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Lattice-boltzmann Method with Immersed Boundary Conditions for Fluid Simulations of Multiples Species

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Abstract: An algorithm to simulate multiples mixtures in single phase with different molecular weights is presented. The coupling of multiple mixtures with the immerse boundary method is proposed. This algorithm is designed to model problems of multiple mixtures using Lattice Boltzmann method which in turn can interact with complex objects modeled with immersed boundaries. The Lattice Boltzmann method is derived from kinetic theory by discretizing multiples fluid Boltzmann equations in which cross-collisions and self-collisions are treated independently. The method is validated against analytical solution in diffusion of binary mixtures and evaluated in ternary mixtures in a curved channel.

Key words: Lattice-boltzmann, immersed boundary, multiples species

INTRODUCTION

The diffusion of multiple species is a very interesting problem in many practical applications, for instance, refrigeration and pollutant dispersion. Since the physics of species diffusion on a macroscopic scale is obtained from microscopics solutions, the Lattice Boltzmann Method (LBM) is widely used for these types of applications. LBM was originated from the lattice-gas automata which the time and space are discretized to solve the Boltzmann equation for particle velocity distribution functions on a regular grid. Recently some LBM models have been proposed (McCracken and Abraham, 2005; Asinari, 2005) which use a discretization of the Bhatnagar-gross-krook models (Bhatnagar *et al*., 1954) (BGK) derived from the continuous kinetic theory, such as the models of (Luo and Girimaji, 2003) and (McCracken and Abraham, 2005).

One of the major weaknesses of LBM, is that an incorrect implementation of the boundaries conditions can decrease the convergence of the system. The boundaries conditions determines how the unknown distribution functions are defined on the nodes adjacent to undefined nodes or interacting objects (Chen and Doolen, 1998). Recently an algorithm combining the features of the LBM and the Immersed Boundary methods (IB) has been introduced to simulate fluid-solid interaction (Boroni *et al*., 2013). Basically the boundary effect into the surrounding fluid is replaced by adding forces to the fluid equations. This algorithm introduces a more efficient iteration procedure to compute the fluid-boundary interaction which facilitates the implementation and improves performance.

In this study an algorithm of IB-LBM-mixtures is presented, with an efficient iteration scheme for calculation of forces at the boundary points. The algorithm allows simulate fluid-object interaction problems with multiples mixtures. The algorithm Furthermore, different problems of multiples mixtures were tested including mixtures with different initial concentration and object-fluid interactions in curved walls.

LATTICE-BOLTZMANN METHOD

The most popular LBM divide the space into a regular lattice (Fig. 1). The grid point of the lattice is called lattice node and the edge connecting two neighboring nodes is called lattice link. In D2Q9 model, for each node, there are a total of 8 neighbors with 8 links to connect them, plus the node itself.

The particles are located on each node and they can move from one node to their neighboring nodes on each computation step. This movement is often called propagation or streaming. So, there are 9 possible motional states for each particle, including the stationary state.

In LBM one real value is used to denote the number of particles on each state and each node at a specific time. This real value is called the particle distribution function value (distribution function for simplicity), denoted as f_α = 0,..,8. These real values

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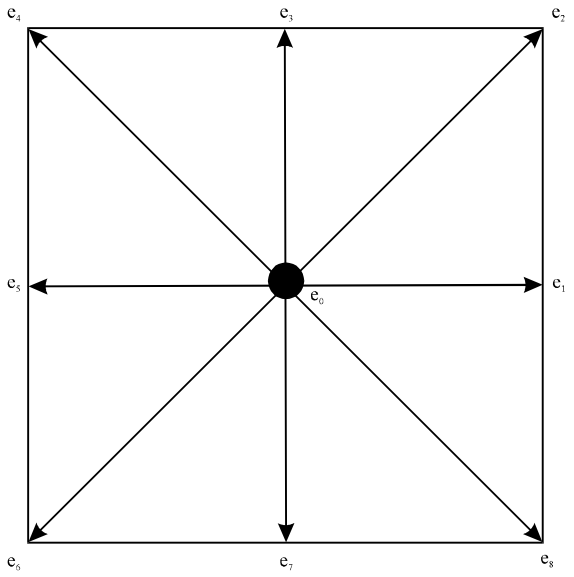

Fig. 1: Space of discrete velocities in LBM-D2Q9, corresponding to the population functions f_α

represent the statistical probabilities of distributions in the specified directions. The macroscopic physical properties density and velocity can be statistically defined as:

$$\rho = \sum_\alpha f_\alpha \tag{1}$$

$$u = \frac{1}{\rho}\sum_\alpha f_\alpha e_\alpha \tag{2}$$

Collision and streaming: From the density and velocity definitions, it can be seen that these variables depend on the distribution functions at each node. The local operations that update these functions are collision and streaming:

$$f_\alpha (x+e_\alpha\delta_t, t+\delta_t)-f_\alpha (x, t) = \Omega_\alpha \tag{3}$$

where, Ω_α is a collision operator, that should ensure that mass and momentum are conserved. The BGK model is the most popular collision operator; with external forces it takes the form:

$$\Omega_\alpha = J_\alpha (x, t)+F_\alpha (x, t)\delta_t \tag{4}$$

$$J_\alpha (x,t) = -\frac{1}{\tau}\left(f_\alpha (x,t)-f_\alpha^0(\rho,u)\right) \tag{5}$$

where, f_α^0 is an equilibrium distribution function, $F_\alpha(x, t)$ is the forcing term and τ is a relaxation time related to viscosity ν:

$$\nu = \frac{1}{3}\left(\tau-\frac{1}{2}\right) \tag{6}$$

The viscosity should be positive (τ>0.5).

LATTICE BOLTZMANN FOR MULTIPLE MIXTURES

The LBM discrete equation for multiple mixtures proposed by Luo and Girimaji (2003) can be represented by:

$$f_{\alpha\Psi}(x+e_\alpha\delta_t, t+\delta_t)-f_{\alpha\Psi}(x,t) = J_{\alpha\Psi}-F_{\alpha\Psi}\delta_t+\sum_{\Lambda\neq\Psi} I_{\alpha\Psi\Lambda}\delta_t \tag{7}$$

where, Ψ and Λ are species, $J_{\alpha\Psi}$ is the self-collision term:

$$\sum_{\Lambda\neq\Psi} I_{\alpha\Psi\Lambda}\delta_t$$

is the cross-collision term and $F_{\alpha\Psi}\delta_t$ represents the effects due to an external force. The self-collision term is derived similar to single fluid LBM:

$$J_{\alpha\Psi} = -\frac{1}{\tau_\Psi}\left(f_{\alpha\Psi}-f_{\alpha\Psi}^0\right) \tag{8}$$

The cross-collision term is derived from the two-fluid theory under the isothermal assumption of the system:

$$I_{\alpha\Psi\Lambda} = -\frac{1}{\tau_\Delta}\frac{\rho_\Lambda}{\rho}\frac{f_{\alpha\Psi}^0}{\delta_t c_s^2}(e_\alpha-u_\Psi)\cdot(u_\Psi-u_\Lambda) \tag{9}$$

where, τ_Δ is the cross-collision coefficients that determine how strong the diffusion effect is of the mixtures, ρ_Ψ, ρ_Λ, u_Ψ, u_Λ are the density and velocity of the each specie, ρ and u are the density and velocity of the mixture, $f_{\alpha\Psi}^0$ is the equilibrium distribution function and $c_s = 1/\sqrt{3}$ is the speed of sound in LBM.

The external force $F_{\alpha\Psi}$ is:

$$F_{\alpha\Psi} = -w_\alpha\rho_\Psi\frac{e_\alpha\cdot a_\Psi}{c_s^2} \tag{10}$$

where a_Ψ represents an external acceleration force and w_α is the weighting function that depends on the discrete velocity set e_α.

The equilibrium distribution function is given by the following equation:

$$f_{\alpha\Psi}^0 = \left[1+\frac{1}{c_s^2}(e_\alpha-u)\cdot(u_\Psi-u)\right]f_{\alpha\Psi}^{eq} \tag{11}$$

where, $f_{\alpha\Psi}^{eq}$ is the equilibrium distribution function to single fluid LBM-BGK, defined by:

$$f_{\alpha\Psi}^{eq} = w_\alpha \rho_\Psi \left[1 + \frac{e_\alpha \cdot u}{c_s^2} + \frac{(e_\alpha \cdot u)^2}{2c_s^4} - \frac{u \cdot u}{2c_s^2}\right] \quad (12)$$

The macroscopic variables for each species are found from the moments of the distribution functions and can be represented by:

$$\rho_\Psi = \sum_\alpha f_{\alpha\Psi} \quad (13)$$

And:

$$\rho_\Psi u_\Psi = \sum_\alpha f_{\alpha\Psi} e_\alpha \quad (14)$$

The total density and mass averaged velocity of mixture are:

$$\rho = \sum_\Lambda \rho_\Lambda \quad (15)$$

$$\rho u = \sum_\Lambda \rho_\Lambda u_\Lambda \quad (16)$$

The pressure in this model is given by:

$$p = c_s^2 \sum_\Lambda \rho_\Lambda \quad (17)$$

And it is equal to the sum of the partial pressures.

The self-collision effect is adjusted with the relaxation coefficient τ_Ψ, so the different viscosities can be represented.

General step of LBM for multiple mixtures: This section briefly describes the algorithm that combines Eq. 7-16 in one step of the LBM method. The main body of the implementation can be described as follows:

For t = 0:

- $f_{\alpha\Psi} = f_{\alpha\Psi 0}$, $\tau_\Psi = \tau_{\Psi 0}$, initialize the distributions functions and select a relaxation coefficient for all species Ψ
- For $t \neq 0$
  For all species Ψ:

$$\rho_\Psi = \sum_\alpha f_{\alpha\Psi}$$

$$u_\Psi = \frac{1}{\rho_\Psi} \sum_\alpha f_{\alpha\Psi} e_\alpha$$

compute the macroscopic density and velocity

- Compute the equilibrium distribution function $f_{\alpha\Psi}^0$, the self-collision term $J_{\alpha\Psi}$ and cross-collision term $\sum_{\Lambda \neq \Psi} I_{\alpha\Psi\Lambda}$ and the external force $F_{\alpha\Psi}$
- Take the propagation and collision operations:

$$f_{\alpha\Psi}(x + e_\alpha \Delta_t, t + \Delta_t) = f_{\alpha\Psi}(x,t) + J_{\alpha\Psi} - F_{\alpha\Psi}\Delta_t + \sum_{\Lambda \neq \Psi} I_{\alpha\Psi\Lambda}\Delta_t$$

and apply boundary conditions

- $t = t + \Delta t$, move forward to next time step

IB METHOD

In this method, the immersed boundary is supposed to consist of massless particles, such that the force generated by distortions of the boundary can be calculated and transferred to the fluid (Cheng and Zhang, 2010).

Figure 2 shows a 2D example with immersed boundary particles (closed). The boundary and the fluid domain are denoted by Γ_b and Ω_f, respectively.

X(s,t) is a Lagrangian vector function of arc length s and time t and returns the location of points on boundary Γ_b. The boundary influence is represented by a force density D(s, t) at the boundary point X(s, t). Thus, D(s, t) is determined by the configuration of X(s, t) and it is transferred into the force term f in the N-S equations which are solved to determine the flow velocity and pressure throughout domain Ω_f.

The immersed boundary moves at the local fluid velocity since it is in contact with the surrounding fluid. This scheme may be expressed by the following equations:

$$\nabla . u = 0 \quad (18)$$

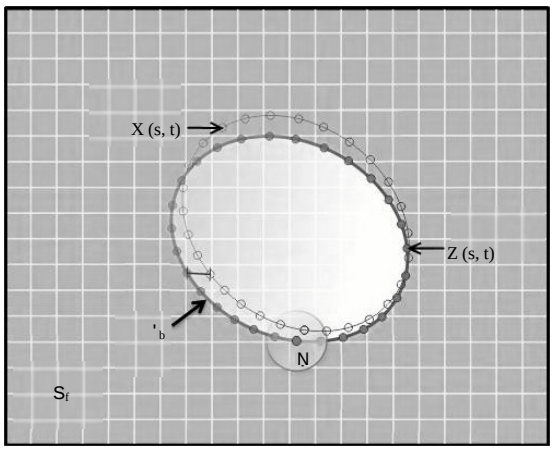

Fig. 2: Immersed Boundary and lattice scheme (the boundary Γ_b, fluid Ω_f, boundary point X(s,t), target position of the boundary Z (s,t) and boundary point influence ϕ)

$$\rho(u_t+(u.\nabla)u) = -\nabla p+\mu.u+F_b \quad (19)$$

$$\frac{dX(s,t)}{dt} = U(X(s,t),t) = \int_{\Omega_f} u(x,t)\delta(x-X(s,t))dx \quad (20)$$

$$D(s,t) = S_f X(s,t) \quad (21)$$

$$F_b(x,t) = \int_{\Gamma_b} D(s,t)\delta(x-X(s,t))ds \quad (22)$$

where, u is the flow velocity, ρ the fluid density, p the flow pressure, μ the fluid viscosity, F_b the external force, X the boundary coordinate, s the boundary fiber length, U the boundary speed, X the fluid flow coordinate, S_f the boundary force generation operator and δ(r) the Dirac delta function.

Equations 18 and 19 are the incompressible N-S equations with external force g while Eq. 20 and 21 are the immersed boundary equations. Equation 22 and the right part of Eq. 20 represent the interaction of boundary and fluid.

Discrete interaction: The interaction between fluid nodes and boundary points is ruled by integration in the continuous Eq. 20 and 22. The discretized equations of Eq. 20 and 22 using a regularized discrete delta function δ_h are:

$$F_{bij} = \sum_k D_k \delta_h(x_{ij} - X_k)\Delta s_k \quad (23)$$

$$\frac{dX_k}{dt} = U_k = \sum_{ij} u_{ij}\delta_h(x_{ij} - X_k)\Delta x\Delta y \quad (24)$$

where, h = ΔX = Δy is the fluid node spacing and Δs_k is the boundary segment length. The delta function δ_h is an approximation to the Dirac delta function δ(r) (Peskin, 2002):

$$\delta_h(x,y) = \frac{1}{h^2}\phi\left(\frac{x}{h}\right)\phi\left(\frac{y}{h}\right) \quad (25)$$

$$\phi(r) = \begin{cases} \frac{1}{8}\left(3-2|r|+\sqrt{1+4|r|-4r^2}\right), & 0 \le |r| < 1, \\ \frac{1}{8}\left(5-2|r|-\sqrt{-7+12|r|-4r^2}\right), & 1 \le |r| < 2, \\ 0, & |r| \ge 2, \end{cases} \quad (26)$$

The boundary force density D is defined by the boundary configuration. For Γ_b with tension, bending and fastening forces, D can be expressed by:

$$D = k_c\frac{\partial^2 X}{\partial s^2} - k_\gamma\frac{\partial^4 X}{\partial s^4} - k_f(X-Z) \quad (27)$$

where, k_c is the tension stiffness, k_γ the bending rigidity, k_f the fastening stiffness and Z the fastening or target position of the boundary. The discretized equations of Eq. 27 can be expressed as:

$$D_k = k_c\left(\frac{X_{k-1}-2X_k+X_{k+1}}{\Delta s^2}\right) - k_\gamma\left(\frac{X_{k-2}-4X_{k-1}+6X_k-4X_{k+1}+X_{k+2}}{\Delta s^4}\right) - k_f(X-Z) \quad (28)$$

IB-LB MULTIPLE MIXTURES COUPLING

For problems with slow moving boundary or flexible boundary with small pressure gradient, the external forcing term $F_{\alpha\Psi}$ (Eq. 7) doesn't affect the result but for fast moving boundary and flexible boundary with large pressure gradient, a higher order method is necessary. For this problem let us consider the solution proposed by Cheng and Zhang (2010), a second-order convergence scheme defined by:

$$F_{\alpha\Psi}\Delta_t = \frac{\Delta_t}{2}\left(F_{b\alpha}(x_{ij},t) + F_{b\alpha}(x_{ij}+e_\alpha\delta_t, t+\delta_t)\right) \quad (29)$$

Where:

$$F_{b\alpha}(x_{ij}, t) = w_\alpha\{3f_{bij}\bullet[(e_\alpha - u_{ij}) + 3(e_\alpha \bullet u_{ij})e_\alpha]\} \quad (30)$$

The Eq. 30 has a second-order accuracy for spatial resolution of fluid, as the original LB model (Boroni *et al*., 2013). As Eq. 29 is implicit, an iterative procedure is used to solve it.

Algorithm:

For t = 0

- $X_k = Z_k, \rho^0_\Psi = \rho_{0\Psi}, u^0_\Psi = u_{0\Psi}; D^0_k = 0, F_{b\alpha} = 0$
- $f_{\alpha\Psi} = f_{\alpha\Psi 0}$, $\tau_\Psi = \tau_{\Psi 0}$ initialize the distributions functions and select a relaxation coefficient for all species Ψ

For t≠0

For all species Ψ

- Execute the collision operation $f^{eq}_{\alpha\Psi}$, compute the equilibrium distribution function $f^0_{\alpha\Psi}$, calculate self-collision term $J_{\alpha\Psi}$ and cross-collision term:

$$\sum_{\Lambda\neq\Psi} I_{\alpha\Psi\Lambda}$$

- $n = o, X^0_k = X_k$

Repeat:

- $n = n+1$
- $X^n_k = X_k + \Delta t\sum_{ij} u^{n-1}_{ij}\delta_h(x_{ij} - X^{n-1}_k)\Delta x\Delta y$
- $D^n_k = k_c\left(\frac{X^n_{k-1}-2X^n_k+X^n_{k+1}}{\Delta s^2}\right) - k_\gamma\left(\frac{X^n_{k-2}-4X^n_{k-1}+6X^n_k-4X^n_{k+1}+X^n_{k+2}}{\Delta s^4}\right) - k_f(X^n_k - Z_k)$

  $f^n_{bij} = \sum_k D^n_k\delta_h(x_{ij} - X^n_k)\Delta s_k$
- $F^n_{boij} = w_\alpha\left\{3f^n_{bij}\cdot\left[(e_\alpha - u^{n-1}_{ij}) + 3(e_\alpha\cdot u^{n-1}_{ij})e_\alpha\right]\right\}$

For all species Ψ

- Take the propagation operation

Algorithm: Continue

$$f^n_{\alpha\Psi}\left(x_{ij}+e_\alpha\Delta t, t+\Delta t\right)=f_{\alpha\Psi ij}+J_{\alpha\Psi ij}-\frac{\Delta_t}{2}\left(F^n_{b\alpha ij}+F_{b\alpha ij}\right)+\sum_{\Lambda\neq\Psi}I_{\alpha\Psi\Lambda}\Delta_t$$

with:

$$f^n_{\alpha\Psi ij}=f^n_{\alpha\Psi}\left(x_{ij},t\right) \text{ and } f_{\alpha\Psi ij}=f_{\alpha\Psi}\left(x_{ij},t\right)$$

- $\rho^n_{\Psi ij}=\sum_\alpha f^n_{\alpha\Psi ij}, \rho^n_{\Psi ij}u^n_{\Psi ij}=\sum_\alpha f^n_{\alpha\Psi ij}e_\alpha$
- $\rho^n_{ij}=\sum_\Lambda \rho^n_{\Lambda ij}, \rho^n_{ij}u^n_{ij}=\sum_\Lambda \rho^n_{\Lambda ij}u^n_{\Lambda ij}$

compute the macroscopic density and velocity

Until $\left\|D^n_k-D^{n-1}_k\right\|<\varepsilon$

- $f_{\alpha\Psi ij}=f^n_{\alpha\Psi ij}, \rho_{ij}=\rho^n_{ij}, u_{ij}=u^n_{ij}, X_k=X^n_k, F_{b\alpha ij}=F^n_{b\alpha ij}$
- t = t+Δt, move forward to next time step

RESULTS AND DISCUSSION

Validation of multiples mixtures: The model has been validated by simulating the diffusion process of two binary mixtures with different initial concentration and comparing the concentration over time with the corresponding analytical solution (Incropera and De Witt, 2002; Arcidiacono *et al*., 2006). Setting $D^n_k=0$, $F^n_{b\alpha ij}=0$ and performing only one iteration in the coupling region, problems without IB contours can be simulated. If m_Ψ is the molecular mass of the specie Ψ, thus:

$$\rho_\Psi=m_\Psi\sum_\alpha f_{\alpha\Psi} \tag{31}$$

$$u_\Psi\rho_\Psi=m_\Psi\sum_\alpha f_{\alpha\Psi}e_\alpha \tag{32}$$

The channel size is 4×400 cells, periodic boundary conditions in the X-direction, bounce-back boundary condition (Chen and Doolen, 1998) in the y-direction, $\tau_\Gamma=\tau_\Lambda$, Γ and Λ are species with m_Λ/m_Γ=100, 60%Λ-40%Γ for x<0, 40% Λ-60% Γ for x≥0. Figure 3 shows the analytical and numerical solutions of the molar fraction $X_\Psi=n_\Psi/n$, where, $n_\Psi=\rho_\Psi/m_\Psi$ the molecules per unit volume and $n=\sum n_\Psi$. The numerical solution agrees fairly well with the analytical solution.

Semi-circular channels with a ternary mixture of species in this experiment the separation of three species through a curved channel is studied. Figure 4 shows the design of a semi-circular channel which is implemented through IB points. The grid dimensions are 100×100 cells. The IB points are spaced by 0.5 cells units. The species are named a, b and c, $\tau_a=\tau_b=\tau_c=0.75$, $m_a=2.0$ $m_b=1.98$ $m_c=0.22$. The channel has a parabolic input velocity profile, with particles uniformly distributed, where the peak velocities are $u_{ai}=u_{bi}=u_{ci}=$ 5e-4. Initial densities are $\rho_{a0}=3.8$ $\rho_{b0}=0.87$ $\rho_{c0}=0.88$. After 5000 time steps, a laminar flow in stationary state is obtained. The channel shape introduces a centrifugal-like force and due to mass difference a redistribution of the particles is produced along the channel (Fig. 5).

Figure 6 show the density profiles (ρ_a, ρ_b, ρ_c) in a flattened graph, where the area with the best separation (with darker colors on the bottom) can be observed and depends on the input speed.

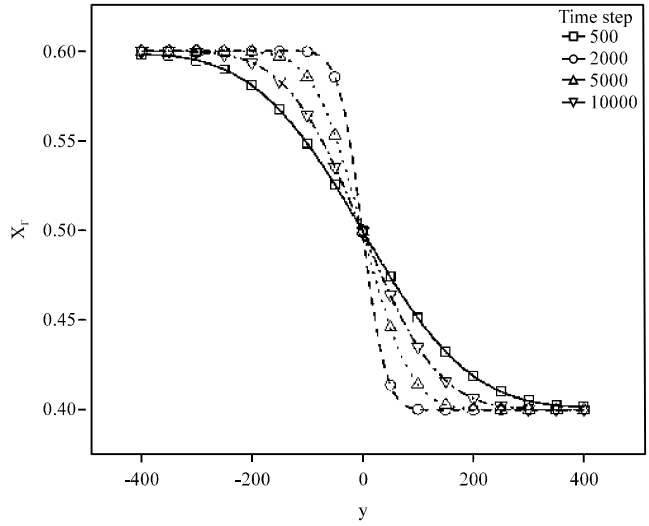

Fig. 3: Diffusion of a binary mixture in transitory state (molar fraction $X\Gamma=n_\Gamma/_n$ with respect to the transverse position Y)

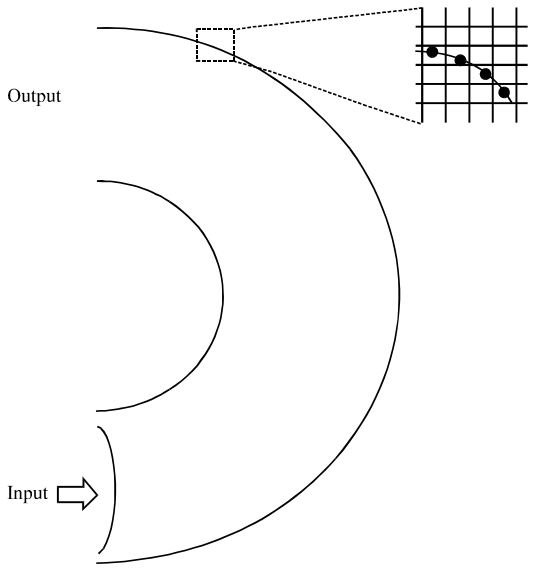

Fig. 4: Representation of a channel by means of Immerse Boundary

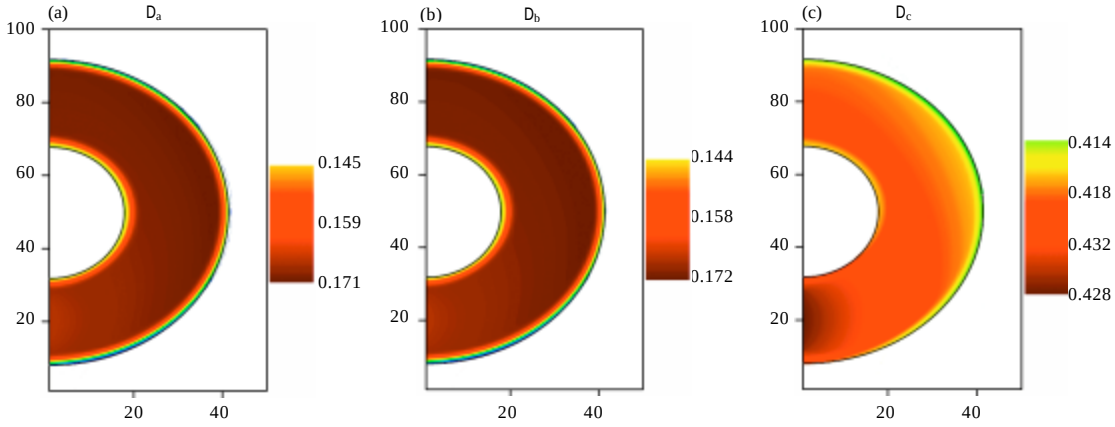

Fig. 5: Density ρ_Ψ (Eq. 13) in the semi-circular channel of (a) specie a, (b) specie b and (c) specie c

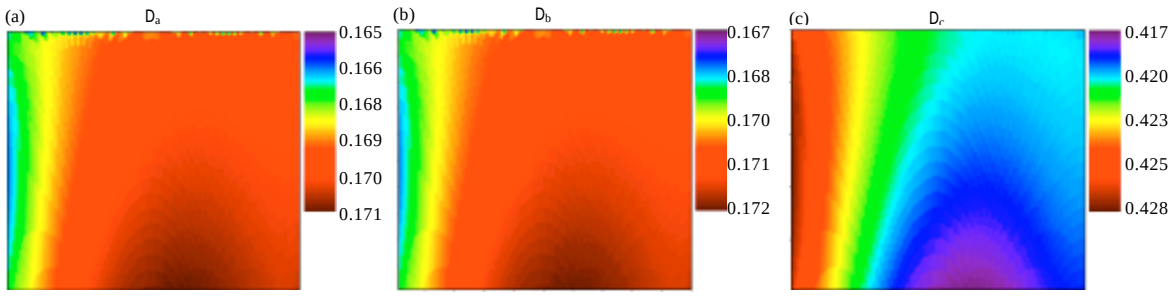

Fig. 6: Density ρ_Ψ (Eq. 13) profiles through channel direction of (a) specie a, (b) specie b and (c) specie c

CONCLUSION

An algorithm to implement the Immersed Boundary method in a Lattice Boltzmann scheme for multiple mixtures was presented. The IB enables the generalization of complex boundaries, instead of LBM regular grids. The model is simple and its implementation is straightforward. Numerical experiments where used to validate results.

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