THERMAL LATTICE BOLTZMANN BGK MODEL FOR IDEAL BINARY MIXTURES

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Abstract. A lattice Boltzmann model for binary mixtures is formally derived from a two-fluid kinetic model for Maxwell molecules by discretizing the Boltzmann equation. In this model, collisions among the same and different species are treated separately, as non-linear BGK terms, enabling the independent management of the species viscosities and thermal conductivities from the binary diffusion coefficient. The velocity space is discretized in accordance with a quadrature method with prescribed abscissas. A Chapman-Enskog analysis is performed for deriving the macroscopic mass, momentum end energy transport equations. The model is verified against the analytical solutions of the diffusion equation for several concentration, velocity and temperature initial conditions.

Keywords: Lattice Boltzmann Method, Gas mixtures, Mass diffusion

1. INTRODUCTION

The mass, momentum and heat transfer in binary fluid systems are of great interest in many engineering applications. Due to the success of new numerical methods on simulating thermohydrodinamics through the solution of the Boltzmann transport equation, e. g. the Lattice Boltzmann Method, in contrast to the traditional methods of Computational Fluid Dynamics, aimed to solve the Navier-Stokes equations, considerably efforts are made to apply this methods to the transport phenomena in gas mixtures.

The most of the first LB models for mixtures were based on a one-fluid theory, where the effects of all encounters were included in a single BGK term. This feature limited their applications to symmetric systems and introduced a heuristic artificial equilibrium velocity (Shan and Doolen, 1995).

Recently, Lattice Boltzmann models, based on the kinetic models of Sirovich and Hamel, were developed (Luo and Girimaji, 2003; Asinari, 2005; Xu, 2005). In these models, a more rigorous connection with the continuous kinetic theory was established but, they lack of a consistent treatment of internal energy transport in system with different molecular masses. Furthermore, the use of constant relaxation times leads to collision terms without the proper symmetries and a constant collision frequency where concentration is spatially non-homogeneous.

In this work a formal procedure is proposed for linking the lattice Boltzmann equation with the kinetic theory. For this purpose the velocity distribution function is developed in series of Hermite polynomial tensors and the discretization of the velocity space is performed using a quadrature method with prescribed abscissas (Philippi et al., 2006). The kinetic model proposed by Hamel (1965) and Morse (1964) was used to account the effect of self and cross collision separately. This approach is similar to the early proposed athermal model by Facin (2004). In addition to the obvious advantages of having a closed relation with existing theories, the present method allows the consistent treatment of the energy transport and the use of a single lattice for systems with components of different molecular masses, without interpolation or reallocation rules. The proposed discretization procedure can be easily extended for the construction of Lattice Boltzmann models for the Boltzmann equation with BGK collision operator, and its linearizations, in multicomponent and reacting systems.

2. TWO-FLUID BGK MODELS

The Boltzmann transport equation for a binary mixture of species a and b, is

$$\frac{\partial f^a}{\partial t} + \mathbf{c} \cdot \nabla f^a = J^{aa} + J^{ab}, \tag{1}$$

where J^{aa} and J^{ab} represent the rate at which the velocity distribution function of species a is modified by self and cross collisions, respectively (Chapman and Cowling, 1970; Ferziger and Kaper, 1972). Roughly speaking, the evolution of a mixture towards the equilibrium is conceived as composed by two processes: the approximation of the velocity distribution function to a local Maxwellian and the equilibrium process of the velocities and temperatures of all species to the same values. These processes could take place simultaneously and involving different time scales.

To avoid the complexity of the full collisional integrals, they are replaced by models that preserve some of its elementary properties. The first simple heuristic model was proposed for single component gases and later extended to a binary plasma (Bathnagar et al., 1954; Gross and Krook, 1956). This model, known as BGK, assumes that the collisions relax the distribution function to a local Maxwellian $f^{(M)}$, at a rate proportional to the collision frequency $n\nu$. In this manner,

the collision integrals in Eq. (1) can be approximated by

$$J_{BGK}^{aa} = n^a \nu^{aa} \left(f^{aa(M)} - f^a \right) \qquad \text{and} \qquad J_{BGK}^{ab} = n^b \nu^{ab} \left(f^{ab(M)} - f^a \right), \tag{2}$$

where

$$f^{ab(M)} = n^{ab} \left(\frac{m^a}{2\pi k T^{ab}} \right)^{D/2} \exp \left(-\frac{m^a \left(\mathbf{c} - \mathbf{u}^{ab} \right)^2}{2k T^{ab}} \right), \tag{3}$$

and $\nu^{ab} = \nu^{ba}$ are constants. The parameters $n^{aa/ab}$, $\mathbf{u}^{aa/ab}$ and $T^{aa/ab}$ into the Maxwellian distribution functions were constructed as linear combinations of the local properties of both species, constrained by the collisional symmetries and the conservation laws. A more detailed model, for molecules with inverse fifth-power force law (Maxwell molecules), was proposed in Hamel (1965) and Morse (1964). The Maxwellian distribution functions were adjusted to reproduce the collisional transfer of momentum and energy or the relaxation processes in a spatially homogeneous system of Maxwell molecules, in a D-dimensional space. For the self collision model, $f^{aa(M)}$ is a function of the local properties of species a and, for the cross collision model, the parameters in $f^{ab(M)}$ are

$$n^{ab} = n^a, \tag{4}$$

$$\mathbf{u}^{ab} = \mu^a \mathbf{u}^a + \mu^b \mathbf{u}^b \tag{5}$$

and

$$T^{ab} = T^a + \mu^a \mu^b \left[2 \left(T^b - T^a \right) + \frac{\mu^b \left(m^a + m^b \right)}{Dk} \left(\mathbf{u}^a - \mathbf{u}^b \right)^2 \right], \tag{6}$$

where $\mu^a = m^a / \left(m^a + m^b \right)$. In circumstances where it is possible to assume that the velocity distribution function has a small deviation from the local equilibrium distribution function of the mixture, the collision operator model can be written as

$$J_{BGKL}^{ab} = n^b \nu^{ab} \left(f^{(M)} \left(n^a, \mathbf{u}, T \right) - f^a \right)$$

$$+ n^b \nu^{ab} \left[\frac{\partial f^{(M)} (n^a, \mathbf{u}, T)}{\partial \mathbf{u}} \cdot \left(\mathbf{u}^{ab} - \mathbf{u} \right) + \frac{\partial f^{(M)} (n^a, \mathbf{u}, T)}{\partial T} \left(T^{ab} - T \right) \right] \tag{7}$$

where $\mathbf{u}$ is the mixture velocity and T is the mixture temperature. With this linearization, the model becomes amenable for a conventional Chapman-Enskog analysis (Chapman and Cowling, 1970; Facin et al., 2004). As shown in Hamel (1965), other linearizations are possible. Particularly, the linearization of the BGK model about a local Maxwellian distribution function of each species corresponds to the model proposed in Sirovich (1962).

Equation (2) is a exact representation of the homogeneous relaxation process and a qualitative approximation of the Maxwellization process. Despite the fact that it have drawbacks, as the relaxation of higher order moments at the same rate, non-indifferentiability of identical molecules and lack of thermal diffusion, it is adequate to be used for the simulation of hydrodynamics and diffusion in moderate conditions.

3. LATTICE BOLTZMANN BGK MODEL FOR BINARY MIXTURES

It was pointed out that the Lattice Boltzmann Equation derived from the lattice gas cellular automata have a close relation with kinetic theory and can be considered as particular discretization of the Boltzmann BGK equation (He and Luo, 1997; Shan and He, 1998; Philippi et al., 2006).

Following Grad's work, the velocity distribution function can be expressed in a infinite series of Hermite polynomial tensors in the molecular velocity (Grad, 1949). The Hermite tensors are an orthonormal basis of the Hilbert space of functions. Choosing a reference speed, defined as $c_0 \equiv \sqrt{\frac{kT_0}{m_0}}$, and the factor $n_0 c_0^{-D}$, for scaling the molecular velocity and the distribution function, respectively, the dimensionless velocity distribution function can be written as

$$f(\mathbf{x}, \mathbf{c}, t) = \omega(\mathbf{c}) \sum_{n=0}^{\infty} \frac{1}{n!} a^{(n)}(\mathbf{x}, t) \mathcal{H}^{(n)}(\mathbf{c}), \tag{8}$$

where n is the order of the tensor and

$$\omega(\mathbf{c}) = \frac{e^{-\frac{c^2}{2}}}{(2\pi)^{D/2}} \tag{9}$$

is the weight function of the inner product in Hilbert space. The coefficients of the series are the velocity moments of the distribution function, calculated as

$$a_{r_n}^{(n)} = \int f \mathscr{H}_{r_n}^{(n)}(\mathbf{c}) \mathrm{d}\mathbf{c}, \tag{10}$$

and the product of the Hermite tensor $\mathscr{H}_{r_n}^{(n)}$ and the coefficient of the series $a_{r_n}^{(n)}$ is a contraction over all the n indexes.

After the polynomial series development of the velocity distribution function, the discretization procedure begins with the proper calculation of a set of dimensionless velocity vectors provided that the velocity moments have the same value of the continuous distribution function, up to a order consistent with a Chapman-Enskog analysis (McNamara and Alder, 1993).

Hydrodynamics description requires exact representation of only the first velocity moments of the distribution function, allowing for a series truncation at the representation order N. Replacing f in Eq. (10) by the truncated expansion and considering that the coefficients of the Hermite polynomials are only functions of macroscopic variables and independent of the integration, a sufficient condition for the correct representation of hydrodynamics is the exact calculation of the inner product of Hermite tensors, with orders up to N, by a quadrature formula with w_i weights

$$\int \omega(\mathbf{c}) \mathscr{H}_{r_n}^{(n)}(\mathbf{c}) \mathscr{H}_{s_m}^{(m)}(\mathbf{c}) \mathrm{d}\mathbf{c} = \sum_i^b W_i \mathscr{H}_{r_n}^{(n)}(\mathbf{c}_i) \mathscr{H}_{s_m}^{(m)}(\mathbf{c}_i), \tag{11}$$

where b is the number of velocities and $W_i = w_i \omega(\mathbf{c}_i)$.

The purpose in the velocity discretization by a quadrature method is to find the minimal number of vectors and weights that satisfies Eq. (11). Some well known quadrature methods could be used but, only a few provide a solution set whose elements could be written as integer factors of the generating vectors of a space filling regular lattice (He and Luo, 1997). To circumvent this problem, a formal procedure to solve the Eq. (11) for a set of prescribed abscissas was proposed by Philippi et al. (2006). The choice of the abscissas allows the use of those solutions in the Lattice Boltzmann Equation framework, where the space and velocity must be coupled, through the relation $\mathbf{c}_i = \Delta\mathbf{x}_i/\Delta t$, to allow a exact *collision* and *stream* sequence.

As a particular case of f, the Maxwellian distribution function, written in dimensionless variables,

$$f^{ab(M)} = \frac{n^{ab}}{(2\pi)^{D/2}} \left(\frac{1}{\theta^{ab}+1} \right)^{D/2} \exp\left(-\frac{1}{2} \frac{(\mathbf{c}-\mathbf{u}^{ab})^2}{(\theta^{ab}+1)} \right), \tag{12}$$

where $\theta^{ab} = \left(\frac{T^{ab}}{T_0} \frac{m_0}{m^a} - 1 \right)$ is a mass-temperature deviation from the references values, can be put in the form of Eq. (8). Then, the calculation of its corresponding velocity moments concludes the construction of the discrete velocity Boltzmann BGK equation for $f_i^a = W_i f^a(\mathbf{x}, \mathbf{c}_i, t)$. Solutions for several truncation representation orders are shown in Philippi et al. (2006).

The advection term in the discrete velocity Boltzmann equation could be discretized with several finite-difference schemes for the time and space derivatives. The Lattice Boltzmann Equation is a particular explicit first order upwind scheme, with unitary CFL number, for uniform cartesian grids. The application of this discretization scheme to Eq. (1) gives

$$f_i^a(\mathbf{x}+\mathbf{c}_i, t+1) = f_i^a(\mathbf{x}, t) + n^a \nu^{aa} \left(f_i^{aa(M)} - f_i^a \right) + n^b \nu^{ab} \left(f_i^{ab(M)} - f_i^a \right). \tag{13}$$

The special conditions of the former LBE allow the absorption of the first order time and space errors into the transport coefficients, attaining second order accuracy on the solution of thermohydrodinamics (Cao et al., 1997).

4. THERMOHYDRODYNAMICS AND DIFFUSION

A Chapman-Enskog analysis of the Lattice Boltzmann Equation with the linearized collision model, in the form of Eq. (7), was developed, introducing the expansions in the small parameter ε (Knudsen number)

$$f_i^a = f_i^{a(0)} + \varepsilon f_i^{a(1)} + \varepsilon^2 f_i^{a(2)} + \cdots, \tag{14}$$

$$\partial_t = \partial_0 + \varepsilon \partial_1 + \cdots \tag{15}$$

The deviations from local equilibrium were considered as Knudsen first order terms. Then, the zero order solution $f^{a(0)}$ is the Maxwellian distribution function with the local velocity and temperature of the mixture. The Knudsen first and second order equations, in the usual notation, are

$$\partial_0 f_i^{a(0)} + c_{i,\alpha} \partial_\alpha f_i^{a(0)} = J_i^{aa(1)} + J_i^{ab(1)}, \tag{16}$$

$$\partial_0 f_i^{a(1)} + \partial_1 f_i^{a(0)} + c_{i,\alpha}\partial_\alpha f_i^{a(1)} + \tfrac{1}{2}\partial_0\left(\partial_0 f_i^{a(0)} + c_{i,\alpha}\partial_\alpha f_i^{a(0)}\right)$$

$$+\tfrac{1}{2}c_{i,\alpha}\partial_\alpha\left(\partial_0 f_i^{a(0)} + c_{i,\beta}\partial_\beta f_i^{a(0)}\right) = J_i^{aa(2)} + J_i^{ab(2)}, \tag{17}$$

constrained by

$$\rho^a = m^a \sum_i f_i^{a(0)}, \qquad \sum_i f_i^{a(l)} = 0 \qquad \forall l \geq 1,$$

$$j_\alpha^{a(l)} = \rho^a\left(u_\alpha^{a(l)} - u_\alpha\right) = m^a \sum_i f_i^{a(l)} c_{i\alpha},$$

$$\rho^a \epsilon^a = \tfrac{1}{2}m^a \sum_i f_i^{a(0)}(C_i^a)^2, \qquad \sum_i f_i^{a(l)}(C_i^a)^2 = 0 \qquad \forall l \geq 1, \tag{18}$$

where ϵ^a is the internal energy and $\mathbf{C}_i^a = \mathbf{c}_i - \mathbf{u}^a$ is the peculiar velocity of species a.

With a set of velocity vectors and a proper Maxwellian function, up to a third truncation order $N = 3$, the m^a moment of Eq. (16) and Eq. (17) leads, exactly, to the mass diffusion equation

$$\partial_t \rho^a + \partial_\alpha \rho^a u_\alpha = -\partial_\alpha j_\alpha^a, \tag{19}$$

$$j_\alpha^a = -\frac{n^2}{\rho}m^a m^b \mathscr{D}^{ab} d_\alpha^a, \tag{20}$$

where the diffusive force is

$$d_\alpha^a = \nabla\frac{n^a}{n} + \left(\frac{n^a}{n} - \frac{\rho^a}{\rho}\right)\nabla\log p, \tag{21}$$

the pressure is $p = nkT$, and the effective binary diffusion coefficient is

$$\mathscr{D}^{ab} = \frac{p\rho}{n^2 m^a m^b}\left(\frac{m^a + m^b}{\rho\nu^{ab}} - \frac{1}{2}\right). \tag{22}$$

In a similar way, the $m^a c_{i\alpha}$ moment of the Knudsen first and second order equations, with a fourth truncation order in the polynomial expansion of f^a, recovers the momentum transport equation for species a. Adding the two momentum equations of species a and b the momentum conservation equation for the mixture is obtained

$$\partial_t \rho u_\beta + \partial_\alpha \rho u_\alpha u_\beta = -\partial_\alpha \Pi_{\alpha\beta}, \tag{23}$$

with the pressure tensor

$$\Pi_{\alpha\beta} = p\delta_{\alpha\beta} - \eta\left(\partial_\alpha u_\beta + \partial_\beta u_\alpha - \frac{2}{D}\partial_\gamma u_\gamma \delta_{\alpha\beta}\right) \tag{24}$$

and the effective dynamic viscosity

$$\eta = kT\left(\frac{n^a}{\Gamma^a} - \frac{n^a}{2} + \frac{n^b}{\Gamma^b} - \frac{n^b}{2}\right), \tag{25}$$

where $\Gamma^a = n^a \nu^{aa} + n^b \nu^{ab}$ and $\Gamma^b = n^b \nu^{bb} + n^a \nu^{ba}$. Mixture viscosity is a function of the local particle densities n^a and n^b, the three parameters ν^{aa}, ν^{ab}, $\nu^{ab} = \nu^{ba}$ and the local mixture temperature. In circumstances when $n^b \to 0$, $n \to n^a$, $T \to T^a$ and we recover the expression for the viscosity of the single component a,

$$\eta^a = p\left(\frac{1}{n^a \nu^{aa}} - \frac{1}{2}\right). \tag{26}$$

Excluding the spurious terms, the binary diffusion coefficient and mixture viscosity are equals to those reported for Maxwell molecules and for the non-linear BGK model (Chapman and Cowling, 1970; Hamel, 1965; Goldman and Sirovich, 1967).

An analogous procedure, using a fifth truncation order velocity distribution function, gives the energy conservation equation for the mixture

$$\partial_t\left(\frac{D}{2}nkT + \frac{u^2}{2}\rho\right) + \partial_\alpha\left(\frac{D}{2}nkTu_\alpha + \frac{u^2}{2}\rho u_\alpha + u_\beta\Pi_{\alpha\beta} + q_\alpha\right) = 0, \tag{27}$$

where the non-convective energy flux vector is

$$q_\alpha = -\kappa \partial_\alpha T + \frac{(D+2)}{2} kT \left(\frac{j_\alpha^a}{m^a} + \frac{j_\alpha^b}{m^b} \right).$$ (28)

The first term in the above expression is the thermal conduction, with effective thermal conductivity

$$\kappa = \frac{(D+2)}{2} k^2 T \left(\frac{n^a}{m^a \Gamma^a} - \frac{n^a}{2m^a} \Delta t + \frac{n^b}{m^b \Gamma^b} - \frac{n^a}{2m^b} \Delta t \right),$$ (29)

and the second is the effective transport of enthalpy by the species diffusive currents. In the limit condition $n^b \rightarrow 0$, the effective thermal conductivity of a single component gas is recovered,

$$\kappa^a = \frac{(D+2)}{2} \frac{pk}{m^a} \left(\frac{1}{n^a \nu^{aa}} - \frac{\Delta t}{2} \right).$$ (30)

5. NUMERICAL RESULTS

Simulation of the convection diffusion equation in a step problem were performed to verify the results of the multiscale analysis, Eqs. (22), (25) and (29). Under special conditions, the mass diffusion, the momentum and the energy equations can be written in the form of the diffusion equation

$$\frac{\partial \phi}{\partial t} + u_x \frac{\partial \phi}{\partial x} = \mathcal{D} \frac{\partial^2 \phi}{\partial x^2},$$ (31)

assuming constant transport coefficients. The analytical solution of the Eq. (31) for a step into the ϕ property,

$$\phi(x, t = 0) = \begin{cases} \phi_0 + \Delta\phi & \text{for} \quad x < 0 \\ \phi_0 & \text{otherwise} \end{cases},$$ (32)

in an infinite medium at rest, is

$$\phi(x, t) = \phi_0 + \frac{1}{2} \Delta\phi \, \text{erfc} \left(\frac{x}{2\sqrt{\mathcal{D}t}} \right).$$ (33)

For a sinusoidal initial distribution with uniform velocity u_x the analitical solution is

$$\phi(x, t) = \frac{1}{2} \Delta\phi \left(e^{-K^2 \mathcal{D}t} \sin(Kx - Ku_x t) + 1 \right),$$ (34)

where K is the wave number.

The former equations were used to verify the expression of the transport coefficients by comparing the evolution of these simplified configurations with the simulations of the concentration, velocity and temperature steps in a one-dimensional domain with periodic boundary conditions in all directions.

For a system of identical particles, at rest, and with initial conditions in mass concentration, in the form of Eq. (32), the binary diffusion coefficient could be considered essentially constant if the total particle density is the same in all sites and fluid pressure and temperature are homogeneous and constant. The evolution of this system is given by the solution of the diffusion equation mentioned above. Several simulations with different relaxation parameters combinations and different initial temperatures were carried out with excellent agreement with the theoretical solutions with the diffusion coefficient $\mathcal{D}$ calculated using initial values of the fluid properties. In the same way, simulations with the second kind of inital conditions were carried out with excellent agreement with the analytical solutions. Figure 1 shows the decaying of a sinusoidal concentration distribution in a system of equal masses every 180 time steps, from the initial configuration to a stage when the wave was travel a half of the computatonal domain, in a simulation with the $D2V53$ lattice. The concentration step problems were simulated also for systems with different molecular masses. In these cases, the assumptions made to obtain the diffusion equation are not valid.

Similar experiments were accomplished for the verification of the mixture viscosity and thermal conductivity. In a system with homogeneous composition and temperature, but different molecular masses and concentrations, the mixture velocity component was set as $u_x = 0$ in all domain, $u_{y0} = 0$ and $\Delta u_y = 0.05$. For small deviations in pressure and concentration, the momentum equation Eq. (23) take the form of the diffusion equation (31). Figure 2 shows a comparison of the evolution of this system with analytical solution, every 200 steps, in a computational domain of 200×1 sites with a $D2V37$ lattice (Philippi et al., 2006). In a system of equal molecular masses, initially at rest and with homogeneous composition, a step in the mixture temperature is also approximately described by Eq. (31). The Figure (3) shown an example of this process in a system with molecular mass ratio $\mu_a/\mu_b = 1.5$, using the $D2V37$ lattice at every 200 time steps. Simulations were carried out using Maxwellian distribution function of several approximation orders and the $D2V17$, $D2V37$, and $D2V53$ lattices.
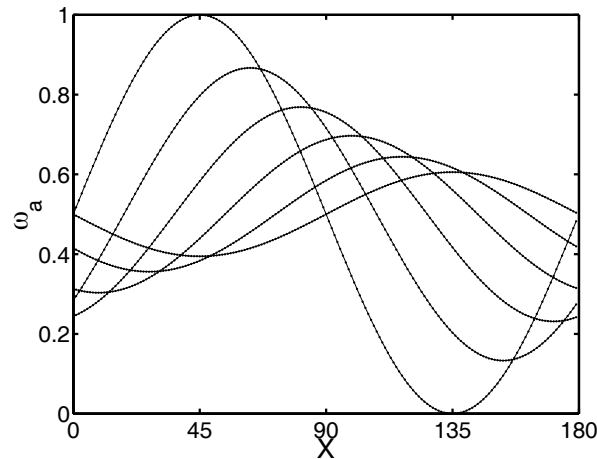
Figure 1. Sinusoidal concentration profile decaying. $\nu^{aa} = 1.0$, $\nu^{bb} = 0.7$, $\nu^{ab} = \nu^{ba} = 1.9$, $n = 0.5$, $\theta^a = \theta^b = 0.0$, $u_x = 0.1$. (•) t = [0 - 900]. Solid lines are the analytical solution.
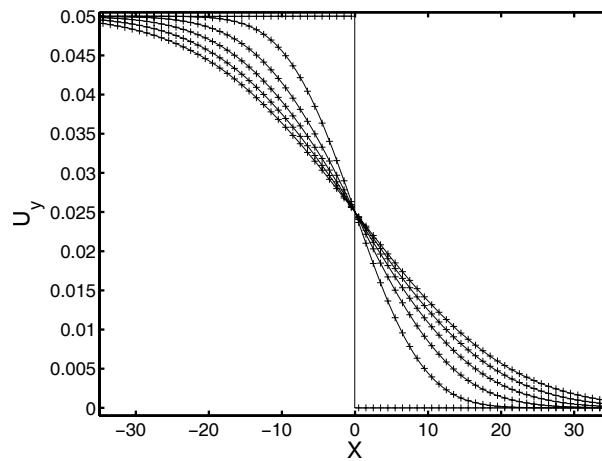

Figure 2. Velocity profile for the step problem. $\nu^{aa} = 1.5$, $\nu^{bb} = 1.0$, $\nu^{ab} = \nu^{ba} = 0.8$, $n^a = 0.5$, $n^b = 1.0$, $\mu^a = 0.6$, $\mu^b = 0.4$, $\theta^a = -0.2$, $\theta^b = 0.2$. (+) t = [0 - 1000]. Solid lines are the analytical solution.

The simulation results of the three kind of problems are in excellent agreement with the theoretical predictions and, for all the parameters combinations tested, the differences are below 0.1%.

Numerical instabilities appear when high mass ratios or high temperature deviation are used, particularly at low values of the transport coefficients.

6. CONCLUSIONS

In this work, a lattice Boltzmann model for binary mixtures was derived from the Boltzmann equation and kinetic models, through a formal procedure of discretization.

The two-fluid theory with a BGK approximation of the collision operator allows to set the binary diffusion coefficient and the species viscosities and thermal conductivities independently. The discretization used also allows simulating diffusion of gases with different molecular weights using the same lattice vectors. A Chapman-Enskog analysis of the linearized model reveals that it reproduces the correct macroscopic hydrodynamic equations and transport coefficients. To verify the results of the multiscale analysis, numerical simulations were carried out for the one-dimensional step in concentration, velocity and temperature. The simulations are in excellent agreement with the analytical solution of the diffusion equation.

Numerical instabilities appear for configurations with large temperature deviation, particularly for high molecular mass ratios.
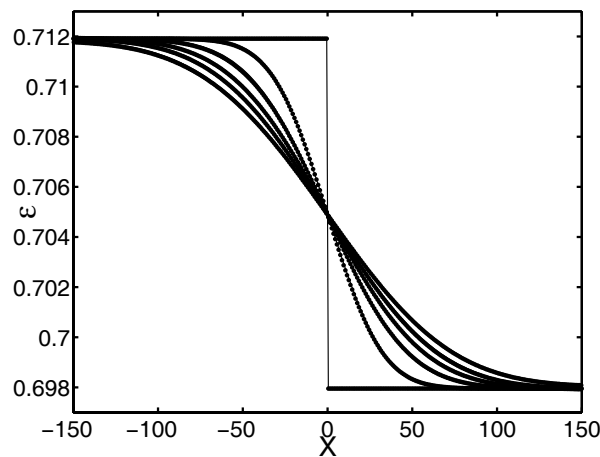
Figure 3. Internal energy profile for the step problem. $\nu^{aa} = 0.7$, $\nu^{bb} = 0.5$, $\nu^{ab} = \nu^{ba} = 0.9$, $n^a = 0.2$, $n^b = 0.3$, $\mu^a = 0.6$, $\mu^b = 0.4$, $\Delta\theta = 0.02$. (•) t = [0 - 1000]. Solid lines are the analytical solution.

7. ACKNOWLEDGMENTS

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