



HAL
open science

**A CFD SOLVER BASED ON THE LATTICE
BOLTZMANN METHOD TO SOLVE
THREE-DIMENSIONAL THERMALLY DRIVEN
FLOWS AND COUPLED MOLECULAR GAS
RADIATION: COMPARISON AND VALIDATION
AGAINST A BENCHMARK SOLUTION**

Félix Schmitt, Frederic Andre, Mathieu Galtier, Etienne Vergnault, Laurent Soucasse, Jerome Jacob, Lucie Merlier

► **To cite this version:**

Félix Schmitt, Frederic Andre, Mathieu Galtier, Etienne Vergnault, Laurent Soucasse, et al.. A CFD SOLVER BASED ON THE LATTICE BOLTZMANN METHOD TO SOLVE THREE-DIMENSIONAL THERMALLY DRIVEN FLOWS AND COUPLED MOLECULAR GAS RADIATION: COMPARISON AND VALIDATION AGAINST A BENCHMARK SOLUTION. 7th Thermal and Fluids Engineering Conference (TFEC), May 2022, Las Vegas, France. pp.409-418, 10.1615/TFEC2022.emt.041362 . hal-04516505

HAL Id: hal-04516505

<https://hal.science/hal-04516505>

Submitted on 22 Mar 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



A CFD SOLVER BASED ON THE LATTICE BOLTZMANN METHOD TO SOLVE THREE-DIMENSIONAL THERMALLY DRIVEN FLOWS AND COUPLED MOLECULAR GAS RADIATION: COMPARISON AND VALIDATION AGAINST A BENCHMARK SOLUTION

Félix Schmitt,^{1,*} Frédéric André,¹ Mathieu Galtier,¹ Etienne Vergnault,¹ Laurent Soucasse,² Jérôme Jacob,³ Lucie Merlier¹

¹Univ Lyon, INSA Lyon, CNRS, CETHIL, UMR5008, 69621 Villeurbanne, France

²Laboratoire EM2C, CNRS, CentraleSupélec, Université Paris-Saclay, 8-10 rue Joliot Curie, 91192 Gif-sur-Yvette, France

³Aix Marseille Univ, CNRS, Centrale Marseille, M2P2 UMR 7340, 13451 Marseille, France

ABSTRACT

Characterizations of heat exchanges and flow structures of thermally driven convection in simple configurations such as enclosed cavities have been intensively carried out both experimentally and numerically for a wide range of Rayleigh numbers. In most cases, the problem is reduced to a thermal conduction-advection flow induced by temperature differences at the boundaries. However, some recent works have emphasized the significant role of radiative transfer in the thermal stratification and stability of the flow. The present work introduces a new solver built from a CFD code based on the lattice Boltzmann method under the Boussinesq approximation coupled with a radiative transfer model solving the Radiative Transfer Equation in participating molecular gases. Simulations are performed in a differentially heated three-dimensional cubical cavity filled with a air/H₂O/CO₂ mixture. Stationary solutions of the resulting laminar flow are obtained and the overall effects of gas radiation on the flow characteristics are obtained. Results are compared to a benchmark solution. Temperature, velocity and radiative heat source profiles in the cavity fit particularly well in all cases, along with convective and radiative heat fluxes at the walls. The present numerical model is shown to be relevant to solve thermal natural convection problems at low Rayleigh numbers with limited computational costs. Results are discussed with the aim of highlighting some modelling features which should be handled with care in order to perform accurate simulations.

KEY WORDS: Natural convection, CFD, Radiative transfer, LBM, Gas mixture radiation

1. INTRODUCTION

Thermally driven natural convection takes place in a wide range of physical flows such as ocean and atmospheric circulations or thermal systems such as heat pipes. Most research focused widely on thermally driven flows in idealized configurations that can be easily reproduced both experimentally and numerically. Among others, differentially heated enclosed cavities with different aspect ratios and heating configurations have been intensively studied. The flow in these conditions is mainly subject to thermal conduction and convection, but in the recent years some studies on Rayleigh-Bénard convection started to investigate the role of radiative transfer on the flow dynamics. In these works in 2D and 3D geometries where two opposite vertical walls are heated and cooled and the lateral walls are adiabatic, it has been shown that absorption

*Corresponding Félix Schmitt: felix.schmitt@insa-lyon.fr

and emission of radiation by the fluid itself modifies the local energy balance resulting in particular in the homogenization of the temperature field and an overall intensification of the flow [1, 2].

Numerical simulations of coupled CFD/gas radiation in enclosed cavities necessitate solving the flow conservation equations on the one hand and the Radiative Transfer Equation (RTE) in the participating medium on the other hand. The radiative heat source in the gas is thus taken into account in the energy equation. Among the models that can be found in the literature, most CFD methods are based on the Navier-Stokes equations solved using in-house codes coupled with RTE solvers either based on ray-tracing or a Discrete Ordinates Method. To the best of the authors' knowledge, until now, no solver has been developed with the aim of solving the lattice Boltzmann equation (LBE) of the flow coupled with real gas mixture absorption in three-dimensional cavities. Such a model and associated numerical tools are introduced in the present paper.

For this purpose, the commercial software ProLB is used. ProLB is a massively parallelizable computational tool developed to solve the LBE for a variety of physical flows, at different scales and in standard or complex geometries [3]. ProLB revealed to be a computationally efficient and reliable numerical solver when applied to combined-mode heat and/or mass transfer problems involving laminar or turbulent flows [4–7]. The present work is motivated by the need to extend the use of ProLB for further simulation and investigation of combined laminar or turbulent thermal flow/radiation problems such as meteorological flows or combustion systems in the framework of the lattice Boltzmann method. This coupling approach is validated hereafter against benchmark solutions obtained by Soucasse et al. [8] considering three-dimensional natural convection at low Rayleigh numbers.

The flow takes place in the cubical cavity of length L depicted on Figure 1. The cavity is filled with a gaseous mixture of air/H₂O/CO₂ at atmospheric pressure, with molar fractions of 0.02 and 0.001 of H₂O and CO₂ respectively. Air is considered as transparent while H₂O and CO₂ can absorb radiation and thus participate to radiative transfer in the cavity. The fluid is subject to natural convection induced by temperature variations inside the cavity. To that end, the two opposite vertical walls located at $x = 0$ (hereafter called hot wall) and $x = L$ (hereafter called cold wall) are kept at the constant temperatures T_h and T_c respectively. T_0 is the mean temperature $\frac{T_h + T_c}{2}$. The hot and cold walls are assumed as black bodies. The other walls of the cavity are adiabatic and isotropically reflect all the incoming radiation, their emissivity is null.

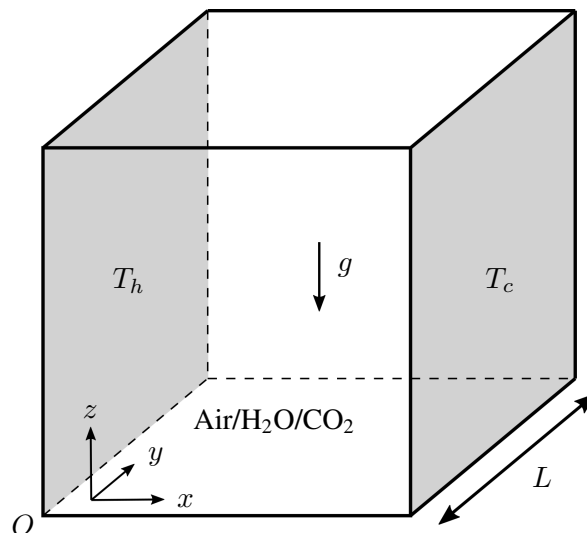


Fig. 1 Problem set-up.

2. METHODS

2.1 Governing equations

The velocity \mathbf{u} and temperature T of the gas are assumed to follow the incompressible mass, momentum and energy conservation equations under the Boussinesq approximation:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\frac{1}{\rho_0} \nabla p + \nu \nabla^2 \mathbf{u} - \mathbf{g} \beta (T - T_0) \quad (2)$$

$$\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T = \alpha \nabla^2 T - \frac{k}{\alpha} \nabla \cdot \dot{\mathbf{q}}_r \quad (3)$$

where ρ_0 is the reference density of the gas, p the pressure deviation from the hydrostatic pressure, \mathbf{g} the gravitational acceleration, ν the kinematic viscosity, $\beta = \frac{1}{T_0}$ the coefficient of volume expansion, α the thermal diffusivity, k the thermal conductivity and $\dot{\mathbf{q}}_r$ the radiative heat flux. The last term in Eq. (3) corresponds to a radiative volumic heat source which results from the local balance between emission and absorption of radiation by the gas mixture given its local thermodynamic state.

T_0 and $\Delta T = T_h - T_c$ are taken equal to 300 K and 0.0109 K respectively, while L is fixed to 1 m. It is assumed that the small amounts of H_2O and CO_2 do not influence the thermophysical properties of the gaseous mixture taken equal to those of the air at atmospheric pressure. In addition, ΔT is very small compared to T_0 so that the thermophysical properties are assumed constant and evaluated at T_0 . The thermal diffusivity, thermal conductivity and Prandtl number are taken equal to $2.25 \times 10^{-5} \text{ m}^2/\text{s}$, $0.0263 \text{ W}/(\text{m}\cdot\text{K})$ and 0.707 respectively to comply with the values used in [8]. The value of g is set to 9.85, so that the Rayleigh number $\text{Ra} = \frac{g\beta\Delta TL^3}{Pr\alpha^2}$ equals the required value of 10^6 . This Ra number is an order of magnitude below the critical value where unsteadiness appears in this specific set-up without radiation [9].

Boundary conditions for the velocity are no-slip on the six walls. On the lateral adiabatic walls, the emissivity is null so that the boundary conditions for the temperature writes

$$\mathbf{n} \cdot \nabla T = 0 \quad (4)$$

where \mathbf{n} is the unit vector normal to the wall directed toward the gas.

In order to evaluate the impact of radiation absorption by the gas mixture, the RTE in a non-scattering and isotropic medium is solved. The RTE takes the form of a Boltzmann equation describing the propagation and change of the spectral radiative intensity I_η at a given point \mathbf{x} in space and along a given direction ω confined within the infinitesimal solid angle $d\Omega$, and writes

$$\omega \cdot \nabla I_\eta(\mathbf{x}, \omega) = \kappa_\eta [I_{b\eta}(T(\mathbf{x})) - I_\eta(\mathbf{x}, \omega)] \quad (5)$$

where $I_{b\eta}$ is the Planck spectral blackbody intensity evaluated at the local gas temperature and κ_η is the spectral absorption coefficient which depends on the local thermodynamic state of the gas. In the present case, gas temperature variations are very small and species concentrations do not vary in the cavity so that κ_η can be considered as constant for a given wavenumber everywhere in the cavity.

At a location \mathbf{x}_w on a wall, the following equation gives the radiative intensity leaving the wall surface at temperature T_w and emissivity ϵ_w :

$$I_\eta(\mathbf{x}_w, \omega) = \epsilon_w I_{b\eta}(T_w) + \frac{(1 - \epsilon_w)}{\pi} \int_{\omega' \cdot \mathbf{n} < 0} |\omega' \cdot \mathbf{n}| I_\eta(\mathbf{x}_w, \omega') d\Omega' \quad (6)$$

The radiative heat source at a given location in the gas is evaluated using the formula

$$\nabla \cdot \dot{\mathbf{q}}_r(\mathbf{x}) = \int_0^\infty \kappa_\eta \left[4\pi I_{b\eta}(T(\mathbf{x})) - \int_{4\pi} I_\eta(\mathbf{x}, \omega) d\Omega \right] d\eta \quad (7)$$

2.2 Numerical aspects

Lattice Boltzmann method. Eq. (1) and (2) are solved using the Lattice Boltzmann method (LBM), which derives from the kinetic theory of gases and aims at solving the Boltzmann equation describing collisions and propagation of a collection of fluid particles from a mesoscale point of view. At this scale, the particles are described through a distribution function affected by inter-particle collisions and body forces modeled using a collision operator, which tends to relax towards an equilibrium state. The Boltzmann equation is solved following a Lagrangian discretization procedure in the velocity space and the physical space and time, on equally spaced nodes arranged on a Cartesian grid called lattice. Resolution is temporal by nature and consists of a succession of collision and propagation steps of the particle distribution function throughout the entire lattice. At each timestep, the macroscopic variables (i.e. density and velocity) are evaluated by computing the zeroth and first order moments of the particle distribution function.

In this study, a Hybrid Recursive Regularized Bhatnagar-Gross-Krook collision model [10] is used for the collision term and the lattice Boltzmann equation is solved on a D3Q19 lattice (i.e. three-dimensional space and 19 discrete velocities). Furthermore it can be shown that through the Chapman-Enskog technique, the lattice Boltzmann equation used in this study recovers the 3D weakly compressible Navier-Stokes equations [11]. More specifically, Eq. (1) and (2) are recovered with the Boussinesq approximation in the present asymptotic regime at very low Mach. Eq. (3) is simultaneously solved using a vertex-based finite volume method together with an explicit temporal resolution on the LBM nodes. Closure between momentum and temperature is ensured by mean of the buoyancy term in Eq. (2).

The LBM mesh is refined near the walls in order to ensure that enough nodes are located in the dynamic and thermal boundary layers and thus accurately capture gradients at these locations. The hybrid LBM/FVM solver for velocity and temperature is implemented in the framework of the commercial software ProLB. Boundaries are managed with an immersed boundary method, so that velocity and temperature on a boundary node are computed using interpolation from its neighbouring nodes and associated surface. Details on the solution method used in ProLB can be found in [5].

Radiative transfer. The discretization procedure of the RTE is based on the so-called Finite Volume Method (FVM) for radiative transfer (hereafter called radiative FVM) [12]. This method consists in integrating the RTE on elementary (or control) volumes and solid angles: the physical and angular spaces are then discretized respectively with a Cartesian mesh and a set of M non-overlapping adjacent control angles whose sum is equal to the 4π steradian unit sphere. For this purpose, the value of the radiative intensity is assumed uniform in a given control volume and angle, so that a set of M discrete equations can be derived for each control volume of the mesh. Each surface of the cavity is discretized using a uniform mesh of square elements matching the faces of the adjacent control volumes. The temperature and the radiative heat flux are uniform within a surface element. Finally, the radiative intensity field is solved using an iterative step-marching method, whose numerical resolution is parallelized on 8 threads. An upwind numerical scheme is used for the divergence term of Eq. (5). Although reliable mesh refinement techniques for the radiative FVM have been developed (see for instance [13]), the spatial discretization is constrained presently to a uniform mesh.

The strong heterogeneity of κ_η with respect to the wavenumber in real gases would imply to solve single RTEs on sufficiently small wavenumber intervals on which spectral absorption properties do not vary significantly. Such an approach being too computationally expensive, global spectral integration models such as the Absorption Distribution Function (ADF) [14], the Spectral Line Weighted-sum-of-gray-gases (SLW) [15] and the Full Spectrum k-distribution (FSK) [16] methods have been developed. These global methods use a distribution function of absorption coefficient weighted by the Planck function (called ALBDF in SLW

modeling) in order to determine a finite number of absorption coefficients κ_j and associated weights a_j . That way a limited number (fixed by the user) of RTEs need to be solved, i.e. one for each "gray" gas represented by the pair $\kappa_j - a_j$. The ADF method for gas mixtures is used hereafter, with 16 gray gases whose coefficients and weights are identical to those used in [8].

In the end, the discretized form of Eq. (7) for a given control volume writes

$$\nabla \cdot \dot{\mathbf{q}}_{\mathbf{r}} = \sum_j \kappa_j \left[4\pi a_j I_b(T) - \sum_m I_j^m \Delta\Omega^m \right] \quad (8)$$

where $\Delta\Omega^m$ is the value of the control angle attached to the m -th direction.

Coupling principle. The radiative solver has been developed as a distinct module of ProLB. Both solvers are coded in the C++ language and the coupling between the two codes is carried out by communicating data via external files written in the computer's hard memory and that can be accessed by both processes.

The pseudo-timestep for LBM calculations depends on the lattice size and does not vary during the simulations, its value being constrained for the sake of stability. It is therefore not optimal to update the radiative field every LBM timestep, as it would result in excessive computational expenses. Thus gas temperatures are communicated to the radiative code at fixed LBM time periods. During the same coupling timestep, radiative heat sources are communicated the other way around to ProLB. Surface temperatures can be updated at shorter LBM time periods, independantly of the radiative field updates. Within a surface element, the convective heat flux is uniform and computed using an average temperature of the boundary nodes facing the element, weighted by their distance from the element center.

The LBM lattice and the radiative FVM mesh being built independently, the temperatures are linearly interpolated at the radiative FVM control volume centers from the enclosing LBM nodes and vice versa for the radiative heat sources. Because the LBM mesh is finer than the radiative FVM mesh close to the walls, radiative heat sources on boundary LBM nodes are extrapolated from the closest radiative nodes. For this purpose, radiative intensities are assumed constant along the space interval separating the LBM node and the radiative node so that the value can be extrapolated from the temperature difference only using Eq. (8).

3. RESULTS

3.1 Simulation parameters

The validation is carried out with stationary solutions obtained from simulations of two study cases taken from [8]: the first without radiation absorption by the gas mixture (thus considered as transparent) and referred to as case A and the second with gas absorption being taken into account, referred to as case B. The results obtained with the present model are systematically compared to the benchmark solutions of [8] in order to assess the model reliability. Soucasse et al. [8] conducted their simulations with a fine enough CFD mesh refined near the walls whose spatial steps were constrained by the collocation method used. The density of radiative nodes was also increased near the walls. The CFD and radiative methods were validated in their paper against benchmark solutions and have shown to be highly accurate and reliable.

The simulation of case A is started from a static and isothermal state. The stationary solution obtained for case A is then used to perform the simulation of case B. Surface temperatures and radiative intensities are updated every 100 and 2000 LBM timesteps respectively. It has been observed that reducing these coupling periods does not necessarily speed up the convergence towards the stationary solutions. Convergence of the solutions is assumed when the difference between two successive values of the velocity, the temperature and the radiative heat source at various locations in the cavity remains lower than a change in the 7th significant digit of the maximum value encountered in the whole domain. Convergence is also checked on average values of the Nusselt numbers and the net radiative heat fluxes at the hot and cold walls.

Values computed in the simulations are made adimensional using the reference length L , the reference time $\frac{L^2}{\alpha\sqrt{Ra}}$, the reference flux $\frac{k\Delta T}{L}$ and the reduced temperature $\theta = \frac{T-T_0}{\Delta T}$.

In order to select suitable LBM and radiative FVM meshes capable of capturing accurately the main characteristics of the flow and the associated heat transfers, a mesh sensitivity analysis is conducted as described below:

- Firstly, case A is simulated without radiative coupling, using a mesh made up of 586,543 (app. 84^3) nodes structured on 3 embedded uniform lattices allowing refinement near the walls. The smallest spatial step is 7.75×10^{-3} m. A simulation is also performed using a finer lattice made up of 1,703,793 (app. 120^3) nodes, built by dividing the spatial step by 1.43. Each surface of the cavity is divided into 43^2 square elements. Relative errors on the maximum velocity encountered in the cavity and on the mean Nusselt number at the hot wall obtained with the 84^3 lattice are 3.95 % and 1.28 % respectively with respect to the ones obtained with the fine lattice. These errors are considered as sufficiently low to use the 84^3 lattice.
- Then, the stationary temperature field in the gas and on the walls obtained in the previous step with the selected lattice is used to compute the corresponding radiative heat sources in the gas along with the net radiative heat fluxes on the walls. Based on preliminary simulations in similar configurations, a sufficiently fine radiative simulation is carried out to obtain a reference solution. Errors are assessed against this reference solution for different tested combinations of spatial steps and numbers of directions. The mean absolute error (MAE) on radiative heat sources at the LBM nodes and the relative error (RE) on the mean radiative heat flux at the hot wall are reported in Table 1. MAE on the radiative heat sources decreases when the mesh is refined. However it stays below 2 with the 43^3 mesh which is low compared to the maximum value encountered in the domain (around 10^2). Hence the 43^3 mesh with 48 directions is selected, as it allows to reach a high level of precision while requiring low computational and memory loads.

Table 1 Sensitivity analysis of the radiative FVM discretization. $\mathbf{n} \cdot \dot{\mathbf{q}}_{r|h}$ is the mean adimensional net radiative heat flux at the hot wall. Errors are evaluated in comparison to the 65^3 mesh with 80 directions.

Mesh	Number of directions	$\mathbf{n} \cdot \dot{\mathbf{q}}_{r h}$	RE on $\mathbf{n} \cdot \dot{\mathbf{q}}_{r h}$	MAE on sources
43^3	24	-116.24	3.04 %	1.78
	48	-118.79	0.91 %	1.47
	80	-120.46	0.48 %	1.47
65^3	24	-115.64	3.54 %	0.74
	48	-118.09	1.49 %	0.23
	80	-119.88		

CFD calculations are parallelized on 25 Intel(R) Xeon(R) E5-2670 v2 @ 2.50GHz processors using MPI and an additional processor is used to run radiative calculations. The step-marching process in the radiative FVM is also parallelized using OpenMP and thus implies multithreading computation. The total CPU time (excluding the pre-processing stage) to reach convergence is 85 h for case A and 39.7 h for case B, for approximately 150,000 and 70,000 LBM timesteps respectively. The actual computational time between the first iteration and the end of the simulation is 3.3 h and 1.5 h for case A and case B respectively. Among the CPU and actual times, approximately 95 % are taken by the CFD calculations. Therefore, limiting the number of radiative coupling timesteps allows to reduce drastically the total simulation time.

3.2 Flow structure and overall characteristics

Figure 2 displays the temperature profiles averaged over y on the central vertical planes of the cavity perpendicular to the x -axis and to the z -axis, obtained for the two test cases. These profiles compare very

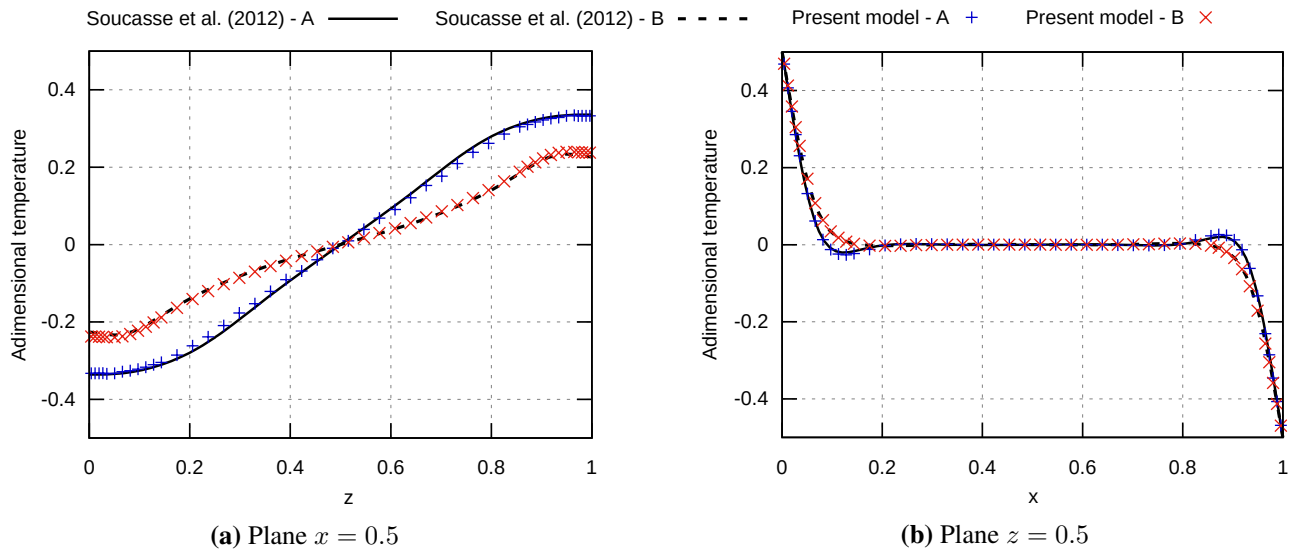


Fig. 2 Adimensional temperature profiles. Results are averaged over y .

well with the reference profiles in each case. Temperatures of the flow advected between the hot and cold walls in case B present smoother gradients compared to case A, which highlights the homogenization effect on the temperature due to gas radiation. Small discrepancies can be noticed on the profiles of Figure 2a. In the central region, the linear slope in case A tends to be slightly underestimated in the present simulation. On the sides of the cavity in case B the temperatures are slightly closer to the wall temperatures. This is probably caused by the use of a coarser mesh close to the walls in the simulation compared to the reference.

Vertical velocity profiles averaged over y on the horizontal planes $z = 0.5$ and $z = 0.75$ are represented on Figure 3. The profile at $z = 0.25$ is not shown for the sake of conciseness, because the velocity field is centrosymmetric with respect to the center of the cavity for a given vertical plane perpendicular to the y -axis. The present simulation succeeds at predicting correct shapes of velocity profiles especially in the dynamic boundary layers, even though the maximum absolute values of the vertical velocity in these layers are slightly lower than the reference ones. In case B vertical velocities are increased in the vertical dynamic boundary layers compared to case A, especially in the downstream part of these layers. Gas radiation has an

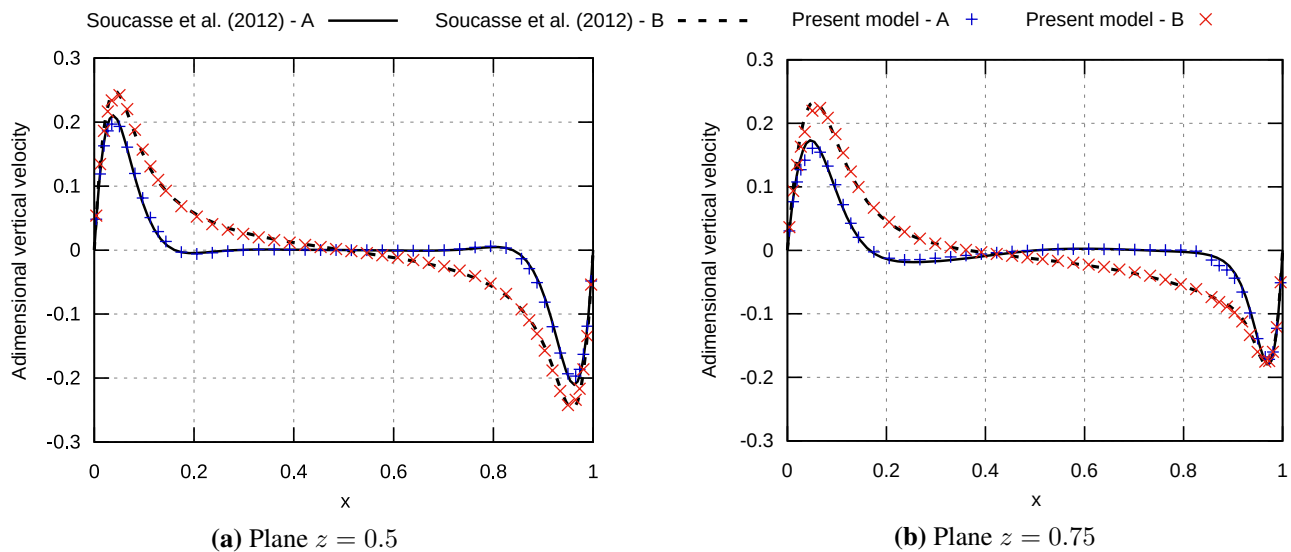


Fig. 3 Adimensional vertical velocity profiles. Results are averaged over y .

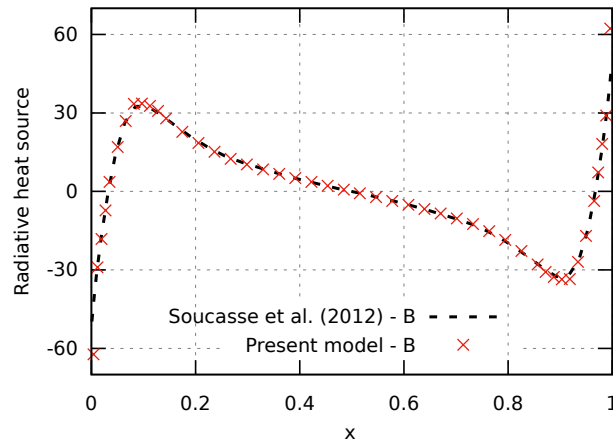


Fig. 4 Adimensional radiative heat source profile along the line $y = z = 0.5$.

intensification effect on the flow in this specific configuration, which can be confirmed by further analysis on the total kinetic energy of the flow (not developed here). In addition, the dynamic boundary layers are thickened when gas radiation is taken into account.

The radiative heat source profile in the gas on the central line $y = z = 0.5$ for case B shown on Figure 4 is also in excellent agreement with the benchmark profile. However the gradients close to the hot and cold walls are slightly overestimated compared to the reference ones. This is likely to be due to the extrapolation technique used close to the walls to determine the radiative heat source on boundary LBM nodes. It is nevertheless of minor importance regarding the fairly good agreement on temperature and velocity distributions in the cavity.

Convective heat transfers taking place at the boundaries of the cavity can be fully characterized by the local Nusselt number computed at the walls, whose adimensional value is given by

$$\text{Nu} = -\mathbf{n} \cdot \nabla \theta \quad (9)$$

Nusselt profiles at the hot wall along z averaged over y are presented on Figure 5a. The global shapes of Nusselt profiles are correctly evaluated with the present simulations, despite the fact that the values close to

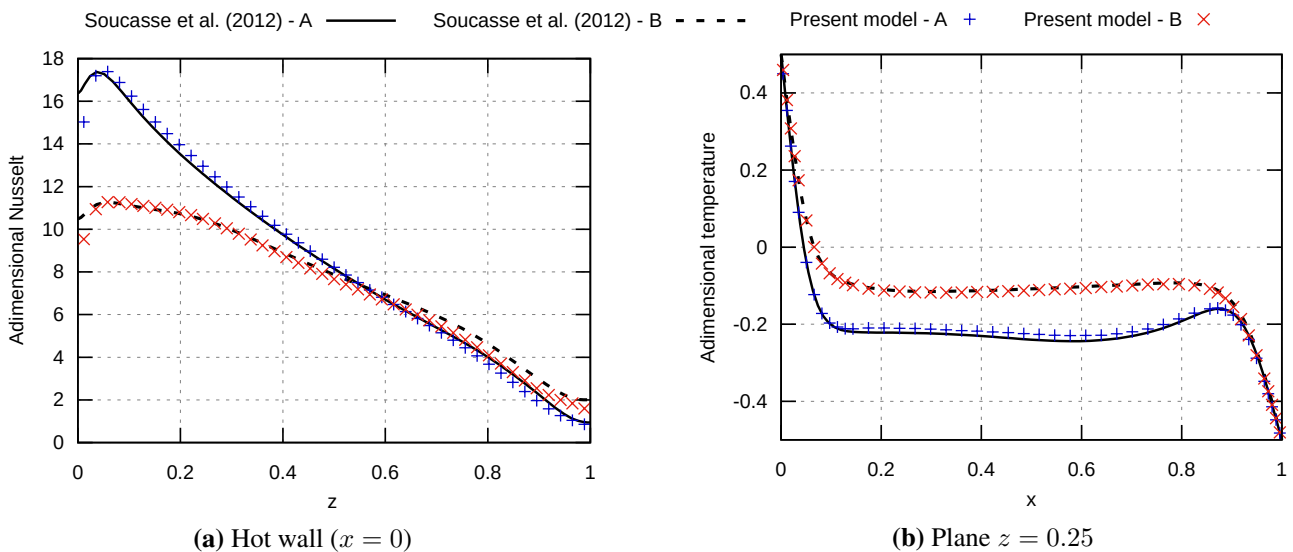


Fig. 5 Adimensional Nusselt and temperature profiles. Results are averaged over y .

the bottom wall and on the the top half of the hot wall are underestimated. These discrepancies are likely to be related to the weak prediction of temperature gradients close to the edges of the cavity caused by the present boundary treatment.

Figure 5b indicates that the gas is pre-heated along the bottom wall in case B due to a net absorption of radiation. Thus temperature gradients tend to be dampened when the flow approaches the hot wall, and therefore convective heat transfers are reduced on the bottom half of the hot wall, which induces a decrease in local Nusselt numbers at this location. The same behaviour is observed by symmetry on the opposite cold wall (not shown here).

Mean radiative net fluxes on the hot and cold walls are in good agreement with the reference ones, with a relative error of 1.96 %. However wall-to-wall radiation has no effect on the flow structure in this specific configuration.

4. DISCUSSION

The overall characteristics of the flow are very satisfactorily recovered by the present model and associated numerical tools, although some discrepancies are noticeable for convective heat fluxes at some key locations in the cavity, e.g. near the edges. Indeed, the main limit of this model lies in the treatment of temperatures at the boundaries. The spatial step of the surface discretization is constrained by the radiative FVM mesh, such that a compromise must be found between the required spatial precision for convective heat fluxes at the walls and the computational costs (a finer surface discretization would require a finer radiative FVM mesh). Additionally, due to the immersed boundary treatment used in ProLB, the temperature value on the boundary nodes is highly dependant on the associated surface, causing unphysical results close to the edges and corners, depending on which surface is assigned for the interpolation step at these locations. This is especially true for adjacent surfaces of different nature, e.g. an isothermal surface adjacent to an adiabatic one, giving rise to large temperature gradients at their junctions.

The present study shows that a combination of LBM for CFD and FVM for radiative transfer is adapted to the modeling of natural convection in enclosed configurations with a non-diffusive and optically thin gas mixture with small ΔT . Refining the radiative FVM mesh near the walls is not necessarily relevant for accurately approximating surface radiative fluxes and heat sources associated to gas radiation, although it may avoid recourse to extrapolation techniques for radiative heat sources close to the walls.

5. CONCLUSIONS

Simulation results obtained with the newly introduced CFD and radiative coupling allow to validate its applicability to natural thermally driven convection flows at low Rayleigh numbers involving real absorbing and emitting gas mixtures. Building relevant and independant LBM lattice and radiative FVM mesh capable of capturing reliable temperature and velocity distributions along with heat transfers at the boundaries can be done in such a way that computational costs and times remain reasonable.

Some bottlenecks concerning the treatment of temperatures at the boundaries located at the edges of the cavity have been highlighted. While treating solid surfaces as immersed boundaries is well suited to complex geometries showing numerous unstructured and/or tilted surfaces, its use in academical configurations such as the ideal enclosure studied here is less straightforward. A possible improvement of the temperature interpolation technique on boundary nodes should take into account the influence of each of the adjacent surface of a boundary node located close to an edge or a corner in order to avoid errors on convective heat fluxes.

ProLB has shown great potential to simulate meteorological flows [5], so that future work will be dedicated to applications of the present model to outdoor atmospherical flows in urban configurations in order to analyse the effects of atmosphere/radiation interactions on urban microclimates.

ACKNOWLEDGMENTS

This work was supported by the Lyon Urban School which benefited from the financial support of the French National Research Agency (ANR) in the framework of the program "Investissements d'avenir: Instituts Convergences" No. ANR-17-CONV-0004. ProLB is developed within a scientific collaboration including CS GROUP, Renault, Airbus, Ecole Centrale de Lyon, CNRS and Aix-Marseille University.

NOMENCLATURE

			SUBSCRIPTS AND SUPERSCRIPTS
\dot{q}_r	radiative heat flux	(W/m ²)	0 reference state
\mathbf{n}	normal to the wall	(-)	η spectral value
\mathbf{x}	vector of space coordinates	(m)	m direction number in the RTE
ω	propagation direction (unit vector)	(-)	b blackbody
θ	adimensional temperature	(-)	w wall
a	gray gas weight	(-)	j j-th gray gas

REFERENCES

- [1] Soucasse, L., Rivière, P., Soufiani, A., Xin, S., and Le Quéré, P., "Transitional regimes of natural convection in a differentially heated cubical cavity under the effects of wall and molecular gas radiation," *Physics of Fluids*, 26(2), pp. 024105, (2014).
- [2] Kogawa, T., Okajima, J., Sakurai, A., Komiya, A., and Maruyama, S., "Influence of radiation effect on turbulent natural convection in cubic cavity at normal temperature atmospheric gas," *International Journal of Heat and Mass Transfer*, 104, pp. 456–466, (2017).
- [3] CS, (2021), URL <http://www.prolb-cfd.com/>
- [4] Merlier, L., Jacob, J., and Sagaut, P., "Lattice-Boltzmann large-eddy simulation of pollutant dispersion in complex urban environment with dense gas effect: Model evaluation and flow analysis," *Building and Environment*, 148, pp. 634–652, (2019).
- [5] Feng, Y., Boivin, P., Jacob, J., and Sagaut, P., "Hybrid recursive regularized lattice boltzmann simulation of humid air with application to meteorological flows," *Physical review. E*, 100(2-1), pp. 023304, (2019).
- [6] Tayyab, M., Zhao, S., Feng, Y., and Boivin, P., "Hybrid regularized Lattice-Boltzmann modelling of premixed and non-premixed combustion processes," *Combustion and Flame*, 211, pp. 173–184, (2020).
- [7] Cheylan, I., Zhao, S., Boivin, P., and Sagaut, P., "Compressible pressure-based Lattice-Boltzmann applied to humid air with phase change," *Applied Thermal Engineering*, 191, pp. 116868, (2021).
- [8] Soucasse, L., Rivière, P., Xin, S., Le Quéré, P., and Soufiani, A., "Numerical study of coupled molecular gas radiation and natural convection in a differentially heated cubical cavity," *Computational Thermal Sciences*, 4(4), pp. 335–350, (2012).
- [9] Labrosse, G., Tric, E., Khallouf, H., and Betrouni, M., "A direct (pseudo-spectral) solver of the 2d/3d stokes problem: transition to unsteadiness of natural-convection flow in a differentially heated cubical cavity," *Numerical Heat Transfer, Part B: Fundamentals*, 31(3), pp. 261–276, (1997).
- [10] Jacob, J., Malaspinas, O., and Sagaut, P., "A new hybrid recursive regularised bhatnagar–gross–krook collision model for lattice boltzmann method-based large eddy simulation," *Journal of Turbulence*, 19(11-12), pp. 1051–1076, (2018).
- [11] Krüger, T., Kusumaatmaja, H., Kuzmin, A., Shardt, O., Silva, G., and Viggen, E. M., (2017). *The Lattice Boltzmann Method: Principles and Practice*. Springer International Publishing.
- [12] Chai, J. C., Lee, H. S., and Patankar, S. V., "Finite volume method for radiation heat transfer," *Journal of Thermophysics and Heat Transfer*, 8(3), pp. 419–425, (1994).
- [13] Howell, L. H., Colella, P., Jessee, P. J., and Pember, R. B., "A conservative adaptive-mesh algorithm for unsteady, combined-mode heat transfer using the discrete ordinates method," *Numerical Heat Transfer, Part B: Fundamentals*, 35(4), pp. 407–430, (1999).
- [14] Pierrot, L., Rivière, P., Soufiani, A., and Taine, J., "A fictitious-gas-based absorption distribution function global model for radiative transfer in hot gases," *Journal of Quantitative Spectroscopy and Radiative Transfer*, 62(5), pp. 609–624, (1999).
- [15] Solovjov, V. P., Andre, F., Lemonnier, D., and Webb, B. W., "The rank correlated SLW model of gas radiation in non-uniform media," *Journal of Quantitative Spectroscopy and Radiative Transfer*, 197, pp. 26–44, (2017).
- [16] Modest, M. F., *Radiative Heat Transfer*, 3rd Edition, Academic Press, (2013).