac{i\pi y}{2a}\right)}{i^3} \tag{25}$$

where $\hat{p}$ is the effective pressure and μ is the viscosity.

In the present simulation, two parametric sets of thermo-physical properties are performed:

- Simulation (1): $C_{psolid} = 3.5,\ C_{pfluid} = 6, k_{solid} = 1.5,\ k_{fluid} = 2$
- Simulation (2): $C_{psolid} = 4,\ C_{pfluid} = 3, k_{solid} = 1.5,\ k_{fluid} = 2.5$

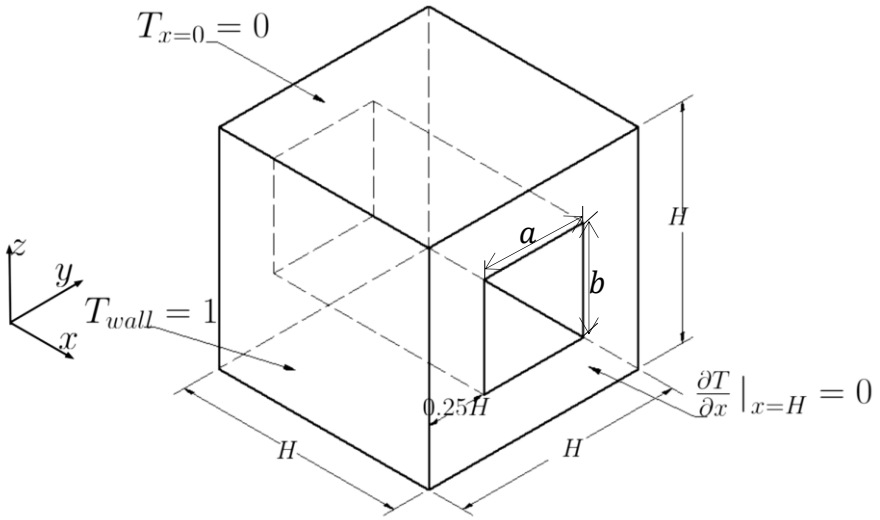


Fig. 1: Schematic of 3d square duct

Initially, the temperature in the whole domain is set to $T = 0$. Elsewhere, the temperature at the entrance section is set to $T_{x=0} = 0$ and for the outlet section, the gradient of temperature is supposed null. The temperature at the external surface of the channel is set to $T_{wall} = 1$.

In modeling boundary condition we adopt a non equilibrium bounce-back concept declaring that the incoming particle toward the solid boundary, bounce back inside the computation domain.

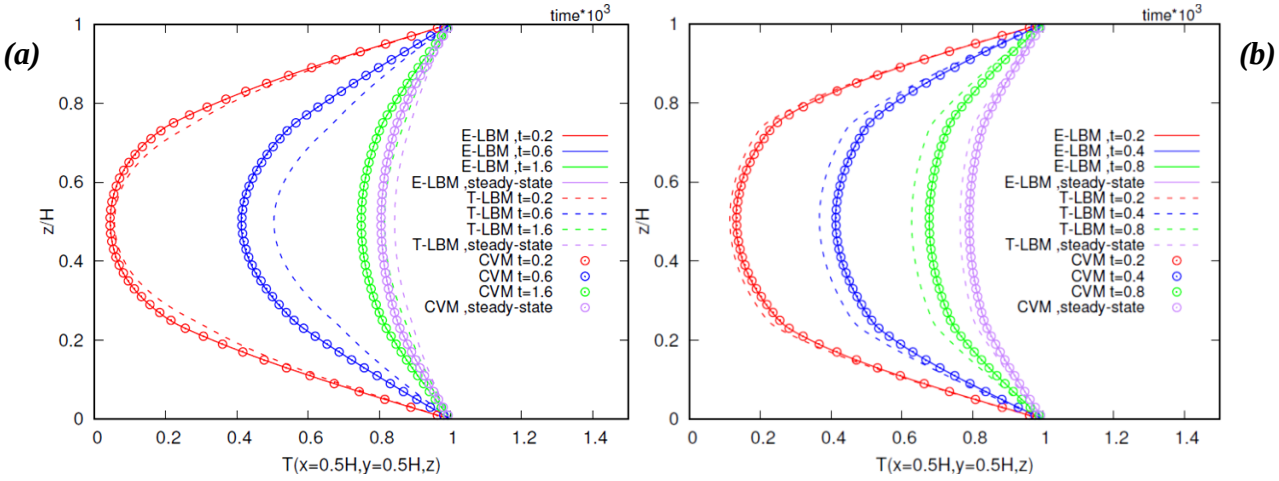


Fig. 2: Comparison between the present enthalpic LB formulation (solid line), CVM (symbol) and conventional LB prediction (dashed line) of temperature distribution for the mid x-axis and mid z-axis at different time steps. (a): $C_{psolid} = 3.5,\ C_{pfluid} = 6, k_{solid} = 1.5, k_{fluid} = 2$, (b): $C_{psolid} = 4,\ C_{pfluid} = 3, k_{solid} = 1.5, k_{fluid} = 2.5$

Fig.2 show a comparison of temperature at mid x-axis and mid z-axis between the proposed enthalpic lattice Boltzmann (E-LBM) formulation, the Control Volume solution (CVM) and the conventional thermal lattice Boltzmann (T-LBM) predictions at transient period as well as steady-state. As intended, we can notice clearly the accordance between the enthalpic formulation and CVM predictions for all the performed tests and during transitional regime as well as steady state, while the conventional T-LBM gives erroneous results towards CVM predictions. In both two parametric simulations, there are no remarkable effects on the accordance between E-LBM predictions and CVM results with the change of thermophysical properties ratios.

Likewise, we mention that the results for the corners or edges interface nodes presents excellent agreement as shown for the temperature profile along the diagonal of the square duct (Fig.3), where $x = y = z$. For this particular locations where two edges meet and form a corner, no additional assumptions or modifications have to be done to the enthalpic LB formulation proposed.

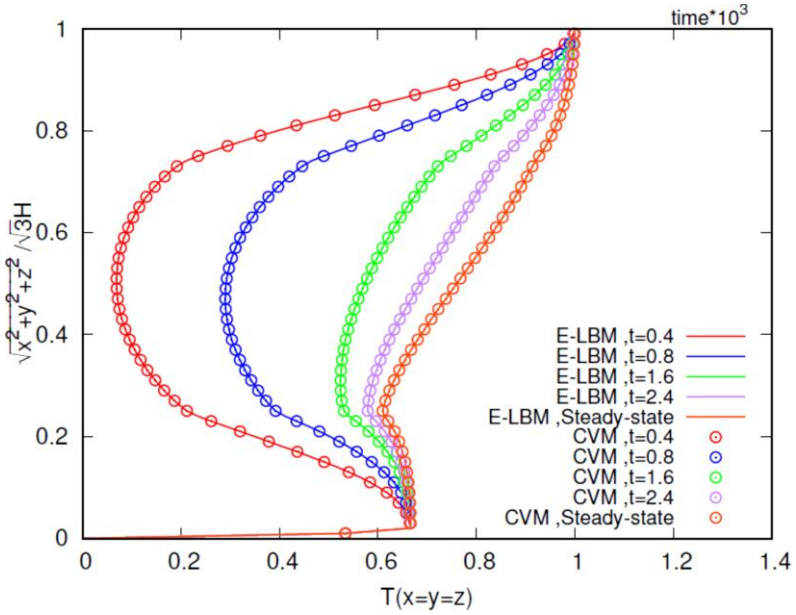


Fig. 3: Comparisons between present enthalpic LB formulation (solid line) and CVM prediction (symbol) of temperature distributions for square's diagonal at different time steps.

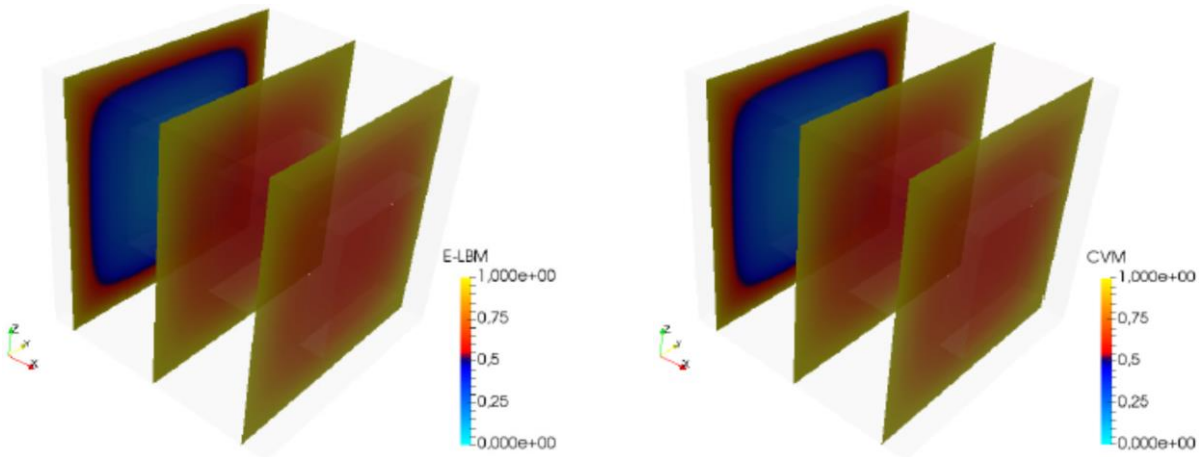


Fig. 4: Sketch of three dimension comparison between the present enthalpic LB formulation (left) and CVM solution (right) temperature prediction for flow in square duct at different slices: $x/H = 0.1, x/H = 0.5$ and $x/H = 0.9$ at $t = 0.8 \times 10^3 s$

Fig.4 shows a three dimensional qualitative comparison between enthalpic formulation and CVM method prediction of temperature distribution at different slice position along x-axis. Very good agreements are shown.

3.2. 3-D Convection-Diffusion heat transfer in a partially heated Couette-Taylor

To demonstrate the ability of the proposed E-LBM formulation to deal with complex geometries, we simulate a 3-D Couette-Taylor conjugate convection-diffusion heat transfer problem. The geometry under consideration is a set of two co-axial cylinders plugged within a 3D square enclosure, where physically we suppose that the length of the enclosure is boundless. For the Couette-Taylor flow, only inner cylinder (C_1) is rotating with an angular velocity equal to ω_α, whereas the external one (C_2) is fixed as show in Fig. 5.
The analytical velocity profile between two co-axial cylinders is given by [29]:

$$u(r) = \frac{\alpha}{r} + \beta r$$

where constants α and β have the following form [29]:

$$\alpha = \frac{r_\alpha^2 r_\beta^2}{\left(r_\beta^2 - r_\alpha^2\right)} \omega_\alpha$$

$$\beta = -\frac{r_\alpha^2}{\left(r_\beta^2 - r_\alpha^2\right)} \omega_\alpha$$

The part of the bottom $(y = 0)$ lateral external surface located between $0.3 < x/H < 0.6$ is heated at $T = 1$, while the remaining surfaces are kept at imposed temperature $T = 0$. At the other external surfaces ($x = 0$ and $x = H$) we impose a zero temperature gradient. Initially the temperature is set to $T = 0$ in the whole domain. This present case put different challenges under investigation in order to demonstrate the capacity of the proposed E-LBM to correctly solve conjugate heat transfer in complex geometries.

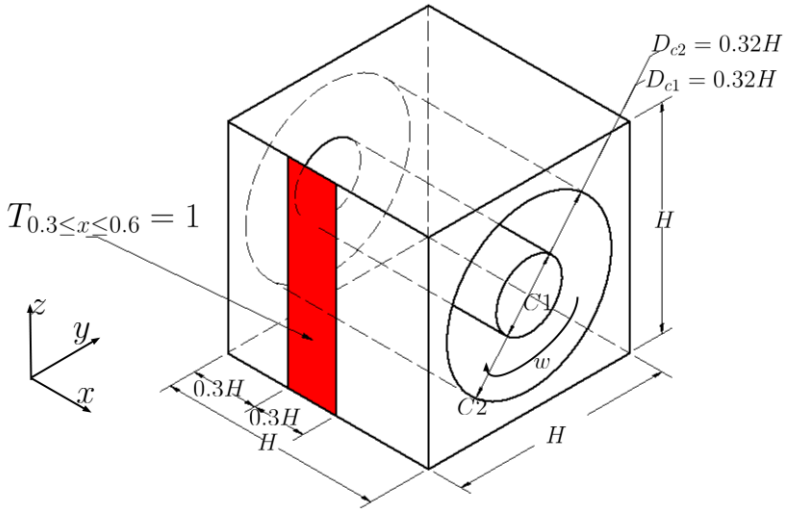


Fig. 5: Schematic of 3D Couette-Taylor problem

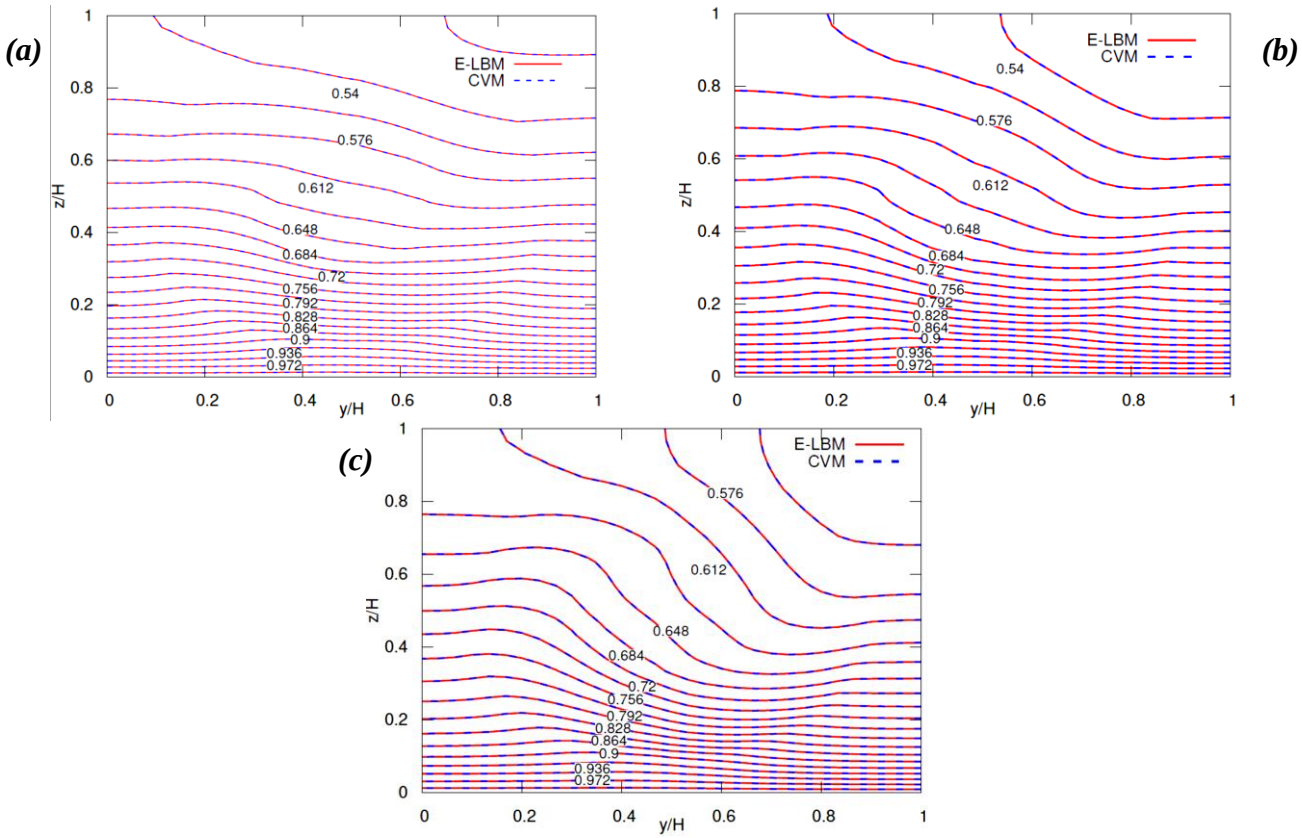
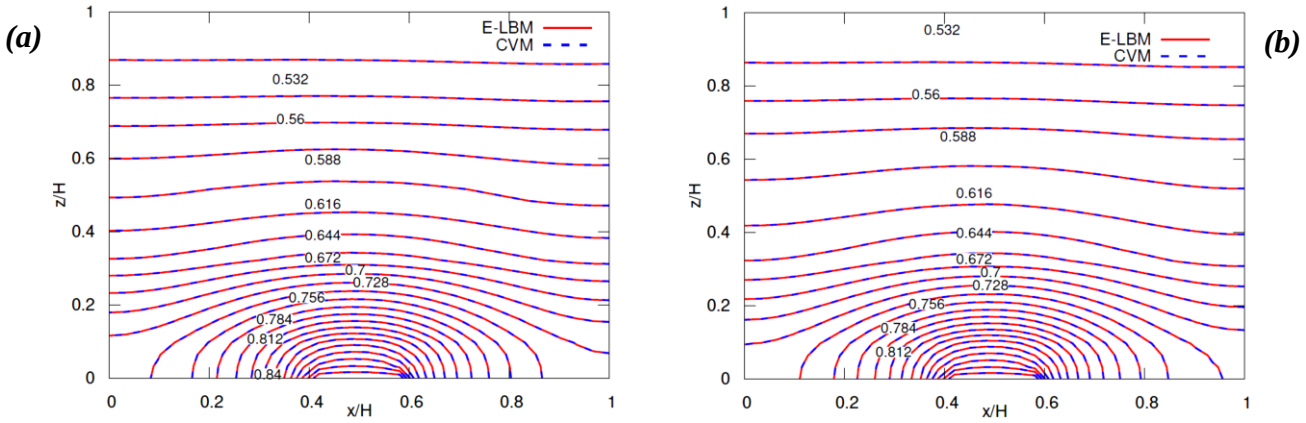


Fig. 6: Comparison between enthalpic LB formulation (red solid line) and CVM (blue dashed line) solution of isotherms at slice $x/H = 0.5$ (a) :$Pe = 0.5$, (b):$Pe = 1$,and (c):$Pe = 2$ at time $t = 0.024s$

In first hand, the two interfaces between fluid and cylinders medium are curved. In the other hand, there are two velocity components in Cartesian coordinate due to the rotation of fluid resulting from the rotation effect of the inner cylinder. Simulations were performed with three different values of the Peclet number, $Pe = \frac{UH}{\alpha}$, where H is the side of the cube, U the velocity and α is the diffusivity.

Fig.6 and 7 show a comparison of isotherms obtained by enthalpic LB formulation and CVM respectively at vertical mid plane and horizontal mid plane slice of the square. Obviously, the present comparison show good agreement. When varying the Peclet number $(Pe = 0.5, 1\ and\ 2)$, the influence of dominated convective flow over diffusive heat transfer, and conversely is obtained.

Fig.8 demonstrates a three dimensional contours results in which we show a three-dimensional quantitative comparison of temperature distribution predicted by the proposed enthalpic LB formulation and CVM solutions and evinces the three-dimensions effect along x-axis.



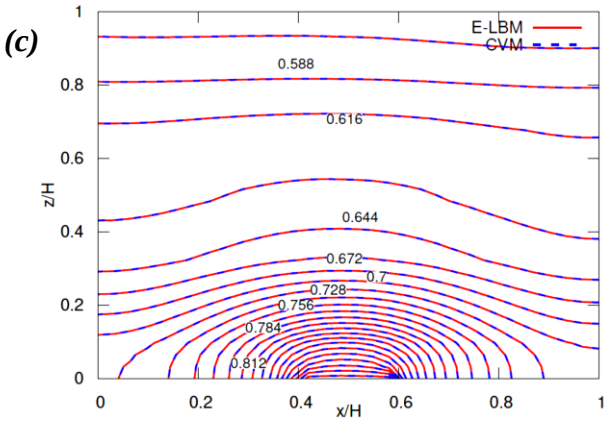


Fig. 7: Comparison between LB enthalpic formulation (red solid line) and CVM (blue dashed line) solution of isotherms at slice $y/H = 0.5$ (a) :$Pe = 0.5$, (b):$Pe = 1$, and (c):$Pe = 2$ at time $t = 0.024s$

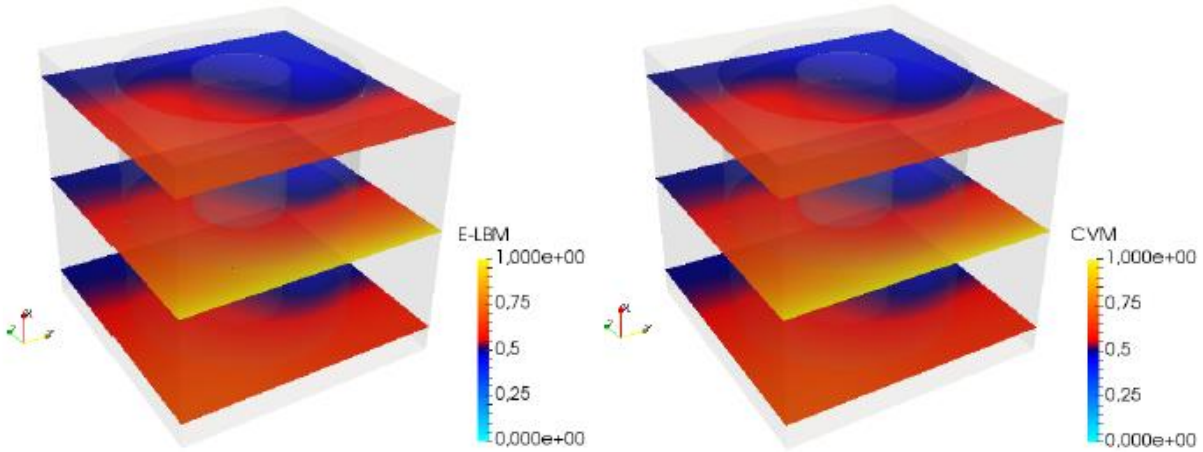


Fig. 8: Sketch of three dimensions comparison between the present enthalpic LBM formulation and CVM solution temperature prediction for flow in Couette-Taylor with $Pe = 2$ at different slice: $x/H = 0.1, x/H = 0.5, x/H = 0.9$ and at time $t = 0.0184s$

Conclusion

A new enthalpic formulation for Lattice Boltzmann method is proposed to overcome discontinuity issues existing with conventional thermal lattice Boltzmann method for heat transfer in heterogeneous medium. The proposed formulation satisfied the jump condition at component interface, by the presence of a correction source term, which as the same time is seen by the conventional thermal LB equation as external source. Then, the enthalpic diffusion-convection equation can be solved directly with standard LB-BGK approximation. Even with his apparent simplicity the proposed E-LBM present no restrictions in correctly solving complex numerical simulations. In different tests released, the enthalpic LB formulation presents an excellent agreement with Control Volume Methods for unsteady-state as well as for the steady regime. The additional source term avoids any extra efforts to implement specific interface treatments owed in other researches. The method feature is validated with different interface type for both curved and straight shape.
Finally, even if in all the presented tests simulated we only take a single-relaxation-time LB model, the extension to its multiple-relaxation-time counterpart is straightforward.

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