C. R. Mecanique 340 (2012) 518–525

Contents lists available at SciVerse ScienceDirect

Comptes Rendus Mecanique

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Analytical and innovative solutions for heat transfer problems involving phase change and interfaces

On the aptitude of the lattice Boltzmann approach for the treatment of the transient heat transfer with crack resistance

Un modèle basé sur la méthode de gaz sur réseaux pour le traitement des contacts thermiques transitoires

M. El Ganaoui [a,*], S. Addakiri [a,b], E. Semma [b]

[a] *Université de Lorraine, Lermab-Longwy, IUT Henri Poincaré, 186, rue de Lorraine, 54400 Cosnes et Romain, France*
[b] *Université Hassan I, Laboratoire de Mécanique, FST de Settat, B.P. 577, Settat, Morocco*

ARTICLE INFO

Article history:
Available online 17 May 2012

Keywords:
Lattice Boltzmann model
Heat transfer
Thermal contact resistance
Numerical simulation
Modelling
Boundary conditions

Mots-clés :
Méthode de gaz sur réseaux
Transferts thermiques
Resistance thermique du contact
Simulation numérique
Modélisation
Conditions aux limites

ABSTRACT

A numerical approach is introduced within the outline of the thermal lattice Boltzmann method developments to solve problems with cracks. It consists on an extension of the termed Partial Bounce Back scheme (PBB) to transient situations. A special case of the scheme leads to account the thermal contact resistance between surfaces. Numerical examples are provided to validate and demonstrate the accuracy of the proposed methodology and its applicative potential.

RÉSUMÉ

Une nouvelle approche numérique est introduite dans le sillage des développements des méthodes de gaz sur réseaux pour résoudre des problèmes en présence de contact imparfait. L'approche consiste en une extension du schéma PBB (Partial Bounce Back) aux situations transitoires. Le développement permet la prise en compte de la nature du contact entre deux milieux solides. Des exemples numériques permettent de valider et de montrer la précision de cette approche ainsi que son potentiel applicatif.

Version française abrégée

Les transferts aux interfaces présentent une importance particulière dans de nombreux problèmes appliqués et posent des défis numériques dans leur modélisation, qui dans la plupart des études, est basée sur des raccordements à base d'éléments discrets (méthodes numériques classiques de type différences finies DF, volumes finis VF, éléments finis EF, ...).

Par ailleurs, les méthodes de gaz sur réseau (LBM) émergent comme une alternative sérieuse aux méthodes conventionnelles (EF, VF, ...). Les développements se focalisent sur les problèmes d'écoulements isothermes puis aux couplages avec les transferts [1–8,26] mais un potentiel important est possible pour des problèmes particuliers (interfaces, contacts, milieux multiphasiques, poreux, ...).

* Corresponding author.
E-mail address: ganaoui@uhp-nancy.fr (M. El Ganaoui).

1631-0721/$ – see front matter © 2012 Published by Elsevier Masson SAS on behalf of Académie des sciences.
http://dx.doi.org/10.1016/j.crme.2012.03.010

Récemment, Han et al. [25] ont utilisé la technique de réflexion partielle (PBB) pour modéliser la résistance de contact par la méthode de gaz sur réseaux. Cette approche donne des résultats acceptables en régime stationnaire mais souffre d'imprécisions en régime transitoire. Dans le présent travail, on propose une nouvelle approche basée sur l'image des fonctions de distribution lors du passage d'un milieu à un autre (IP). Les résultats basés sur cette technique sont comparés avec la solution analytique et permettent de bien prédire le comportement thermique à l'interface.

Le principe de traitement dans un schéma LBM est présenté sur la Fig. 2 pour la transmission entre deux milieux en vue d'une application à un bicouche Fig. 3.

L'étude comparative en régime stationnaire, est portée sur une large gamme de temps de relaxation allant de 0,55 à 1. Les Figs. de 4 à 7 montrent la distribution spatiale de la température pour les deux méthodes comparée à la solution analytique. Les deux modèles donnent le même comportement thermique avec une bonne précision en comparaison avec la solution analytique. Les résultats issus du modèle PBB pour $\tau = 1$ sont expliqués par les hypothèses de base adoptées par Han et al. concernant les conditions aux limites portant sur les fonctions (f_i) [25].

Cette condition n'est vérifiée que pour les régimes permanents ou un temps de relaxation égal à 1. Le modèle PBB ne produit plus un profile proche à la solution analytique (voir par exemple pour l'instant $t = 5000$ lu pour $\tau = 0{,}8$, $R_C^l = 1000$, Fig. 5). Ceci s'explique par le fait que lorsque le temps de relaxation s'éloigne de la valeur unité, le modèle s'éloigne des hypothèses adoptées par les auteurs en régime stationnaire et la sous estimation des fonctions (f_i) introduit des imprécisions au niveau du calcul pas seulement pour le gradient thermique sur l'interface mais aussi la distribution de la température dans les deux corps et par conséquent induit une erreur sur les résultats de simulation.

1. Introduction

In recent years, the lattice Boltzmann method (LBM) has emerged as an alternative to conventional computational fluid dynamics methods employing the Navier–Stokes equations. It has found extensive applications in simulating isothermal flows of various complexities; see for instance [1–8]. There has also been an ongoing effort in the construction of stable lattice Boltzmann methods to solve heat transfer problems (TLBM) [9]. In the early works, the isothermal lattice Boltzmann model is extended with additional velocities to obtain the temperature evolution. The LBM leads to numerical instabilities and hence the temperature variation is limited to a narrow range. To overcome the defects, He et al. [9] introduced a double population approach by using a density distribution function to simulate hydrodynamics for fluid flows and an internal energy distribution function to simulate thermodynamics for heat transfer. This model has better numerical stability and the viscous heat dissipation and compression work done by the pressure can be solved fundamentally.

As a result, it has been extensively adopted by researchers to solve various thermo-hydrodynamic problems [10–12]. With regard to the thermal boundary conditions, several methods have been developed. D'Orazio et al. [10] propose a thermal counter-slip approach, in which a counter-slip thermal energy density is assumed for boundary nodes and is determined consistently with Dirichlet or Neumann boundary constraints. Tang et al. [11] introduce a thermal boundary treatment by decomposing the internal energy distribution functions at the boundary nodes into equilibrium and no equilibrium parts.

Huang et al. [12] propose a thermal curved wall boundary scheme based on the idea of non-slip wall boundary treatment for isothermal LBM. In this work, we attempt to incorporate thermal contact resistance into the thermal lattice Boltzmann framework. Thermal contact resistance exists when two solid bodies come in contact. Heat flows from the hotter body to the colder body, and a temperature drop is usually observed at the interface between the two surfaces in contact. Thermal contact resistance can be very important in a number of applications [13–22]. Loulou et al. [23,24] present an experimental study of the evolution of thermal contact conditions (temperature jump at the interface, heat flux and transient thermal contact resistance) during solidification of a liquid metal drop on water-cooled wall. Laraqi et al. [13] propose an exact analytical solution to calculate the thermal constriction resistance due to moving heat sources on semi-infinite bodies. An extension to finite media has been developed in [14,15]. It is however a stiff phenomenon influenced by many factors, among which surface roughness is believed to play a central role as no real surface is perfectly smooth. Unfortunately there is no satisfactory theory which will predict thermal contact resistance for all situations.

2. Crack problem formulation and analytical solution

The task here is to make a model for evolution crack problem, then some basic considerations related to the methods and key parameters will be given followed by a test case treatment:

$$\frac{\partial T_i}{\partial t} = \frac{\partial}{\partial x}\left[k(T)\frac{\partial T_i}{\partial x}\right] \tag{1}$$

x refers to space [m], t to time [s], T to the temperature [K], k is the thermal conductivity [W/m.K]. The transmission conditions at the interface can be written:

$$[q_i]_\Sigma = -\frac{[T]_\Sigma}{R_C}, \quad i = 1, 2 \tag{2}$$

$q_i = k_i \partial T_i / \partial x$ is the heat flux and $[\ ]_\Sigma$ indicates a jump at the interface and R_C represents the value of thermal resistance contact. The two layers are two different initial temperatures (T_{i0} is the initial temperature for the layer i) and the contact is located at $x = 0$. In perfect contact case, the temperature jump at the interface is null (continuity of the thermal field).

The analytical solution gives:

$$T_i(y,t) = T_{i0} + \frac{A_i}{B}\left[erfc\left((-1)^{i+1}\frac{1}{2}\frac{x}{\sqrt{\alpha_i t}}\right) - \exp\left((-1)^{i+1}\frac{xB}{\sqrt{\alpha_i}} + B^2 t\right) erfc\left((-1)^{i+1}\frac{1}{2}\frac{x}{\sqrt{\alpha_i t}} + B\sqrt{t}\right)\right] \tag{3}$$

with:

$$A_1 = \frac{-T_e\sqrt{a_1}}{k_1 R_C}, \qquad A_2 = \frac{\sqrt{\alpha_2/\alpha_1}\, T_e\sqrt{\alpha_1}}{k_2 R_C}, \qquad B = \left(\frac{k_2\sqrt{\alpha_1} + k_1\sqrt{\alpha_2}}{k_2 k_1 R_C}\right)$$

erf and *erfc* represent respectively the error function and the complementary of error function. $T_e = T_{10} - T_{20}$ ($T_{10} = 1$ and $T_{20} = 0$ in dimensionless form more practical for comparisons). See Fig. 3.

This time dependent solution will serve for comparison between existing models in the literature and present developments.

3. The LB computational solution method

3.1. Basic considerations

The LBM method is an original based on a distribution function $f_i(x,t)$ which expresses the probability to locate a particle in x point at time t, taking a velocity $e_i = \Delta x_i/\Delta t$ (with Δx_i and Δt the space and time steps respectively). The LBM equation writes:

$$\partial_t f_i(x,t) + e_i.\nabla f_i(x,t) = \Omega_i(f) \tag{4}$$

Based on two steps (collision) modelled in the term $\Omega_i(f)$, in a linearized form:

$$\Omega_i(f) = \frac{1}{\tau}\left(f_i^{eq}(x,t) - f_i(x,t)\right) \tag{5}$$

Introducing τ the relaxation time (toward the equilibrium state), and $f_i^{eq}(x,t)$ the equilibrium distribution function leads to LBGK model:

$$\partial_t f_i(x,t) + e_i.\nabla f_i(x,t) = \frac{1}{\tau}\left(f_i^{eq}(x,t) - f_i(x,t)\right) \tag{6}$$

The time integration leads to:

$$f_i(\mathrm{x} + \mathrm{e}_i\Delta t, t + \Delta t) = f_i(\mathrm{x},t) + \frac{\Delta t}{\tau}\left(f_i^{eq}(\mathrm{x},t) - f_i(\mathrm{x},t)\right) \tag{7}$$

Then the LBM model is completely defined by the choice of the equilibrium distribution function [9]. For FHP model (D2Q9), this function is given by:

$$f_i^{eq} = \omega_i\rho\left[1 + 3\frac{e_i.u}{c^2} + \frac{9}{2}\frac{(e_i.u)^2}{c^4} - \frac{3}{2}\frac{u.u}{c^4}\right] \tag{8}$$

where ω_i are the weighting coefficients relating to D2Q9 model, u the velocity vector and c the lattice speed.

Hydrodynamic macroscopic quantities such as density ρ [kg m^{-3}] and velocity u [m s^{-1}] are recovered by:

$$\rho(x,t) = \sum_i f_i(x,t) \tag{9}$$

$$\rho u(x,t) = \sum_i e_i f_i(x,t) \tag{10}$$

3.2. Transmission models

It consists on determining the distribution functions traducing the transmission conditions at the interface (Eq. (2)). We will focus on the PBB model introduced in [25] and our present model.

To fix the purpose, let us consider the heat transfer in a rectangular cavity submitted to heat flux (q_{ix}) through two media in contact (Fig. 1).

D2Q9 LBM scheme allows one to write:

$$q_{ix} = \sum_{\alpha=0}^{8} f_\alpha e_\alpha$$

$$q_{ix} = f_1 - f_3 + f_5 - f_6 + f_8 - f_7$$

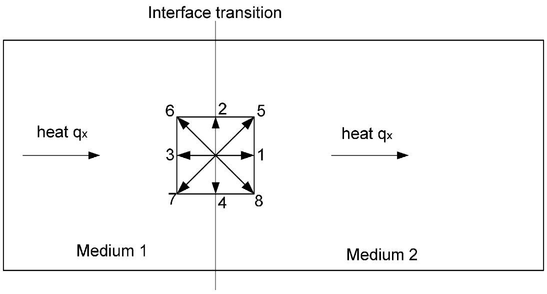

Fig. 1. Heat conduction in a fully adiabatic rectangular cavity.

Knowing that f_3, f_6 and f_7 of the medium 1 reaches two the medium 2 through f_1, f_5 and f_8 allows one to write:

$$q_{ix} = f_1^2 + f_5^2 + f_8^2 - f_3^1 - f_6^1 - f_7^1$$

Then:

$$f_1^2 + f_5^2 + f_8^2 = q_{ix} + f_3^1 + f_6^1 + f_7^1$$

For the determination of each distribution function in the medium 2, a relationship between the two medias is needed.

4. Extended transitional model and comparisons

4.1. The PBB model

This model is based on a partial reflexion of the particle energy at the contact area. Only a part of the internal energy of the body 1 is allowed to be transmitted to the adjacent node in the body 2, there is a rebound in the opposite direction. This model consists in determining the distribution functions at the time crossing from a medium to another by considering a partial reflexion of the energy of the particle on the contact line. Only part of the internal energy of a node of border of body 1 is allowed to be propagated with its adjacent node of border of body 2 and the remaining part is rebounded again with the node itself with the opposite direction. Measurement of contact resistance according to δ (partial bounce back parameter) is based on the steady assumption of the thermal transfer to the level of the interface of contact.

Then in this model the thermal contact resistance is linked to LBM parameters [25] by:

$$R_C = \frac{3\delta}{1-\delta} \tag{11}$$

Namely if f_α^{I,M_1} denotes the distribution function of the internal energy in the node I of the boundary in the direction α, and δ the control parameter varying continuously between 0 and 1, then $(1-\delta) f_\alpha^{1,M_1}$ is the quantity to be absorbed in the node J of the body M and $\delta f_\alpha^{1,M_1}$ is bounce at the node I in the direction α. The choice of α is achieved in such a way that the thermal contact resistance been represented. It is based on a stationary assumption (relaxation time equal to unity).

4.2. The particle image (PI model)

In order to take into account the transient state for a large relaxation time range, we assume that both borders in contact are juxtaposed and their distribution functions during the propagation phase are proportional. The proportionality factor is independent on the direction of propagation (assumption of isotropy) but just of the medium considered. Fig. 2 represents the distribution functions. In the isotropic case, these functions are recovered by two matrix relationships:

$$\begin{pmatrix} f_3^{e1} \\ f_6^{e1} \\ f_7^{e1} \end{pmatrix} = \alpha I_d \begin{pmatrix} f_3^{e2} \\ f_6^{e2} \\ f_7^{e2} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} f_1^{e2} \\ f_5^{e2} \\ f_8^{e2} \end{pmatrix} = \beta I_d \begin{pmatrix} f_1^{e1} \\ f_5^{e1} \\ f_8^{e1} \end{pmatrix} \tag{12}$$

where I_d is the 3×3 identity matrix. Model leads on evaluating α and β conserving the interface transmission conditions (Eq. (2)). (See Fig. 3.)

About boundary conditions, the reader can find in the literature various LBM possibilities of treatment. The Bao et al. [26] treatment is used here. It consists on determining a fictive density $\rho(x_P, t)$ based on the conservation hypothesis. The unknown distribution functions are:

$$f_\alpha^{unknown}(x,t) = \omega_\alpha \rho(x_P, t) \tag{13}$$

At the wall/interface singularity, the same procedure is adopted.

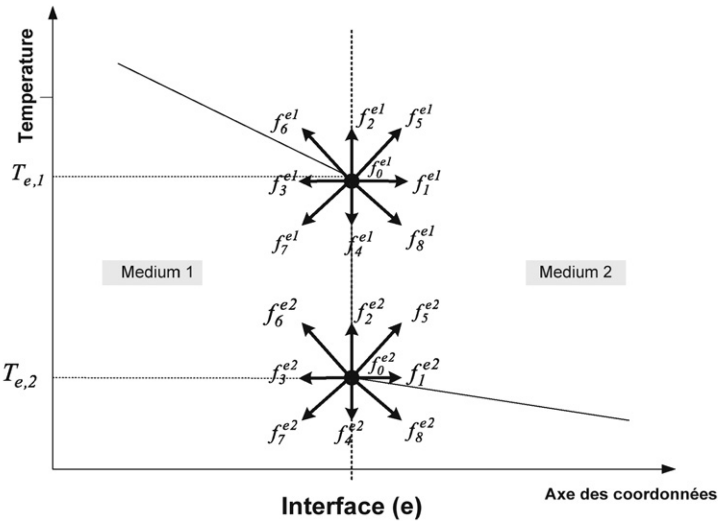

Fig. 2. Configuration diagram for the new model LBM.

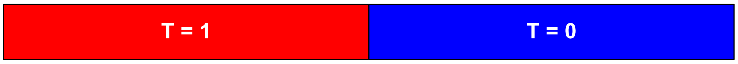

Fig. 3. Diagram simplified for a semi-infinite bi-layer material.

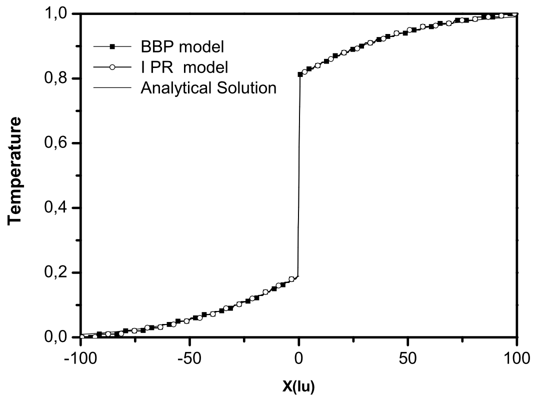

Fig. 4. Temperature distribution in space ($\tau = 1$, $t = 10\,000$ lu, $R_C^l = 1000$).

4.3. Comparisons

This article is focusing on the validation of the proposed model and its accuracy, $\tau_1 = \tau_2 = \tau$, inducing the dimensionless diffusion coefficients $\alpha_1 = \alpha_2 = (\tau - 1/2)/3$. The comparative study covers a range of relaxation time from 0.55 to 1. The spatial temperature distribution for $t = 10\,000$ lu, $\tau = 1$ and $R_C^l = 1000$ (Fig. 4). The two models exhibit accurate agreement with the analytical solution. The PBB model for $\tau = 1$ corresponds to the hypothesis of Han et al. [25]:

$$f_2 = f_4 = f_2^{eq} = \frac{1}{6}T \tag{14}$$

This hypothesis corresponds to permanent regimes or relaxation time of unity.

A temperature profile is given (Fig. 5) at $t = 5000$ lu for $\tau = 0.8$, $R_C^l = 1000$. The BBP model exhibits a difference with the analytical. One can explain by the relaxation time to the value of one underlying a limit of the steady regime the underestimate of the functions f_2 and f_4 introducing inaccuracy in the computations of thermal gradients and temperature fields in the two bodies in contact.

For a weak relaxation time, Figs. 6 and 7 present a comparison of PBB model to analytical one, the present model reaches the analytical one but BBP exhibits more deviation to the analytical solution.

To test the model regarding the contact quality (R_C value), Fig. 8 shows the temperature distribution for 0 and 10 000. It is shown the perfect contact and a right behaviour of the temperature gap with bad contact.

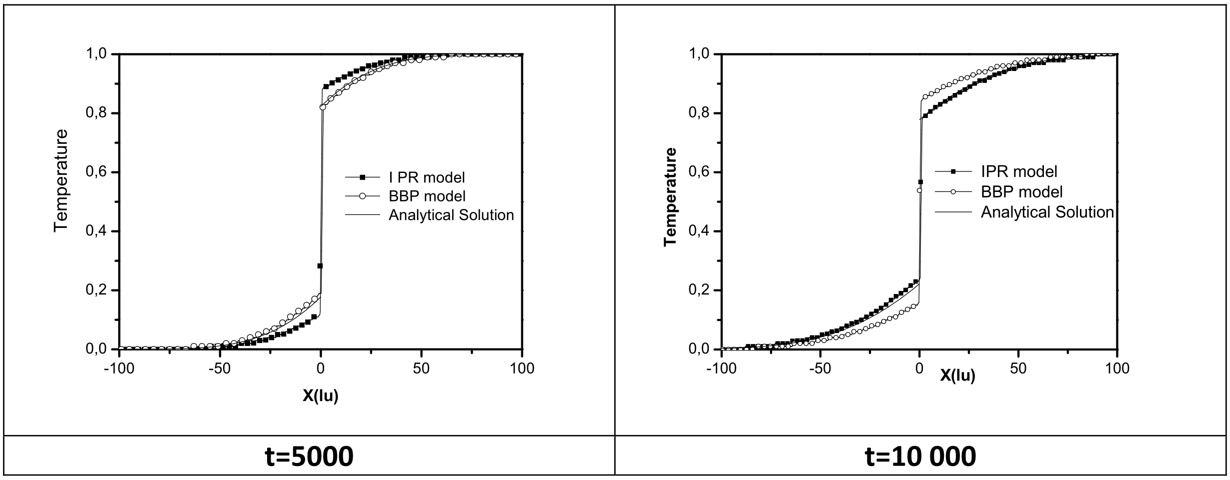

Fig. 5. Temperature distribution in space ($\tau = 0.8$, $R_C^l = 1000$).

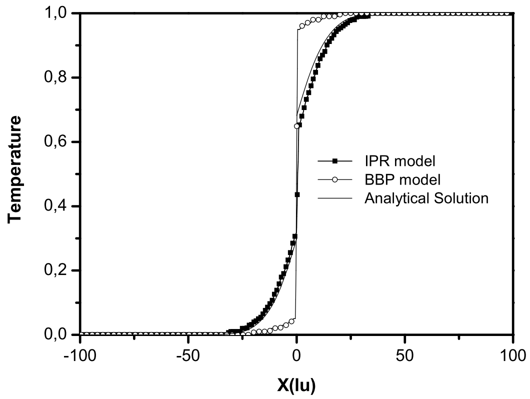

Fig. 6. Temperature profile for $\tau = 0.55$, $R_C^l = 1000$, $t = 5000$.

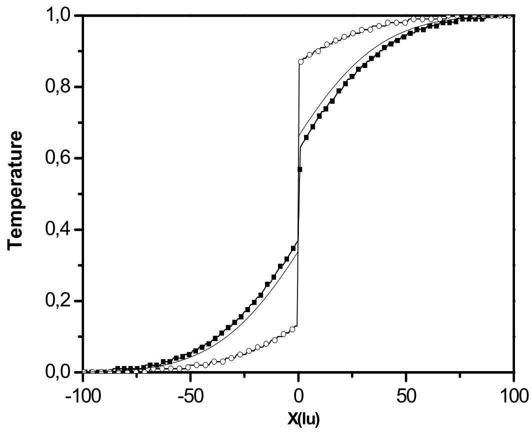

Fig. 7. Temperature profile for $\tau = 0.6$, $R_C^l = 1000$, $t = 20\,000$.

5. Conclusion

This article is in framework of the ability of the LBM model to solve two layer problems with imperfect contact, such as the case of the temperature field shown in Fig. 9. The model is based on coupled PBB (partial bounce back) and PI (particle image) approaches. This work is a step ahead to solve problems with crack resistance by using LBM method.

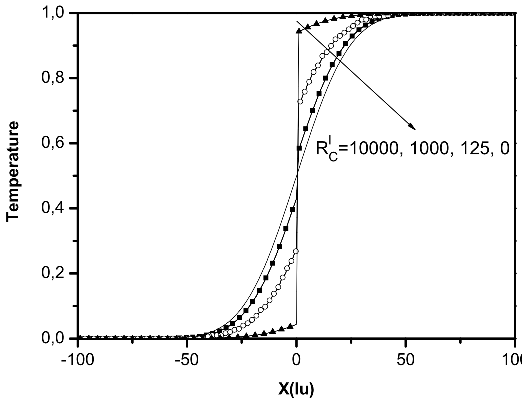

Fig. 8. Temperature profile at time step $t = 5000$ for various values of the contact resistance ($\tau = 0.6$).

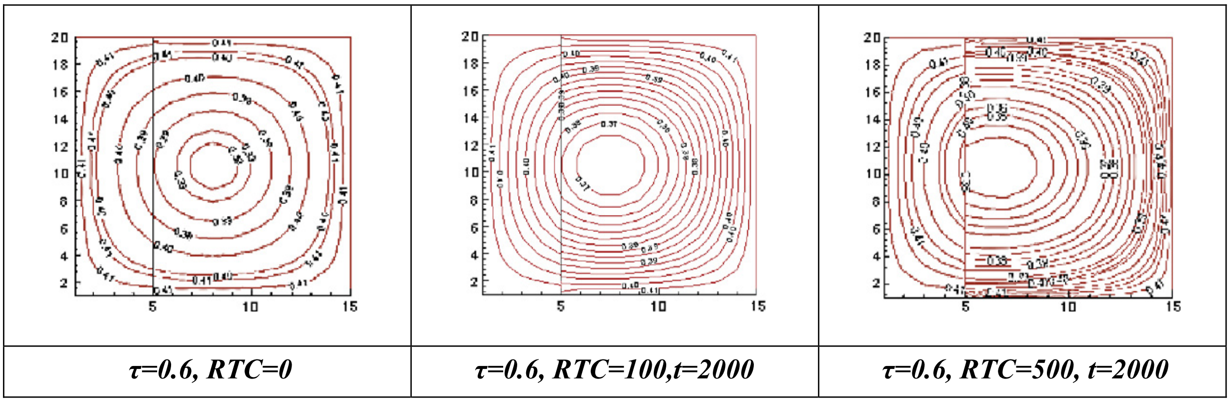

Fig. 9. Thermal field showing the capture of the temperature jump for imperfect contact.

A potential applicative domain is the composite material synthesis where droplet (known as also splat) generally hot in liquid phase is applied to a cold support (known also as substrate). In fact, during the process of solidification of the splat, the contact of the two bodies is never perfect and present irregularities. The high heat flux will have a tendency to pass through the contacts solid/solid. This phenomenon tends to increase the heat gradient through the interface of contact. The work follows on investigating this domain.

Acknowledgements

Prof. A.A. Mohamad (Univ. Calgary) and R. Bennacer (ENS Cachan) are acknowledged for very enlightening discussions concerning the LBM during visits. B. Pateyron from the SPCTS – University of Limoges is also acknowledged for advise and recommendations. Our thanks go also to France–Maghreb Hubert-Curien program of exchange.

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