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Pietro Asinari

Department of Energetics, Politecnico di Torino
Corso Duca degli Abruzzi 24, Zip Code 10129, Torino, Italy
Tel. +39-011-564-4413, Fax. +39-011-564-4499

Abstract

A new lattice Boltzmann model for simulating ideal mixtures has been developed by means of the multiple-relaxation-time (MRT) approach. If compared with the previous single-relaxation-time (SRT) formulation of the same model, based on the continuous kinetic theory, the new model offers the possibility to independently tune the mutual diffusivity and the effects of cross collisions on the effective stress tensor. The additional degrees of freedom, due to the increased set of relaxation time constants used for modeling the cross collisions, allows us to match the experimental data on macroscopic transport coefficients. Two different integration rules, i.e. the forward Euler and the modified mid-point integration rule, were used in order to numerically integrate the developed model. Unfortunately the simpler forward Euler integration rule violates the mass conservation and there is no way to fix the problem by changing the definition of the macroscopic velocity. On the other hand, a small correction has been purposely designed for compensating this error by means of the mid-point integration rule. Some numerical simulations are reported for proving the effectiveness of the proposed corrective factor. For the considered application, the asymptotic analysis, recently suggested as an effective tool for analyzing the macroscopic equations corresponding to the lattice Boltzmann schemes, offers a remarkable advantage in comparison with the classical Chapman-Enskog technique, because it easily deals with leading terms in the distribution functions, which are no more Maxwellian.

Key words: mixture modeling, cross collisions, lattice Boltzmann method, asymptotic analysis

Email address: `pietro.asinari@polito.it` (Pietro Asinari).

1 Introduction

In the last years, the lattice Boltzmann method (LBM) has become very popular among the discretization techniques for solving simplified kinetic models. Starting from some pioneer works [1–3], the method has reached a more systematic fashion [4,5] by means of a better understanding of the connections with the continuous kinetic theory [6,7] and by widening the set of applications, which can benefit from this numerical technique. When complex geometries are considered and the inter-particle interactions must be taken into account, the discretized models derived by means of the lattice Boltzmann method offer some computational advantages over continuum based models, particularly for large parallel computing. A more complete and recent coverage of various previous contributions on LBM is beyond the purposes of the present paper, but can be found in some books [8–10] and some review papers [11,12].

A promising application for lattice Boltzmann models seems to be the analysis of reactive mixtures in porous catalysts [13,14]. For this reason, a lot of work has been performed in recent years in order to produce reliable lattice Boltzmann models for multi-component fluids and, in particular, for mixtures composed by miscible species. The problem is to find a proper way, within the framework of a simplified kinetic model, for describing the interactions among particles of different types, i.e. cross collisions. Once this milestone is defined, the extension of the model to reactive flows is straightforward [15,16] and it essentially involves additional source terms in the species equations according to the reaction rate.

Unfortunately, most existing lattice Boltzmann models for mixtures are based on pseudo-potential interactions [17–20] or heuristic free energies [21–24] in order to realize the so-called *single-fluid approach* [25,26]. Essentially, the averaged effect due to both self-collisions and cross-collisions is described by means of a total BGK-like collisional operator. Considering some special kind of mixture properties in the Maxwellian distribution function of the BGK-like collisional operator, each species will be forced to evolve towards the mixture equilibrium conditions. For almost a decade now, diffusions driven by concentrations, pressure, temperature and external forces have been studied by this kind of models for arbitrary number of components with non-ideal interactions. Even though the single-fluid approach proved to be an accurate numerical tool for solving some macroscopic equations in a large number of applications, it provides a mesoscopic picture of the phenomena which shows some limits.

On the other hand, some models based on the *two-fluid approach* have been proposed. According to this approach, each species relaxes towards its equilib-

rium configuration according to its specific relaxation time and some coupling must be considered in order to describe the collisions among different species. Some models [27,28] adopt a *force coupling* in the momentum equations, which derives from a linearized kinetic term, while other models [29,30] adopt a *viscous coupling*, which is an additional coupling effect in the effective stress tensor.

In particular, the Hamel model [31–33], originally developed within the framework of the continuous kinetic theory, implies that cross collisions realize both an internal coupling force, proportional to the diffusion velocity, and an additional coupling effect in the effective stress tensor. For this reason, Hamel model is the natural forerunner of all linearized models and allows us to describe mixtures at different limiting regimes consistently. An LB discrete formulation of the continuous kinetic model proposed by Hamel has been recently proposed [30]. Unfortunately in the original LB formulation, the macroscopic mutual diffusivity and the mixture kinematic viscosity could not be independently tuned because only a single cross-collision relaxation time was available. Tuning strategies based on diffusivity or on mixture kinematic viscosity were proposed, but it is worth pointing out that in that formulation the viscous relaxation process and the diffusion process were inseparable.

The goal of this paper is twofold:

(1) to extend the previous LB formulation of the Hamel model by means of the multiple-relaxation-time [34,35] (MRT) approach in order to independently tune both mutual diffusivity and mixture kinematic viscosity, which, according to the experimental data, differs from the elementary mass averaged kinematic viscosity;
(2) to prove that, for the considered application, the asymptotic analysis [36], recently suggested as an effective tool for analyzing the macroscopic equations corresponding to LB schemes, offers some advantages if compared with the classical Chapman-Enskog expansion.

Even though the MRT formulation represents a remarkable progress, the well-known drawback of Hamel model of the Boltzmann system for gas mixtures is the lack of differentiability. The indifferentiability principle [37] prescribes that, if a BGK-like equation for each species is assumed, this set of equations should reduce to a single BGK-like equation, when mechanically identical components are considered. This essentially means that, when all the species are identical, one should recover the equation governing the single component gas dynamics. This principle can be considered one of the basic physical properties in the design of simplified kinetic models for mixture modeling [38]. From the macroscopic point of view, the consequences due to the lack of differentiability will be discussed (see Section 4 for details). However this paper still considers the original formulation of the Hamel model. The development of an

MRT model for mixture modeling fully consistent with the indifferentiability principle is discussed in another paper [39].

This paper is organized as follows. Section 2 summarizes the previous single-relaxation-time formulation of the Hamel model. Section 3 generalizes the previous formulation by means of the multiple-relaxation-time approach for the continuous case. Section 4 recovers the macroscopic equations which correspond to the continuous model by means of the asymptotic analysis. Section 5 recovers the macroscopic equations for the discrete model based on the forward Euler integration rule. Since this simple implementation does not satisfy the continuity equation, Section 6 discusses a modified integration scheme based on the modified mid-point integration rule for ensuring the mass conservation. Section 7 reports some numerical simulations for proving that the modified integration scheme is effective and, finally, Section 8 summarizes the conclusions of this work.

2   Single-relaxation-time (SRT) formulation of the Hamel model on the D2Q9 lattice

According to the Hamel model [31–33], the distribution function g_σ for the generic species σ satisfies the following equation,

$$\frac{\partial_t g_\sigma}{\partial t} + \mathbf{v} \cdot \nabla g_\sigma = \frac{1}{\tau_\sigma} \left(g_\sigma^e - g_\sigma \right) + \frac{1}{\tau_m} \left(g_{\sigma\,m}^e - g_\sigma \right), \tag{1}$$

where $g_\sigma^e = g_*^e(\mathbf{u}_\sigma)$, $g_{\sigma\,m}^e = g_*^e(\mathbf{u})$ and $g_*^e(\mathbf{u}_*)$ is defined as

$$g_*^e(\mathbf{u}_*) = \frac{\rho_\sigma}{m_\sigma \left(2\pi e_\sigma \right)^{D/2}} \exp\left[-\frac{(\mathbf{v} - \mathbf{u}_*)^2}{2\,e_\sigma} \right]. \tag{2}$$

In particular $\mathbf{u}_\sigma$ is the single species velocity and $\mathbf{u}$ is the barycentric velocity, defined as the mass average of the single species velocities, i.e. $\mathbf{u} = \sum_\sigma x_\sigma \mathbf{u}_\sigma$ where x_σ is the generic concentration. The relaxation time constants τ_σ and τ_m describe the equilibration process due to self collisions and cross collisions, respectively. Introducing a proper two-dimensional lattice (D2Q9) for the microscopic velocity and considering the limiting case $U/c \ll 1$, where U is a characteristic macroscopic flow speed and c is the lattice speed, yield to the single-relaxation-time (SRT) formulation of the Hamel model [30], namely

$$\frac{\partial f_\sigma^i}{\partial t} + \mathbf{v}^i \cdot \nabla f_\sigma^i = \lambda_\sigma \left(f_\sigma^{e\,i} - f_\sigma^i \right) + \lambda_m \left(f_m^{e\,i} - f_\sigma^i \right), \tag{3}$$

4

where $f_\sigma^{e\,i} = f_\sigma^{e\,i}(\mathbf{u}_\sigma)$ is the equilibrium distribution function centered on the species velocity and $f_m^{e\,i} = f_m^{e\,i}(\mathbf{u})$ is the equilibrium distribution function centered on the barycentric velocity, defined as the mass average of the species velocities.

It is possible to reformulate the previous equation in a more simple way,

$$\frac{\partial f_\sigma^i}{\partial t} + \mathbf{v}^i \cdot \nabla f_\sigma^i = (\lambda_\sigma + \lambda_m) \left(f_{\sigma m}^{e\,i} - f_\sigma^i \right), \tag{4}$$

where $f_{\sigma m}^{e\,i} = (1 - \alpha_\sigma) f_\sigma^{e\,i} + \alpha_\sigma f_m^{e\,i}$ and $\alpha_\sigma = \lambda_m / (\lambda_\sigma + \lambda_m)$. The modified equilibrium distribution function is defined as

$$f_{\sigma m}^{e\,i} = \rho_\sigma \, \varsigma^i \left\{ \frac{(9 - 5\,s_\sigma)}{4} - \frac{3}{2\,c^2} \left[(1 - \alpha_\sigma) \, \mathbf{u}_\sigma^2 + \alpha_\sigma \, \mathbf{u}^2 \right] \right\}, \tag{5}$$

for $i = 0$,

$$
\begin{aligned}
f_{\sigma m}^{e\,i} = \rho_\sigma \, \varsigma^i \Big\{ & s_\sigma + \frac{3}{c^2} \, \mathbf{v}^i \cdot \left[(1 - \alpha_\sigma) \, \mathbf{u}_\sigma + \alpha_\sigma \, \mathbf{u} \right] \\
& + \frac{9}{2\,c^4} \left[(1 - \alpha_\sigma) \, (\mathbf{v}^i \cdot \mathbf{u}_\sigma)^2 + \alpha_\sigma \, (\mathbf{v}^i \cdot \mathbf{u})^2 \right] \\
& - \frac{3}{2\,c^2} \left[(1 - \alpha_\sigma) \, \mathbf{u}_\sigma^2 + \alpha_\sigma \, \mathbf{u}^2 \right] \Big\},
\end{aligned} \tag{6}
$$

for $1 \leq i \leq 8$ and $s_\sigma = 3\,e_\sigma / c^2$. The constants ς^i are the usual weight factors for this lattice [5] and e_σ is the internal energy. The previous equations can be written in vectorial form, namely

$$\frac{\partial \mathbf{f}_\sigma}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{f}_\sigma = (\lambda_\sigma + \lambda_m) \, \mathbf{I} \, (\mathbf{f}_{\sigma m}^e - \mathbf{f}_\sigma), \tag{7}$$

where $\mathbf{V}$ is defined as

$$\mathbf{V}^T = c \begin{bmatrix} 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \end{bmatrix}. \tag{8}$$

It is possible to consider an equivalent moment system of the previous model by defining a proper set of moments. The lower-order moments are the conserved hydrodynamic moments, but the higher-order non-hydrodynamic moments are unknown. Since the final goal of the moment formulation is to decouple the different moments in order to differently relax them, it seems

natural to consider an orthogonalization procedure: in the following, the well-known Graham-Schmidt procedure will be considered. For this procedure two elements are needed: the generalized scalar product and the starting non-orthogonal basis. Concerning the first issue, it has been shown that the scalar product, which includes the weight factors, namely

$$< \mathbf{x}_1, \mathbf{x}_2 >= \sum_{i=0}^{8} \varsigma^i \, x_1^i \, x_2^i, \tag{9}$$

generates orthogonal basis clearly separating the terms in the distribution function according to the power of macroscopic velocities [36]. Concerning the starting non-orthogonal basis, it is essentially a matter of convenience: for simplicity, a simple monomial basis will be considered $\{1, \hat{v}_x, \hat{v}_y, \}$ and $\left\{ \hat{v}_x \hat{v}_y, \hat{v}_x^2, \hat{v}_y^2, \hat{v}_x \hat{v}_y^2, \hat{v}_y \hat{v}_x^2, \hat{v}_x^2 \hat{v}_y^2 \right\}$, where $\hat{v}_x = v_x/c$ and $\hat{v}_y = v_y/c$. These assumptions yield the following linear mapping

$$\mathbf{M}_A = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\ 0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\ -1/3 & 2/3 & -1/3 & 2/3 & -1/3 & 2/3 & 2/3 & 2/3 & 2/3 \\ -1/3 & -1/3 & 2/3 & -1/3 & 2/3 & 2/3 & 2/3 & 2/3 & 2/3 \\ 0 & -1 & 0 & 1 & 0 & 2 & -2 & -2 & 2 \\ 0 & 0 & -1 & 0 & 1 & 2 & 2 & -2 & -2 \\ 1 & -2 & -2 & -2 & -2 & 4 & 4 & 4 & 4 \end{bmatrix}, \tag{10}$$

which allows us to define the full set of equilibrium moments for self collisions

$$\mathbf{m}_\sigma^e = \mathbf{M}_A \, \mathbf{f}_\sigma^e = \rho_\sigma \left[1, \hat{u}_{\sigma x}, \hat{u}_{\sigma y}, \hat{u}_{\sigma x} \hat{u}_{\sigma y}, \right.$$
$$\left. (s_\sigma - 1)/3 + \hat{u}_{\sigma x}^2, (s_\sigma - 1)/3 + \hat{u}_{\sigma y}^2, 0, 0, 1 - s_\sigma \right]^T, \tag{11}$$

and cross collisions

$$\mathbf{m}_m^e = \mathbf{M}_A \, \mathbf{f}_m^e = \rho_\sigma \left[1, \hat{u}_x, \hat{u}_y, \hat{u}_x \hat{u}_y, \right.$$
$$\left. (s_\sigma - 1)/3 + \hat{u}_x^2, (s_\sigma - 1)/3 + \hat{u}_y^2, 0, 0, 1 - s_\sigma \right]^T. \tag{12}$$

The same mapping $\mathbf{M}_A$ can be used in order to define the generic non-equilibrium moments, namely

$$\mathbf{m}_\sigma = \mathbf{M}_A\,\mathbf{f}_\sigma = \left[\rho_\sigma, \rho_\sigma\,\hat{u}_{\sigma x}, \rho_\sigma\,\hat{u}_{\sigma y}, \hat{T}_{\sigma xy}, \hat{T}_{\sigma xx}, \hat{T}_{\sigma yy}, \hat{q}_{\sigma x}, \hat{q}_{\sigma y}, \hat{h}_\sigma\right]^T, \qquad (13)$$

where all the previous quantities were rescaled by means of the lattice speed in order to ensure that all the moments have the physical dimensions equal to those of the density. Finally, the equivalent moment system corresponding to Eq. (7) is

$$\frac{\partial \mathbf{m}_\sigma}{\partial t} + \mathbf{M}_A\,\mathbf{V}\cdot\left(\mathbf{M}_A^{-1}\,\nabla\mathbf{m}_\sigma\right) = (\lambda_\sigma + \lambda_m)\,\mathbf{I}\,(\mathbf{m}^e_{\sigma\,m} - \mathbf{m}_\sigma), \qquad (14)$$

where $\mathbf{m}^e_{\sigma\,m} = (1 - \alpha_\sigma)\,\mathbf{m}^e_\sigma + \alpha_\sigma\,\mathbf{m}^e_m$.

These preliminary results, which are equivalent to those reported in the paper discussing the SRT formulation of the Hamel model [30], will be generalized in the following section.

3   Multiple-relaxation-time (MRT) formulation of the Hamel model on the D2Q9 lattice

The previous vectorial equation (7) can be formally generalized as

$$\frac{\partial \mathbf{f}_\sigma}{\partial t} + \mathbf{V}\cdot\nabla\mathbf{f}_\sigma = \mathbf{A}_\sigma\,(\mathbf{f}^e_\sigma - \mathbf{f}_\sigma) + \mathbf{A}_m\,(\mathbf{f}^e_m - \mathbf{f}_\sigma), \qquad (15)$$

where $\mathbf{A}_\sigma = \mathbf{M}_D^{-1}\mathbf{D}_\sigma\mathbf{M}_D$, $\mathbf{A}_m = \mathbf{M}_D^{-1}\mathbf{D}_m\mathbf{M}_D$ and $\mathbf{M}_D$ defines a proper orthonormal basis. In particular, $\mathbf{D}_\sigma$ and $\mathbf{D}_m$ are diagonal matrices,

$$diag(\mathbf{D}_\sigma)^T = [\lambda^0_\sigma, \lambda^I_\sigma, \lambda^I_\sigma, \lambda^{II}_{\sigma\,1}, \lambda^{II}_{\sigma\,2}, \lambda^{II}_{\sigma\,3}, \lambda^{III}_\sigma, \lambda^{III}_\sigma, \lambda^{IV}_\sigma]$$
$$diag(\mathbf{D}_m)^T = [\lambda^0_m, \lambda^I_m, \lambda^I_m, \lambda^{II}_{m\,1}, \lambda^{II}_{m\,2}, \lambda^{II}_{m\,3}, \lambda^{III}_m, \lambda^{III}_m, \lambda^{IV}_m], \qquad (16)$$

collecting the generalized relaxation time constants for self and cross collisions.

In the equivalent moment space, the previous equation can be reformulated as

$$\frac{\partial \mathbf{m}_\sigma}{\partial t} + \mathbf{M}_A\,\mathbf{V}\cdot\left(\mathbf{M}_A^{-1}\,\nabla\mathbf{m}_\sigma\right) = \mathbf{E}_\sigma\,(\mathbf{m}^e_\sigma - \mathbf{m}_\sigma) + \mathbf{E}_m\,(\mathbf{m}^e_m - \mathbf{m}_\sigma), \qquad (17)$$

where $\mathbf{E}_\sigma = \mathbf{M}_A \mathbf{A}_\sigma \mathbf{M}_A^{-1}$ and $\mathbf{E}_m = \mathbf{M}_A \mathbf{A}_m \mathbf{M}_A^{-1}$. The choice of $\mathbf{M}_D$ strongly effects the coupling among the moments and the final system of macroscopic equations. The easiest choice is obviously $\mathbf{M}_D = \mathbf{M}_A$, because in this case $\mathbf{E}_\sigma = \mathbf{D}_\sigma$ and $\mathbf{E}_m = \mathbf{D}_m$. Unfortunately this choice does not allow one to freely tune the bulk viscosity of the fluid, which can strongly effect the stability of the calculation when the diffusion phenomena are considered. For this reason, a slightly different choice was adopted and the practical consequences will be discussed by the asymptotic analysis discussed in the next paragraph. Assuming $\mathbf{M}_D$ as

$$
\mathbf{M}_D = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\
0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\
0 & 1/2 & -1/2 & 1/2 & -1/2 & 0 & 0 & 0 & 0 \\
-2/3 & -1/6 & -1/6 & -1/6 & -1/6 & 1/3 & 1/3 & 1/3 & 1/3 \\
0 & -1 & 0 & 1 & 0 & 2 & -2 & -2 & 2 \\
0 & 0 & -1 & 0 & 1 & 2 & 2 & -2 & -2 \\
1 & -2 & -2 & -2 & -2 & 4 & 4 & 4 & 4
\end{bmatrix}, \tag{18}
$$

implies

$$
\mathbf{E}_\sigma = \begin{bmatrix}
\lambda_\sigma^0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \lambda_\sigma^I & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \lambda_\sigma^I & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \lambda_{\sigma 1}^{II} & 0 & 0 & 0 & 0 & 0 \\
-\mu_{3m0} & 0 & 0 & 0 & \mu_{3p2} & \mu_{3m2} & 0 & 0 & 0 \\
-\mu_{3m0} & 0 & 0 & 0 & \mu_{3m2} & \mu_{3p2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \lambda_\sigma^{III} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda_\sigma^{III} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \lambda_\sigma^{IV}
\end{bmatrix}, \tag{19}
$$

where $\mu_{3m0} = (\lambda_{\sigma 3}^{II} - \lambda_\sigma^0)/3$, $\mu_{3p2} = (\lambda_{\sigma 3}^{II} + \lambda_{\sigma 2}^{II})/2$ and $\mu_{3m2} = (\lambda_{\sigma 3}^{II} - \lambda_{\sigma 2}^{II})/2$. In order to reduce the truncation errors, some relaxation time constants will be assumed equal to zero: $\lambda_\sigma^0 = \lambda_\sigma^I = 0$ because $m_\sigma^{ei} = m_\sigma^i$ for $i = 0, 1, 2$ and

$\lambda_m^0 = 0$ $m_m^{e\,i} = m_\sigma^i$ for $i = 0$ respectively.

As previously done for the SRT formulation, it is possible to search for a more compact form. In particular, let us introduce the matrix $\mathbf{X}_\sigma$, defined as

$$\mathbf{X}_\sigma = \mathbf{M}_A\,\mathbf{M}_D^{-1}\,\mathbf{X}_\sigma^0\,\mathbf{M}_D\,\mathbf{M}_A^{-1}, \tag{20}$$

where $\mathbf{X}_\sigma^0$ is a diagonal matrix such as

$$diag(\mathbf{X}_\sigma^0)^T = [1, 1, 1, \alpha_{\sigma\,1}^{II}, \alpha_{\sigma\,2}^{II}, \alpha_{\sigma\,3}^{II}, \alpha_\sigma^{III}, \alpha_\sigma^{III}, \alpha_\sigma^{IV}], \tag{21}$$

and $\alpha_{\sigma\,j}^k = \lambda_{m\,j}^k/(\lambda_{\sigma\,j}^k + \lambda_{m\,j}^k)$ for $k \geq 2$. It is possible to prove that the following equivalences hold

$$\mathbf{E}_\sigma = (\mathbf{E}_\sigma + \mathbf{E}_m)\,(\mathbf{I} - \mathbf{X}_\sigma), \tag{22}$$
$$\mathbf{E}_m = (\mathbf{E}_\sigma + \mathbf{E}_m)\,\mathbf{X}_\sigma. \tag{23}$$

Introducing the previous relations in the Eq. (17) yields

$$\frac{\partial \mathbf{m}_\sigma}{\partial t} + \mathbf{M}_A\,\mathbf{V} \cdot \left(\mathbf{M}_A^{-1}\,\nabla \mathbf{m}_\sigma\right) = (\mathbf{E}_\sigma + \mathbf{E}_m)\,(\mathbf{m}_{\sigma\,m}^e - \mathbf{m}_\sigma), \tag{24}$$

where $\mathbf{m}_{\sigma\,m}^e = (\mathbf{I} - \mathbf{X}_\sigma)\,\mathbf{m}_\sigma^e + \mathbf{X}_\sigma\,\mathbf{m}_m^e$. Coming back in the discrete velocity space, the compact form becomes

$$\frac{\partial \mathbf{f}_\sigma}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{f}_\sigma = \mathbf{A}_*\,(\mathbf{f}_*^e - \mathbf{f}_\sigma), \tag{25}$$

where $\mathbf{A}_* = \mathbf{M}_A^{-1}\,(\mathbf{E}_\sigma + \mathbf{E}_m)\,\mathbf{M}_A$ and

$$\mathbf{f}_*^e = \left(\mathbf{I} - \mathbf{M}_D^{-1}\,\mathbf{X}_\sigma^0\,\mathbf{M}_D\right)\mathbf{f}_\sigma^e + \mathbf{M}_D^{-1}\,\mathbf{X}_\sigma^0\,\mathbf{M}_D\,\mathbf{f}_m^e. \tag{26}$$

The matrix $\mathbf{A}_*$ is singular, then a pseudo-inverse has been defined as

$$\mathbf{A}_*^\dagger \mathbf{A}_* = \mathbf{A}_* \mathbf{A}_*^\dagger = \mathbf{I} - \mathbf{Q}, \tag{27}$$

where $Q_{ij} = 1/9$. This definition differs from that reported in the paper by Junk et al. [36], because the kernel of the generalized matrix $\mathbf{A}_*$ is smaller, since the single species momentum is not conserved (at least for $\lambda_m^I > 0$).

In the next paragraph, the asymptotic analysis will be applied in order to recover the macroscopic equations, which derive from the generalized MRT formulation of the Hamel model.

4 Asymptotic analysis of the MRT Hamel model by the diffusive scaling

For most of the diffusion phenomena, the characteristic velocities are usually much smaller than the sound speed. For this reason, the diffusive scaling [40] can be properly applied.

There are three characteristic time scales in this system: the time scale T_C, which properly describes the collision phenomenon, i.e. $O(\tau_\sigma/T_C) = 1$; the time scale T_F, which properly describes the particle dynamics on the lattice, i.e. $O[(L/c)/T_F] = 1$ where L is the system size and, finally, the time scale T_S, which properly describes the slow fluid dynamics, i.e. $O[(L/U)/T_S] = 1$. The fast fluid dynamics (acoustic waves) was neglected. Since a lot of collisions are needed in order to travel across the system, then $T_C/T_F = \epsilon$, where ϵ is a small number. Moreover since $U/c \ll 1$, then $T_F/T_S = \epsilon$ and then consequently $T_C/T_S = \epsilon^2$. Once the characteristic time scales are defined, the basic idea is to express the previous equation in terms of some normalized quantities, in order to analyze the slow fluid dynamics only. Applying the diffusive scaling to Eq. (25) yields

$$
\epsilon^2 \, \frac{\partial \mathbf{f}_\sigma}{\partial \hat{t}} + \epsilon \, \hat{\mathbf{V}} \cdot \hat{\nabla} \mathbf{f}_\sigma = \hat{\mathbf{A}}_* \, (\mathbf{f}_*^e - \mathbf{f}_\sigma) \,, \tag{28}
$$

where $\hat{x} = x/L$, $\hat{t} = t/T_S$, $\hat{\mathbf{A}}_* = T_C \, \mathbf{A}_*$ (which implies $\hat{\mathbf{E}}_\sigma = T_C \, \mathbf{E}_\sigma$ and $\hat{\mathbf{E}}_m = T_C \, \mathbf{E}_m$) and $\hat{\mathbf{V}} = \mathbf{V}/c$. Let us introduce the following regular expansion

$$
\mathbf{f}_\sigma = \sum_{k=0}^{\infty} \epsilon^k \, \mathbf{f}_\sigma^{(k)}, \tag{29}
$$

and then consequently

$$
\mathbf{m}_\sigma = \sum_{k=0}^{\infty} \epsilon^k \, \mathbf{m}_\sigma^{(k)}. \tag{30}
$$

In particular, for the density and the momentum

$$
\rho_\sigma = \sum_{k=0}^{\infty} \epsilon^k \, \rho_\sigma^{(k)}, \tag{31}
$$

$$
\hat{\mathbf{j}}_\sigma = \sum_{k=0}^{\infty} \epsilon^k \, \hat{\mathbf{j}}_\sigma^{(k)}, \tag{32}
$$

where $\hat{\mathbf{j}}_\sigma = \rho_\sigma \, \hat{\mathbf{u}}_\sigma$. Consequently it is possible to define a regular expansion for the velocity, namely

$$\hat{\mathbf{u}}_\sigma = \frac{\mathbf{j}_\sigma}{\rho_\sigma} = \frac{\sum_{k=0}^{\infty} \epsilon^k \, \hat{\mathbf{j}}_\sigma^{(k)}}{\sum_{k=0}^{\infty} \epsilon^k \, \rho_\sigma^{(k)}} = \frac{\hat{\mathbf{j}}_\sigma^{(0)}}{\rho_\sigma^{(0)}} + \epsilon \left(\frac{\hat{\mathbf{j}}_\sigma^{(1)}}{\rho_\sigma^{(0)}} - \frac{\hat{\mathbf{j}}_\sigma^{(0)}}{\rho_\sigma^{(0)}} \frac{\rho_\sigma^{(1)}}{\rho_\sigma^{(0)}} \right) + O(\epsilon^2). \tag{33}$$

In the following, the coefficients of the regular expansion for the momentum $\hat{\mathbf{j}}_\sigma^{(k)}$ will be considered as functions of the coefficients of the regular expansions for the density and the velocity, i.e. $\rho_\sigma^{(k)}$ and $\hat{\mathbf{u}}_\sigma^{(k)}$. This means that the expansion given by Eq. (32) means

$$\hat{\mathbf{j}}_\sigma = \rho_\sigma \, \hat{\mathbf{u}}_\sigma = \left(\sum_{k=0}^{\infty} \epsilon^k \, \rho_\sigma^{(k)} \right) \left(\sum_{k=0}^{\infty} \epsilon^k \, \hat{\mathbf{u}}_\sigma^{(k)} \right) = \sum_{k=0}^{\infty} \epsilon^k \left[\sum_{p+q=k} \rho_\sigma^{(p)} \hat{\mathbf{u}}_\sigma^{(q)} \right]. \tag{34}$$

Introducing the previous expansions in the Eq. (28) yields

$$\frac{\partial \mathbf{f}_\sigma^{(k)}}{\partial \hat{t}} + \hat{\mathbf{V}} \cdot \hat{\nabla} \mathbf{f}_\sigma^{(k+1)} = \hat{\mathbf{A}}_* \, \mathbf{f}_*^{e0} \left[\rho_\sigma^{(k+2)} \right] + \hat{\mathbf{A}}_* \sum_{p+q=k+2} \mathbf{f}_*^{e1} \left[\rho_\sigma^{(p)}, \hat{\mathbf{u}}_\sigma^{(q)} \right]$$

$$+ \hat{\mathbf{A}}_* \sum_{p+q+r=k+2} \mathbf{f}_*^{e2} \left[\rho_\sigma^{(p)}, \hat{\mathbf{u}}_\sigma^{(q)}, \hat{\mathbf{u}}_\sigma^{(r)} \right] - \hat{\mathbf{A}}_* \, \mathbf{f}_\sigma^{(k+2)}, \tag{35}$$

where the equilibrium distribution vector $\mathbf{f}_*^e$ was split by grouping together the same monomial terms with regards to the velocity, i.e. $\mathbf{f}_*^e = \mathbf{f}_*^{e0} + \mathbf{f}_*^{e1} + \mathbf{f}_*^{e2}$. In particular $\mathbf{f}_*^{ej} = \mathbf{M}_A^{-1} \mathbf{m}_*^{ej}$ and

$$\mathbf{m}_*^{e0} = \rho_\sigma \left[1, 0, 0, 0, (s_\sigma - 1)/3, (s_\sigma - 1)/3, 0, 0, (1 - s_\sigma) \right]^T, \tag{36}$$

$$\mathbf{m}_*^{e1} = \rho_\sigma \left[0, u_x, u_y, 0, 0, 0, 0, 0, 0 \right]^T, \tag{37}$$

$$\mathbf{m}_*^{e2} = \rho_\sigma \begin{bmatrix} 0 \\ 0 \\ 0 \\ (1 - \alpha_{\sigma 1}^{II}) \, u_{\sigma x} \, u_{\sigma y} + \alpha_{\sigma 1}^{II} \, u_x \, u_y \\ (1 - \beta_{3p2}) \, u_{\sigma x}^2 - \beta_{3m2} \, u_{\sigma y}^2 + \beta_{3p2} \, u_x^2 + \beta_{3m2} \, u_y^2 \\ -\beta_{3m2} \, u_{\sigma x}^2 + (1 - \beta_{3p2}) \, u_{\sigma y}^2 + \beta_{3m2} \, u_x^2 + \beta_{3p2} \, u_y^2 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \tag{38}$$

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where $\beta_{3p2} = (\alpha^{II}_{\sigma 3} + \alpha^{II}_{\sigma 2})/2$ and $\beta_{3m2} = (\alpha^{II}_{\sigma 3} - \alpha^{II}_{\sigma 2})/2$. Conventionally the dependence on the single species velocity was explicitly reported, even when the barycentric velocity appears in the previous expressions, because the barycentric velocity is the mass average of the species velocity. Since $U/c \ll 1$, then $O(|\mathbf{u}|/c) = \epsilon$ and consequently $\hat{\mathbf{u}}^{(0)}_\sigma = 0$. It has been proved [36] that the expansion coefficients of the moments satisfy the following property

$$\rho^{(2n+1)}_\sigma = 0, \quad \hat{\mathbf{u}}^{(2n)}_\sigma = 0, \tag{39}$$

for $n \geq 0$. Taking into account this property, Eq. (35) for $k = -2$ yields $\mathbf{f}^{(0)}_\sigma = \mathbf{f}^{e0}_*[\rho^{(0)}_\sigma] = \rho^{(0)}_\sigma \mathbf{s}_0$, where $\mathbf{s}_0$ is defined as

$$\mathbf{s}_0 = [(1 - 5/9\,s_\sigma), s_\sigma/9, s_\sigma/9, s_\sigma/9, s_\sigma/9, s_\sigma/36, s_\sigma/36, s_\sigma/36, s_\sigma/36]^T, \tag{40}$$

and $\rho^{(0)}_\sigma$ is unknown. In order to find what macroscopic equation the function $\rho^{(0)}_\sigma$ must satisfy, the equivalent moment formulation with the diffusive scaling will be considered, namely

$$\epsilon^2 \frac{\partial \mathbf{m}_\sigma}{\partial \hat{t}} + \epsilon\, \mathbf{M}_A\, \hat{\mathbf{V}} \cdot \left(\mathbf{M}^{-1}_A \hat{\nabla} \mathbf{m}_\sigma \right) = \left(\hat{\mathbf{E}}_\sigma + \hat{\mathbf{E}}_m \right) \left(\mathbf{m}^e_* - \mathbf{m}_\sigma \right). \tag{41}$$

In particular, introducing the usual expansions in the equations for the lower order moments and separating the scales yields

$$\frac{\partial \rho^{(k)}_\sigma}{\partial \hat{t}} + \hat{\nabla} \cdot \sum_{p+q=k+1} \rho^{(p)}_\sigma \hat{\mathbf{u}}^{(q)}_\sigma = 0, \tag{42}$$

$$\frac{\partial \hat{\mathbf{j}}^{(k)}_\sigma}{\partial \hat{t}} + \hat{\nabla} \cdot \hat{\mathbf{T}}^{(k+1)}_\sigma = \hat{\lambda}^I_m \sum_{p+q=k+2} \rho^{(p)}_\sigma \left[\hat{\mathbf{u}}^{(q)} - \hat{\mathbf{u}}^{(q)}_\sigma \right], \tag{43}$$

where the tensor $\hat{\mathbf{T}}^{(k+1)}_\sigma$ can be considered as the result of a proper operator $\mathbf{T}$ working on $\mathbf{f}^{(k+1)}_\sigma$, i.e. $\hat{\mathbf{T}}^{(k+1)}_\sigma = \mathbf{T}\left[\mathbf{f}^{(k+1)}_\sigma \right]$ where

$$\mathbf{T}\left[\mathbf{f}^{(k+1)}_\sigma \right] = \begin{bmatrix} \sum_{i=0}^8 M_{5i}\, f^{(k+1)}_{\sigma i} & \sum_{i=0}^8 M_{4i}\, f^{(k+1)}_{\sigma i} \\ \sum_{i=0}^8 M_{4i}\, f^{(k+1)}_{\sigma i} & \sum_{i=0}^8 M_{6i}\, f^{(k+1)}_{\sigma i} \end{bmatrix}, \tag{44}$$

and

$$
\mathbf{M} = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
0 & 1 & 0 & -1 & 0 & 1 & -1 & -1 & 1 \\
0 & 0 & 1 & 0 & -1 & 1 & 1 & -1 & -1 \\
0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 \\
0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 \\
0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \\
0 & 1/2 & 1/2 & 1/2 & 1/2 & 1 & 1 & 1 & 1 \\
0 & 1/2 & 0 & -1/2 & 0 & 1 & -1 & -1 & 1 \\
0 & 0 & 1/2 & 0 & -1/2 & 1 & 1 & -1 & -1
\end{bmatrix}.
\tag{45}
$$

According to the general property given by Eqs. (39), the Eqs. (42) for $k = -1, +1$ are meaningless. For $k = 0, +2$, the same equation yields

$$
\frac{\partial \rho_\sigma^{(0)}}{\partial \hat{t}} + \hat{\nabla} \cdot \left[\rho_\sigma^{(0)} \hat{\mathbf{u}}_\sigma^{(1)} \right] = 0,
\tag{46}
$$

$$
\frac{\partial \rho_\sigma^{(2)}}{\partial \hat{t}} + \hat{\nabla} \cdot \hat{\mathbf{j}}_\sigma^{(3)} = 0.
\tag{47}
$$

According to the general property given by Eqs. (39), the Eqs. (43) for $k = -2, 0$ are meaningless. The equations for $k = -1, +1$ can be recovered

$$
\hat{\nabla} \cdot \hat{\mathbf{T}}_\sigma^{(0)} = \hat{\lambda}_m^I \rho_\sigma^{(0)} \left[\hat{\mathbf{u}}^{(1)} - \hat{\mathbf{u}}_\sigma^{(1)} \right],
\tag{48}
$$

$$
\frac{\partial}{\partial \hat{t}} \left[\rho_\sigma^{(0)} \hat{\mathbf{u}}_\sigma^{(1)} \right] + \hat{\nabla} \cdot \hat{\mathbf{T}}_\sigma^{(2)} = \hat{\lambda}_m^I \left[\hat{\mathbf{j}}^{(3)} - \hat{\mathbf{j}}_\sigma^{(3)} \right],
\tag{49}
$$

Recalling the definition of $\mathbf{f}_\sigma^{(0)}$, then $\hat{\mathbf{T}}_\sigma^{(0)} = s_\sigma/3 \, \rho_\sigma^{(0)} \, \mathbf{I}$ and consequently

$$
s_\sigma/3 \, \hat{\nabla} \rho_\sigma^{(0)} = -\hat{\lambda}_m^I \rho_\sigma^{(0)} \, \hat{\mathbf{w}}_\sigma^{(1)},
\tag{50}
$$

where $\hat{\mathbf{w}}_\sigma^{(1)} = \hat{\mathbf{u}}_\sigma^{(1)} - \hat{\mathbf{u}}^{(1)}$ is the diffusion velocity. Hence in general the leading term of the density field is due to the sum of a constant value ρ_σ^0 and a proper field due to the diffusion velocity $\rho_\sigma^D(\hat{\mathbf{x}})$ satisfying the previous equation, i.e. $\rho_\sigma^{(0)} = \rho_\sigma^0 + \rho_\sigma^D(\hat{\mathbf{x}})$. Eqs. (35) for $k = -1$ yields

$$
\mathbf{f}_\sigma^{(1)} = \mathbf{f}_*^{e1} \left[\rho_\sigma^{(0)}, \hat{\mathbf{u}}_\sigma^{(1)} \right] - \hat{\mathbf{A}}_*^\dagger \hat{\mathbf{V}} \cdot \hat{\nabla} \mathbf{f}_\sigma^{(0)},
\tag{51}
$$

and recalling the definition of $\mathbf{f}_\sigma^{(0)}$,

$$\mathbf{f}_\sigma^{(1)} = 3\,\rho_\sigma^{(0)}\,\hat{\mathbf{V}}\cdot\left[\mathbf{s}_I \otimes \hat{\mathbf{u}}^{(1)}\right] - \hat{\mathbf{A}}_*^\dagger\,\hat{\mathbf{V}}\cdot\left[\mathbf{s}_0 \otimes \hat{\nabla}\rho_\sigma^{(0)}\right], \tag{52}$$

where $\mathbf{s}_I$ is defined as

$$\mathbf{s}_I = [4/9, 1/9, 1/9, 1/9, 1/9, 1/36, 1/36, 1/36, 1/36]^T. \tag{53}$$

It is easy to prove that if $s_\sigma = 1$ then $\mathbf{s}_0 = \mathbf{s}_I$. Applying Eq. (50) yields

$$\mathbf{f}_\sigma^{(1)} = 3\,\rho_\sigma^{(0)}\,\hat{\mathbf{V}}\cdot\left[\mathbf{s}_I \otimes \hat{\mathbf{u}}^{(1)}\right] + 3\,\rho_\sigma^{(0)}\,\frac{\hat{\lambda}_m^I}{s_\sigma}\,\hat{\mathbf{A}}_*^\dagger\,\hat{\mathbf{V}}\cdot\left[\mathbf{s}_0 \otimes \hat{\mathbf{w}}_\sigma^{(1)}\right], \tag{54}$$

and consequently

$$\mathbf{f}_\sigma^{(1)} = 3\,\rho_\sigma^{(0)}\,\hat{\mathbf{V}}\cdot\left[\mathbf{s}_I \otimes \hat{\mathbf{u}}_\sigma^{(1)}\right]. \tag{55}$$

This result is identical to that obtained by Junk et al [36]. Recalling Eq. (35) for $k = 0$ and taking into account the general property given by Eq. (39), the last expansion coefficient can be recovered

$$\mathbf{f}_\sigma^{(2)} = \rho_\sigma^{(2)}\,\mathbf{s}_I + \mathbf{f}_*^{e2}\left[\rho_\sigma^{(0)}, \hat{\mathbf{u}}_\sigma^{(1)}, \hat{\mathbf{u}}_\sigma^{(1)}\right] - \hat{\mathbf{A}}_*^\dagger\left\{\frac{\partial \mathbf{f}_\sigma^{(0)}}{\partial \hat{t}} + \hat{\mathbf{V}}\cdot\left[\hat{\nabla}\mathbf{f}_\sigma^{(1)}\right]\right\}. \tag{56}$$

Assuming $\hat{\lambda}_{\sigma 2}^{II} = \hat{\lambda}_{\sigma 1}^{II}$ and $\hat{\lambda}_{m 2}^{II} = \hat{\lambda}_{m 1}^{II}$ yields

$$\begin{aligned}
\hat{\mathbf{T}}_\sigma^{(2)} = {} & \left[\frac{s_\sigma}{3}\,\rho_\sigma^{(2)} + \frac{(2 - s_\sigma)}{3\,(\hat{\lambda}_{\sigma 3}^{II} + \hat{\lambda}_{m 3}^{II})}\frac{\partial \rho_\sigma^{(0)}}{\partial \hat{t}}\right]\mathbf{I} \\
& + (1 - \alpha_{\sigma 1}^{II})\,\rho_\sigma^{(0)}\,\mathbf{u}_\sigma^{(1)} \otimes \mathbf{u}_\sigma^{(1)} + \alpha_{\sigma 1}^{II}\,\rho_\sigma^{(0)}\,\mathbf{u}^{(1)} \otimes \mathbf{u}^{(1)} \\
& - \frac{1}{3\,(\hat{\lambda}_{\sigma 1}^{II} + \hat{\lambda}_{m 1}^{II})}\left\{\hat{\nabla}\left[\rho_\sigma^{(0)}\,\hat{\mathbf{u}}_\sigma^{(1)}\right] + \hat{\nabla}\left[\rho_\sigma^{(0)}\,\hat{\mathbf{u}}_\sigma^{(1)}\right]^T - \hat{\nabla}\cdot\left[\rho_\sigma^{(0)}\,\hat{\mathbf{u}}_\sigma^{(1)}\right]\mathbf{I}\right\} \\
& + \beta_{3m1}\,\rho_\sigma^{(0)}\left\{\left[\hat{\mathbf{u}}^{(1)}\right]^2 - \left[\hat{\mathbf{u}}_\sigma^{(1)}\right]^2\right\}\mathbf{I},
\end{aligned} \tag{57}$$

where $\beta_{3m1} = (\alpha_{\sigma 3}^{II} - \alpha_{\sigma 1}^{II})/2$. In order to ensure the Galilean invariance of the pressure, $\beta_{3m1} = 0$ is assumed and this implies

$$\frac{\hat{\lambda}_{m 1}^{II}}{\hat{\lambda}_{\sigma 1}^{II}} = \frac{\hat{\lambda}_{m 3}^{II}}{\hat{\lambda}_{\sigma 3}^{II}}. \tag{58}$$

The asymptotic analysis allows to define some constraints in the relaxation time constants in order to ensure the desired structure of the macroscopic

equations. Taking into account these assumptions, the Eq. (49) explicitly becomes

$$
\frac{\partial}{\partial \hat{t}} \left[\rho_\sigma^{(0)} \hat{\mathbf{u}}_\sigma^{(1)} \right] + \hat{\nabla} \cdot \left[\left(1 - \alpha_{\sigma 1}^{II} \right) \rho_\sigma^{(0)} \, \hat{\mathbf{u}}_\sigma^{(1)} \otimes \hat{\mathbf{u}}_\sigma^{(1)} + \alpha_{\sigma 1}^{II} \, \rho_\sigma^{(0)} \, \hat{\mathbf{u}}^{(1)} \otimes \hat{\mathbf{u}}^{(1)} \right]
$$

$$
+ s_\sigma / 3 \, \hat{\nabla} \rho_\sigma^{(2)} = \hat{\nabla} \cdot \left\{ \hat{\nu}_{\sigma m} \, \hat{\nabla} \left[\rho_\sigma^{(0)} \, \hat{\mathbf{u}}_\sigma^{(1)} \right] + \hat{\nu}_{\sigma m} \left[\rho_\sigma^{(0)} \, \hat{\nabla} \hat{\mathbf{u}}_\sigma^{(1)} \right]^T \right\}
$$

$$
+ \hat{\nabla} \left\{ \hat{\eta}_{\sigma m} \, \hat{\nabla} \cdot \left[\rho_\sigma^{(0)} \, \hat{\mathbf{u}}_\sigma^{(1)} \right] \right\} + \frac{s_\sigma}{3 \, \hat{D}_\sigma} \left[\hat{\mathbf{j}}^{(3)} - \hat{\mathbf{j}}_\sigma^{(3)} \right], \tag{59}
$$

where $\hat{D}_\sigma$, $\hat{\nu}_{\sigma m}$ and $\hat{\eta}_{\sigma m}$ are respectively the diffusivity, the kinematic viscosity and the second coefficient of the kinematic viscosity for the generic species in the mixture, defined as

$$
\hat{D}_\sigma = \frac{s_\sigma}{3 \, \hat{\lambda}_m^I}, \tag{60}
$$

$$
\hat{\nu}_{\sigma m} = \frac{1}{3 \left(\hat{\lambda}_{\sigma 1}^{II} + \hat{\lambda}_{m 1}^{II} \right)}, \tag{61}
$$

$$
\hat{\eta}_{\sigma m} = \frac{2 - s_\sigma}{3 \left(\hat{\lambda}_{\sigma 3}^{II} + \hat{\lambda}_{m 3}^{II} \right)} - \frac{1}{3 \left(\hat{\lambda}_{\sigma 1}^{II} + \hat{\lambda}_{m 1}^{II} \right)}. \tag{62}
$$

The following simplifications yield

$$
\hat{\nabla} \left[\rho_\sigma^{(0)} \, \hat{\mathbf{u}}_\sigma^{(1)} \right] = \rho_\sigma^{(0)} \, \hat{\nabla} \hat{\mathbf{u}}_\sigma^{(1)} - 3 \, \rho_\sigma^{(0)} \, \frac{\hat{\lambda}_m^I}{s_\sigma} \, \hat{\mathbf{u}}_\sigma^{(1)} \otimes \hat{\mathbf{w}}_\sigma^{(1)} \approx \rho_\sigma^{(0)} \, \hat{\nabla} \hat{\mathbf{u}}_\sigma^{(1)}, \tag{63}
$$

$$
\hat{\nabla} \cdot \left[\rho_\sigma^{(0)} \, \hat{\mathbf{u}}_\sigma^{(1)} \right] = \rho_\sigma^{(0)} \, \hat{\nabla} \cdot \hat{\mathbf{u}}_\sigma^{(1)} - 3 \, \rho_\sigma^{(0)} \, \frac{\hat{\lambda}_m^I}{s_\sigma} \, \hat{\mathbf{u}}_\sigma^{(1)} \cdot \hat{\mathbf{w}}_\sigma^{(1)} \approx \rho_\sigma^{(0)} \, \hat{\nabla} \cdot \hat{\mathbf{u}}_\sigma^{(1)}, \tag{64}
$$

because the neglected terms are of the same order of magnitude of the inertial terms and the latter are much smaller than the velocity gradients in the low Mach number limit. Collecting the previous results yields

$$
\epsilon^2 \frac{\partial}{\partial \hat{t}} \left[\rho_\sigma^{(0)} + \epsilon^2 \, \rho_\sigma^{(2)} \right] + \epsilon \, \hat{\nabla} \cdot \left[\epsilon \, \rho_\sigma^{(0)} \hat{\mathbf{u}}_\sigma^{(1)} + \epsilon^3 \, \hat{\mathbf{j}}_\sigma^{(3)} \right] = 0, \tag{65}
$$

$$
\epsilon^2 \frac{\partial}{\partial \hat{t}} \left[\epsilon \, \rho_\sigma^{(0)} \hat{\mathbf{u}}_\sigma^{(1)} \right] + \epsilon \, \hat{\nabla} \cdot \left[\epsilon^2 \left(1 - \alpha_{\sigma 1}^{II} \right) \rho_\sigma^{(0)} \, \hat{\mathbf{u}}_\sigma^{(1)} \otimes \hat{\mathbf{u}}_\sigma^{(1)} + \epsilon^2 \, \alpha_{\sigma 1}^{II} \, \rho_\sigma^{(0)} \, \hat{\mathbf{u}}^{(1)} \otimes \hat{\mathbf{u}}^{(1)} \right]
$$

$$
+ \epsilon \, s_\sigma / 3 \, \hat{\nabla} \left[\rho_\sigma^{(0)} + \epsilon^2 \, \rho_\sigma^{(2)} \right] = \epsilon \, \hat{\nabla} \left[\rho_\sigma^{(0)} \, \hat{\eta}_{\sigma m} \, \epsilon \, \hat{\nabla} \cdot \epsilon \, \hat{\mathbf{u}}_\sigma^{(1)} \right]
$$

$$
+ \epsilon \, \hat{\nabla} \cdot \left\{ \rho_\sigma^{(0)} \, \hat{\nu}_{\sigma m} \, \epsilon \, \hat{\nabla} \epsilon \, \hat{\mathbf{u}}_\sigma^{(1)} + \rho_\sigma^{(0)} \, \hat{\nu}_{\sigma m} \left[\epsilon \, \hat{\nabla} \epsilon \, \hat{\mathbf{u}}_\sigma^{(1)} \right]^T \right\}
$$

$$
+ \frac{s_\sigma}{3 \, \hat{D}_\sigma} \left[\rho_\sigma^{(0)} \, \epsilon \, \hat{\mathbf{u}}^{(1)} - \rho_\sigma^{(0)} \, \epsilon \, \hat{\mathbf{u}}_\sigma^{(1)} + \epsilon^3 \, \hat{\mathbf{j}}^{(3)} - \epsilon^3 \, \hat{\mathbf{j}}_\sigma^{(3)} \right]. \tag{66}
$$

Coming back to the original quantities expressed in physical units, it is easy to verify that, if terms $O(\epsilon^3)$ are neglected, then $\tilde{\rho}_\sigma = \rho_\sigma^{(0)} + \epsilon^2 \rho_\sigma^{(2)}$ and $\tilde{\mathbf{u}}_\sigma = \epsilon \, \mathbf{u}_\sigma^{(1)}$ satisfy the Navier-Stokes system of equations, namely

$$\frac{\partial \tilde{\rho}_\sigma}{\partial t} + \nabla \cdot (\tilde{\rho}_\sigma \, \tilde{\mathbf{u}}_\sigma) = 0, \tag{67}$$

$$\begin{aligned}
\frac{\partial}{\partial t} \left(\tilde{\rho}_\sigma \tilde{\mathbf{u}}_\sigma \right) + \nabla \cdot & \left[(1 - \alpha_{\sigma 1}^{II}) \, \tilde{\rho}_\sigma \, \tilde{\mathbf{u}}_\sigma \otimes \tilde{\mathbf{u}}_\sigma + \alpha_{\sigma 1}^{II} \, \tilde{\rho}_\sigma \, \tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}} \right] \\
& = -s_\sigma/3 \, \nabla \tilde{\rho}_\sigma + \nabla \left(\tilde{\rho}_\sigma \, \eta_{\sigma m} \, \nabla \cdot \tilde{\mathbf{u}}_\sigma \right) \\
& \quad + \nabla \cdot \left[\tilde{\rho}_\sigma \, \nu_{\sigma m} \, \nabla \tilde{\mathbf{u}}_\sigma + \tilde{\rho}_\sigma \, \nu_{\sigma m} \, (\nabla \tilde{\mathbf{u}}_\sigma)^T \right] \\
& \quad - \frac{s_\sigma}{3 \, D_\sigma} \, \tilde{\rho}_\sigma \, (\tilde{\mathbf{u}}_\sigma - \tilde{\mathbf{u}}),
\end{aligned} \tag{68}$$

where $D_\sigma = T_C \, c^2 \, \hat{D}_\sigma$, $\nu_{\sigma m} = T_C \, c^2 \, \hat{\nu}_{\sigma m}$ and $\eta_{\sigma m} = T_C \, c^2 \, \hat{\eta}_{\sigma m}$.

From the macroscopic point of view, the consequences due to the lack of differentiability of the Hamel model are evident in Eq. (68). As a matter of fact, if one sums over the single species momentum equations, then the mixture momentum equation is not recovered. This is due to the additional quadratic term appearing in the left hand side of Eq. (68), which depends on the single species velocities. Sometimes this undesired feature of the Hamel model (and consequently of the Sirovich model) is omitted by considering this additional quadratic term negligible in comparison with that depending on the mixture velocity [41]: however, this is clearly not correct by taking into account the considerations discussed in the asymptotic analysis. The development of an MRT model for mixture modeling fully consistent with the indifferentiability principle is discussed in another paper [39].

In the next paragraph, some integration rules will be compared in order to analyze the performance of the numerical implementations of the previous model.

5 Asymptotic analysis of the MRT Hamel model integrated by the forward Euler integration rule

The easiest way to integrate the previous model is by means of the forward Euler integration rule. According to this technique, the operative formula is

$$\mathbf{f}_\sigma(\hat{t} + \epsilon^2, \hat{\mathbf{X}} + \epsilon \, \hat{\mathbf{V}}) - \mathbf{f}_\sigma(\hat{t}, \hat{\mathbf{X}}) = \hat{\mathbf{A}}_* \left[\mathbf{f}_*^e(\hat{t}, \hat{\mathbf{X}}) - \mathbf{f}_\sigma(\hat{t}, \hat{\mathbf{X}}) \right]. \tag{69}$$

The difference in the left hand side is transformed in differential operators by means of the Taylor expansion, namely

$$\sum_{k=1}^{\infty} \epsilon^k \, D_k(\partial/\partial \hat{t}, \hat{\mathbf{V}} \cdot \hat{\nabla}) \, \mathbf{f}_\sigma = \hat{\mathbf{A}}_* \left(\mathbf{f}_*^e - \mathbf{f}_\sigma \right), \tag{70}$$

where $D_k(x_1, x_2)$ are polynomials defined as

$$D_k(x_1, x_2) = \sum_{2a+b=k \geq 1} \frac{x_1^a \, x_2^b}{a! \, b!}. \tag{71}$$

Introducing the previous expansions in the Eq. (70) yields

$$\sum_{p+q=k+2} D_p(\partial/\partial \hat{t}, \hat{\mathbf{V}} \cdot \hat{\nabla}) \, \mathbf{f}_\sigma^{(q)} = \hat{\mathbf{A}}_* \, \mathbf{f}_*^{e0} \left[\rho_\sigma^{(k+2)} \right] + \hat{\mathbf{A}}_* \sum_{p+q=k+2} \mathbf{f}_*^{e1} \left[\rho_\sigma^{(p)}, \hat{\mathbf{u}}_\sigma^{(q)} \right]$$
$$+ \hat{\mathbf{A}}_* \sum_{p+q+r=k+2} \mathbf{f}_*^{e2} \left[\rho_\sigma^{(p)}, \hat{\mathbf{u}}_\sigma^{(q)}, \hat{\mathbf{u}}_\sigma^{(r)} \right] - \hat{\mathbf{A}}_* \, \mathbf{f}_\sigma^{(k+2)}, \tag{72}$$

or explicitly

$$\mathbf{f}_\sigma^{(k+2)} = \mathbf{f}_*^{e0} \left[\rho_\sigma^{(k+2)} \right] + \sum_{p+q=k+2} \mathbf{f}_*^{e1} \left[\rho_\sigma^{(p)}, \hat{\mathbf{u}}_\sigma^{(q)} \right]$$
$$+ \sum_{p+q+r=k+2} \mathbf{f}_*^{e2} \left[\rho_\sigma^{(p)}, \hat{\mathbf{u}}_\sigma^{(q)}, \hat{\mathbf{u}}_\sigma^{(r)} \right] - \hat{\mathbf{A}}_*^\dagger \sum_{p+q=k+2} D_p(\partial/\partial \hat{t}, \hat{\mathbf{V}} \cdot \hat{\nabla}) \, \mathbf{f}_\sigma^{(q)}. \tag{73}$$

Even though we are using the simple forward Euler integration rule, the same expansion coefficients are recovered for $\mathbf{f}_\sigma^{(0)}$ and $\mathbf{f}_\sigma^{(1)}$, while for the $\mathbf{f}_\sigma^{(2)}$ the following relation holds

$$\mathbf{f}_{\sigma \, d}^{(2)} = \mathbf{f}_\sigma^{(2)} - \frac{1}{2} \, \hat{\mathbf{A}}_*^\dagger \hat{\mathbf{V}} \cdot \hat{\nabla} \left[\hat{\mathbf{V}} \cdot \hat{\nabla} \mathbf{f}_\sigma^{(0)} \right]. \tag{74}$$

In the moment space, the system of equations becomes

$$\sum_{k=1}^{\infty} \epsilon^k \, \mathbf{M}_A \, D_k(\partial/\partial \hat{t}, \hat{\mathbf{V}} \cdot \hat{\nabla}) \, \mathbf{M}_A^{-1} \mathbf{m}_\sigma = \left(\hat{\mathbf{E}}_\sigma + \hat{\mathbf{E}}_m \right) \left(\mathbf{m}_*^e - \mathbf{m}_\sigma \right), \tag{75}$$

Introducing the usual expansions in the equations for the lower order moments and separating the scales yields that for $k = 0$ the contribution to the continuity equation is

$$\frac{\partial \rho_\sigma^{(0)}}{\partial \hat{t}} + \hat{\nabla} \cdot \left[\rho_\sigma^{(0)} \hat{\mathbf{u}}_\sigma^{(1)} \right] + \frac{s_\sigma}{6} \, \hat{\nabla}^2 \rho_\sigma^{(0)} = 0, \tag{76}$$

and for $k = -1$ the contribution to the momentum equation is identical to that given by Eq. (48). Unfortunately this means that the continuity equation is no more satisfied. In order to solve this problem, a modified vector $\mathbf{m}_{*d}^{e\,1}$ and consequently $\mathbf{f}_{*d}^{e1}$ can be introduced, where

$$\mathbf{m}_{*d}^{e\,1} = \rho_\sigma \left[0, u_x + d\,w_{\sigma\,x}, u_y + d\,w_{\sigma\,y}, 0, 0, 0, 0, 0, 0\right]^T. \tag{77}$$

The reason to choose such modification is due to the undesired term appearing in Eq. (76). This additional term is the divergence of the density gradient, but the last gradient is proportional to the diffusion velocity $\mathbf{w}_\sigma$. Hence it is reasonable to try to delete the undesired term by modifying the definition of the macroscopic momentum, since this quantity will appear in the divergence part of the continuity equation. Moreover this correction should be proportional to the diffusion velocity for producing a term identical to that we want to delete.

For this reason, the second expansion coefficient will be modified

$$\mathbf{f}_{\sigma\,d}^{(1)} = \mathbf{f}_{*d}^{e1} \left[\rho_\sigma^{(0)}, \hat{\mathbf{u}}_\sigma^{(1)}\right] - \hat{\mathbf{A}}_*^\dagger \, \hat{\mathbf{V}} \cdot \hat{\nabla} \mathbf{f}_\sigma^{(0)}, \tag{78}$$

and then consequently

$$\hat{\mathbf{A}}_* \left\{ \mathbf{f}_{\sigma\,d}^{(1)} - \mathbf{f}_{*d}^{e1} \left[\rho_\sigma^{(0)}, \hat{\mathbf{u}}_\sigma^{(1)}\right] \right\} = -\hat{\mathbf{V}} \cdot \hat{\nabla} \mathbf{f}_\sigma^{(0)}. \tag{79}$$

Calculating the zero-order moment of the previous expression yields

$$s_\sigma/3 \, \hat{\nabla} \rho_\sigma^{(0)} = -\hat{\lambda}_m^I \, (1 - d) \, \rho_\sigma^{(0)} \, \hat{\mathbf{w}}_\sigma^{(1)}, \tag{80}$$

which generalizes the Eq. (50). Introducing Eq. (80) into Eq. (76) yields

$$\frac{\partial \rho_\sigma^{(0)}}{\partial \hat{t}} + \hat{\nabla} \cdot \left[\rho_\sigma^{(0)} \hat{\mathbf{u}}^{(1)} + d\, \rho_\sigma^{(0)} \, \hat{\mathbf{w}}_\sigma^{(1)} - \frac{s_\sigma}{3\,\hat{\lambda}_m^I} \, \hat{\nabla} \rho_\sigma^{(0)} \right] + \frac{s_\sigma}{6} \, \hat{\nabla}^2 \rho_\sigma^{(0)} = 0, \tag{81}$$

which is equivalent to Eq. (76). There is no way to tune d, in such a way to restore the continuity equation.

For this reason, in the next paragraph a proper corrective factor will be discussed.

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6 Asymptotic analysis of the MRT Hamel model integrated by the modified mid-point integration rule

Let us suppose to modify the operative formula due to the forward Euler integration rule by adding a proper corrective factor. Recalling the Eq. (73), it is easy to prove that any corrective factor taken from the kernel of $\hat{\mathbf{A}}_*^\dagger$ does not effect the expansion coefficients of the discrete models. A generic vector from the kernel of $\hat{\mathbf{A}}_*^\dagger$ is proportional to

$$\mathbf{s}_{II} = [0, 1/6, 1/6, 1/6, 1/6, 1/12, 1/12, 1/12, 1/12]^T. \tag{82}$$

When the definition of the moments are considered, the generic vector $\mathbf{s}_{II}$ produces an unit source term in the continuity equation and a zero source in the momentum equation. The corrected equation will be

$$\mathbf{f}_\sigma(\hat{t} + \epsilon^2, \hat{\mathbf{X}} + \epsilon\,\hat{\mathbf{V}}) - \mathbf{f}_\sigma(\hat{t}, \hat{\mathbf{X}}) = \epsilon^2\,\frac{s_\sigma}{6}\,\hat{\nabla}^2\rho_\sigma^{(0)}\,\mathbf{s}_{II} + \hat{\mathbf{A}}_*\,(\mathbf{f}_*^e - \mathbf{f}_\sigma). \tag{83}$$

Taking into account the following property

$$\mathbf{s}_{III}^T \cdot \left\{ \hat{\mathbf{V}} \cdot \hat{\nabla}\left[\hat{\mathbf{V}} \cdot \hat{\nabla}\mathbf{f}_\sigma^{(0)}\right]\right\} = \frac{s_\sigma}{3}\,\hat{\nabla}^2\rho_\sigma^{(0)}, \tag{84}$$

where $\mathbf{s}_{III}$ is

$$\mathbf{s}_{III} = [3, 3/2, 3/2, 3/2, 3/2, 0, 0, 0, 0]^T, \tag{85}$$

it is possible to express the Eq. (83) in terms of the discrete distribution function

$$\begin{aligned}
\mathbf{f}_\sigma(\hat{t} + \epsilon^2, \hat{\mathbf{X}} + \epsilon\,\hat{\mathbf{V}}) - \mathbf{f}_\sigma(\hat{t}, \hat{\mathbf{X}}) = \\
\frac{1}{2}\,\epsilon^2\,\mathbf{s}_{II} \otimes \mathbf{s}_{III}\,\left\{\hat{\mathbf{V}} \cdot \hat{\nabla}\left[\hat{\mathbf{V}} \cdot \hat{\nabla}\mathbf{f}_\sigma^{(0)}\right]\right\} + \hat{\mathbf{A}}_*\,(\mathbf{f}_*^e - \mathbf{f}_\sigma).
\end{aligned} \tag{86}$$

Finally, neglecting the terms $O(\epsilon^4)$ yields

$$\begin{aligned}
\mathbf{f}_\sigma(\hat{t} + \epsilon^2, \hat{\mathbf{X}} + \epsilon\,\hat{\mathbf{V}}) = \mathbf{f}_\sigma(\hat{t}, \hat{\mathbf{X}}) + \hat{\mathbf{A}}_*\,(\mathbf{f}_*^e - \mathbf{f}_\sigma) \\
+ 1/2\,\mathbf{s}_{II} \otimes \mathbf{s}_{III}\,\left[\mathbf{f}_\sigma(\hat{t}, \hat{\mathbf{X}} + \epsilon\,\hat{\mathbf{V}}) - 2\,\mathbf{f}_\sigma(\hat{t}, \hat{\mathbf{X}}) + \mathbf{f}_\sigma(\hat{t}, \hat{\mathbf{X}} - \epsilon\,\hat{\mathbf{V}})\right].
\end{aligned} \tag{87}$$

The modified scheme satisfies Eq. (46), as the continuous model does. The contribution to the continuity equation for $k = +2$ can be expressed by means

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of the following operator $\hat{\mathbf{j}}_\sigma^{(k+1)} = \mathbf{j}\left[\mathbf{f}_\sigma^{(k+1)}\right]$, where

$$\mathbf{j}\left[\mathbf{f}_\sigma^{(k+1)}\right] = \begin{bmatrix} \sum_{i=0}^{8} M_{2i} f_{\sigma i}^{(k+1)} \\ \sum_{i=0}^{8} M_{3i} f_{\sigma i}^{(k+1)} \end{bmatrix}. \tag{88}$$

In particular, the discrete flux is

$$\hat{\mathbf{j}}_{\sigma d}^{(3)} = \hat{\mathbf{j}}_\sigma^{(3)} + \mathbf{j}\left\{ 1/2\,\hat{\mathbf{V}}\cdot\hat{\nabla}\mathbf{f}_\sigma^{(2)} + \partial\mathbf{f}_\sigma^{(1)}/\partial\hat{t} + 1/6\,\hat{\mathbf{V}}\cdot\hat{\nabla}\left(\hat{\mathbf{V}}\cdot\hat{\nabla}\mathbf{f}_\sigma^{(1)}\right) \right.$$
$$\left. + 1/24\,\hat{\mathbf{V}}\cdot\hat{\nabla}\left[\hat{\mathbf{V}}\cdot\hat{\nabla}\left(\hat{\mathbf{V}}\cdot\hat{\nabla}\mathbf{f}_\sigma^{(0)}\right)\right] \right\}. \tag{89}$$

Summing the contributions for $k = 0$ and $k = +2$ to the continuity equation, an expression similar to Eq. (65), but involving the discrete flux, is recovered. Since the discrete flux produces some terms $O(\epsilon^3)$, it can be neglected and this ensures that the continuity equation is satisfied with second order spatial accuracy.

The contribution to the momentum equation for $k = -1$ is identical to that of the continuous model, given by Eq. (50). This means that if the terms $O(\epsilon^3)$ are neglected, the discrete model produces a diffusion velocity which is proportional to the concentration gradient by means of the diffusion coefficient. The contribution to the momentum equation for $k = +1$ can be expressed by means of a modified tensor $\hat{\mathbf{T}}_{\sigma d}^{(2)}$, namely

$$\hat{\mathbf{T}}_{\sigma d}^{(2)} = \hat{\mathbf{T}}_\sigma^{(2)} + \mathbf{T}\left\{ -1/2\,\hat{\mathbf{A}}_*^\dagger\,\hat{\mathbf{V}}\cdot\hat{\nabla}\left[\hat{\mathbf{V}}\cdot\hat{\nabla}\mathbf{f}_\sigma^{(0)}\right] + 1/2\,\hat{\mathbf{V}}\cdot\hat{\nabla}\mathbf{f}_\sigma^{(1)} + \partial\mathbf{f}_\sigma^{(0)}/\partial\hat{t} \right.$$
$$\left. 1/6\,\hat{\mathbf{V}}\cdot\hat{\nabla}\left[\hat{\mathbf{V}}\cdot\hat{\nabla}\mathbf{f}_\sigma^{(0)}\right] \right\}. \tag{90}$$

After some simple algebra, the final expression is recovered

$$\hat{\mathbf{T}}_{\sigma d}^{(2)} = \hat{\mathbf{T}}_\sigma^{(2)} + \frac{1}{6}\,\hat{\nabla}\cdot\left[(1 - 2\,s_\sigma)\,\rho_\sigma^{(0)}\,\hat{\mathbf{u}}_\sigma^{(1)} - \frac{1}{3}\,\hat{\lambda}_m^I\,\rho_\sigma^{(0)}\,\hat{\mathbf{w}}_\sigma^{(1)}\right]\mathbf{I}$$
$$+ \frac{\hat{\lambda}_m^I}{6\,(\hat{\lambda}_{\sigma 1}^{II} + \hat{\lambda}_{m 1}^{II})}\left\{ \hat{\nabla}\left[\rho_\sigma^{(0)}\,\hat{\mathbf{w}}_\sigma^{(1)}\right] + \hat{\nabla}\left[\rho_\sigma^{(0)}\,\hat{\mathbf{w}}_\sigma^{(1)}\right]^T - \hat{\nabla}\cdot\left[\rho_\sigma^{(0)}\,\hat{\mathbf{w}}_\sigma^{(1)}\right]\mathbf{I} \right\}$$
$$+ \frac{1}{6}\left\{ \hat{\nabla}\left[\rho_\sigma^{(0)}\,\hat{\mathbf{u}}_\sigma^{(1)} - \frac{1}{3}\,\hat{\lambda}_m^I\,\rho_\sigma^{(0)}\,\hat{\mathbf{w}}_\sigma^{(1)}\right] \right.$$
$$\left. + \hat{\nabla}\left[\rho_\sigma^{(0)}\,\hat{\mathbf{u}}_\sigma^{(1)} - \frac{1}{3}\,\hat{\lambda}_m^I\,\rho_\sigma^{(0)}\,\hat{\mathbf{w}}_\sigma^{(1)}\right]^T \right\}. \tag{91}$$

Summing over all the species and assuming that the mixture velocity based on the volumetric concentration $[\sum_\sigma e_\sigma \rho_\sigma \hat{\mathbf{u}}^{(1)}]/\sum_\sigma e_\sigma \rho_\sigma$ does not differ too much

from the barycentric velocity, i.e. $[\sum_\sigma e_\sigma \rho_\sigma \hat{\mathbf{u}}^{(1)}]/\sum_\sigma e_\sigma \rho_\sigma \approx \hat{\mathbf{u}}^{(1)} = \sum_\sigma x_\sigma \hat{\mathbf{u}}_\sigma^{(1)}$ yields

$$
\hat{\mathbf{T}}_d^{(2)} = \sum_\sigma \hat{\mathbf{T}}_{\sigma d}^{(2)} = \sum_\sigma \hat{\mathbf{T}}_\sigma^{(2)} + \frac{1}{6}\left(1 - 2\sum_\sigma s_\sigma x_\sigma\right)\hat{\nabla}\cdot\left[\rho^{(0)}\,\hat{\mathbf{u}}^{(1)}\right]\mathbf{I}
$$
$$
+ \frac{1}{6}\left\{\hat{\nabla}\left[\rho^{(0)}\,\hat{\mathbf{u}}^{(1)}\right] + \hat{\nabla}\left[\rho^{(0)}\,\hat{\mathbf{u}}^{(1)}\right]^T\right\},
\tag{92}
$$

and consequently

$$
\hat{\mathbf{T}}_d^{(2)} = \frac{1}{3}\sum_\sigma s_\sigma \rho_\sigma^{(2)}\mathbf{I} - \hat{\eta}_{md}\,\hat{\nabla}\cdot\left[\rho^{(0)}\,\hat{\mathbf{u}}^{(1)}\right]\mathbf{I}
$$
$$
+ \sum_\sigma\left[(1 - \alpha_{\sigma 1}^{II})\,\rho_\sigma^{(0)}\,\mathbf{u}_\sigma^{(1)}\otimes\mathbf{u}_\sigma^{(1)} + \alpha_{\sigma 1}^{II}\,\rho_\sigma^{(0)}\,\mathbf{u}^{(1)}\otimes\mathbf{u}^{(1)}\right]
$$
$$
- \hat{\nu}_{md}\left\{\hat{\nabla}\left[\rho^{(0)}\,\hat{\mathbf{u}}^{(1)}\right] + \hat{\nabla}\left[\rho^{(0)}\,\hat{\mathbf{u}}^{(1)}\right]^T\right\},
\tag{93}
$$

where $\hat{\nu}_{md}$ and $\hat{\eta}_{md}$ are defined as

$$
\hat{\nu}_{md} = \sum_\sigma \hat{\nu}_{\sigma m} - \frac{1}{6},
\tag{94}
$$
$$
\hat{\eta}_{md} = \sum_\sigma \hat{\eta}_{\sigma m} - \frac{1}{6}\left(1 - 2\sum_\sigma s_\sigma x_\sigma\right).
\tag{95}
$$

Collecting the previous results, the final system of equation is

$$
\frac{\partial \tilde{\rho}_\sigma}{\partial t} + \nabla\cdot(\tilde{\rho}_\sigma\,\tilde{\mathbf{u}}_\sigma) = 0,
\tag{96}
$$
$$
\tilde{\rho}_\sigma\,\tilde{\mathbf{w}}_\sigma = -D_\sigma\,\nabla\tilde{\rho}_\sigma,
\tag{97}
$$

$$
\frac{\partial}{\partial t}(\tilde{\rho}\tilde{\mathbf{u}}) + \nabla\cdot\sum_\sigma\left[\left(1 - \alpha_{\sigma 1}^{II}\right)\tilde{\rho}_\sigma\,\tilde{\mathbf{u}}_\sigma\otimes\tilde{\mathbf{u}}_\sigma + \alpha_{\sigma 1}^{II}\,\tilde{\rho}_\sigma\,\tilde{\mathbf{u}}\otimes\tilde{\mathbf{u}}\right]
$$
$$
= -1/3\,\nabla(\sum_\sigma s_\sigma\tilde{\rho}_\sigma) + \nabla\,(\tilde{\rho}\,\eta_{md}\,\nabla\cdot\tilde{\mathbf{u}})
$$
$$
+ \nabla\cdot\left[\tilde{\rho}\,\nu_{md}\,\nabla\tilde{\mathbf{u}} + \tilde{\rho}\,\nu_{md}\,(\nabla\tilde{\mathbf{u}})^T\right],
\tag{98}
$$

where $\nu_{md} = T_C\,c^2\,\hat{\nu}_{md}$ and $\eta_{md} = T_C\,c^2\,\hat{\eta}_{md}$.

In the next paragraph, some numerical results are reported in order to prove that the modified integration scheme is effective for ensuring the mass conservation.

7 Numerical simulations

In this section, some numerical results are reported for the suggested discrete lattice model. Some carefully conducted benchmarking computations were performed in order to verify the transport coefficients of the proposed lattice Boltzmann model and to verify the mass conservation.

The transient method [18] is a very popular method for measuring the effective numerical diffusivity. Essentially by combining Eq. (97) and Eq. (96), the following equation can be recovered

$$\frac{\partial \tilde{\rho}_\sigma}{\partial t} + \nabla \cdot (\tilde{\rho}_\sigma \, \tilde{\mathbf{u}}) = D_\sigma \, \nabla^2 \tilde{\rho}_\sigma. \tag{99}$$

Let us consider a one dimensional concentration field. In the case $\tilde{u}_x$ is a constant and D_σ is a constant as well, a solution of the Eq. (99), describing a decaying sine wave flowing along in the x direction with velocity $\tilde{u}_x$, is given as

$$\tilde{\rho}_\sigma[x,t] = \tilde{\rho}_\sigma^0 + (\tilde{\rho}_\sigma' - \tilde{\rho}_\sigma^0) \, \exp\left[-k^2 \, D_\sigma \, t\right] \, \sin\left[k \, (x - \tilde{u}_x \, t)\right], \tag{100}$$

where $\tilde{\rho}_\sigma^0$ is the constant averaged density of the σ species, $\tilde{\rho}_\sigma'$ is the maximum value of the initial perturbation applied to the density and $1/k$ is the wave length of the perturbation. Since periodic boundary conditions were used, the ratio between the computational domain length along x axis and the wave length was an integer. Assuming $\tilde{u}_x = 0$ (this can be done by starting with a proper initial concentration field), the numerical diffusivity can be measured by considering the sine wave maximum decay, namely

$$D_\sigma^{MT} = \frac{1}{k^2 \, t} \, \ln \left\{ \frac{\tilde{\rho}_\sigma[\pi/(2\,k), 0] - \tilde{\rho}_\sigma^0}{\tilde{\rho}_\sigma[\pi/(2\,k), t] - \tilde{\rho}_\sigma^0} \right\}. \tag{101}$$

This is not the only way to numerically measure the actual diffusivity. Another way is to directly apply the definition, namely

$$D_\sigma^{MF} = -\frac{\tilde{\rho}_\sigma \, (\tilde{u}_{\sigma\,x} - \tilde{u}_x)}{\partial \tilde{\rho}_\sigma/\partial x} = -\frac{\tilde{\rho}_\sigma \, \tilde{u}_{\sigma\,x}}{\partial \tilde{\rho}_\sigma/\partial x}. \tag{102}$$

The previous numerical experiments allow us to appreciate the limits of the forward Euler integration rule for the present application. The key point is that it is always possible to tune d in Eq. (81) in such a way that D_σ^{MT} recovers the theoretical result, i.e. $D_\sigma^{MT} = D_\sigma$. However this implies $D_\sigma^{MF} \neq D_\sigma$ and consequently the mass is not conserved. A numerical implementation

will satisfy the desired transport coefficient and the mass conservation, if and only if $D_\sigma^{MT} = D_\sigma^{MF} = D_\sigma$ at the same time.

The results of the numerical simulations are reported in Fig. 1 and Fig. 2 for the transient technique [18] and for the direct application of flux definition, respectively. The modified mid-point integration rule proves to be an effective way to ensure both the desired transport coefficient D_σ and the mass conservation. In particular, satisfying the condition given by Eq. (102) is more difficult, particularly for small λ_m^I, i.e. for decoupled species dynamics. This is consistent with the previous analysis which assumed that $O(\lambda_m^I) = 1$ and this is no more valid for small λ_m^I.
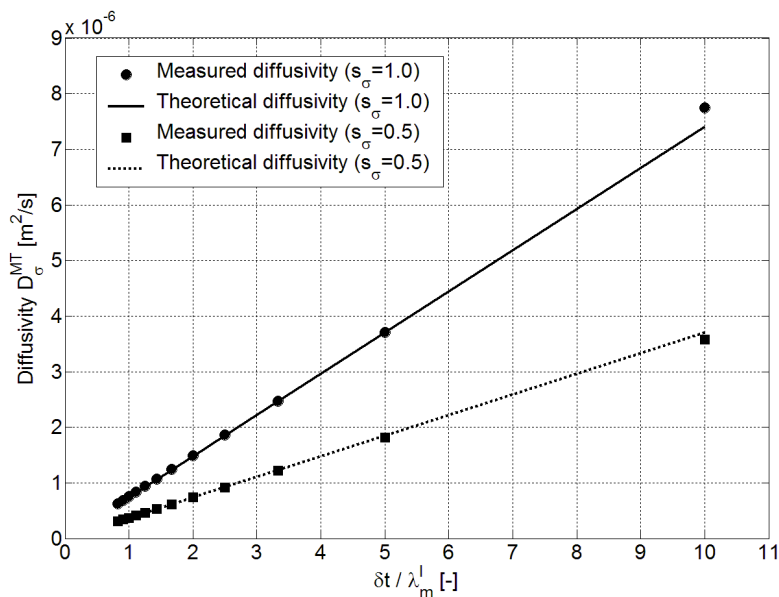

Fig. 1. Comparison between numerically measured diffusivity, obtained by means of the transient technique given by Eq. (101), and the theoretical diffusivity, given by Eq. (60).

8 Conclusions

In this paper, a new lattice Boltzmann model for simulating ideal mixtures has been developed by means of the multiple-relaxation-time (MRT) approach. If compared with the previous single-relaxation-time (SRT) formulation of the same model, based on the Hamel work, the new model offers the possibility to independently tune the mutual diffusivity, driven by the relaxation parameter λ_m^I, and the effects of cross collisions on the effective stress tensor, in terms of additional kinematic viscosity $\nu_{\sigma m} - \nu_\sigma$ and additional bulk viscosity $(\nu_{\sigma m} + \eta_{\sigma m}) - (\nu_\sigma + \eta_\sigma)$, driven by the relaxation parameter λ_{m1}^{II} and λ_{m3}^{II}
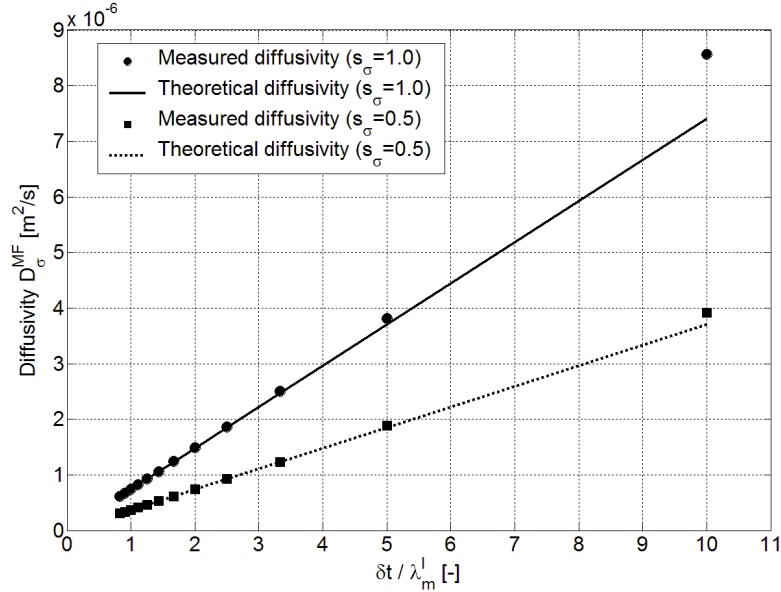
Fig. 2. Comparison between numerically measured diffusivity, obtained by means of the direct application of flux definition given by Eq. (102), and the theoretical diffusivity, given by Eq. (60).

respectively. However an additional constraint, given by Eq. (58), must be taken into account in order to ensure the Galilean invariance.

For the considered application, the asymptotic analysis [36], recently suggested as an effective tool for analyzing the macroscopic equations corresponding to LB schemes, offers the possibility to easily deal with leading terms in the distribution functions, which are no more Maxwellian. This represents a remarkable advantage in comparison with the classical Chapman-Enskog technique. In fact the Chapman-Enskog approach can be generalized for the present application [30], by using some heuristic assumption about the fact that, if the leading terms are no more Maxwellian, higher order terms of the expansion only effect the conserved quantities in order to ensure the conservation laws. The results obtained by the asymptotic analysis does not seem to confirm this assumption. In fact the higher order terms of the expansion effect the conserved quantities in order to ensure the conservation laws, as recovered for the expansion coefficient $\mathbf{f}_\sigma^{(1)}$ given by Eqs. (54, 55), but they also effect the non-conserved quantities like the stress tensor components, as proved by Eq. (56).

Acknowledgments

References

[1] G.R. McNamara, G. Zanetti, "Use of the Boltzmann equation to simulate lattice-gas automata", Phys. Rev. Lett. **61**, 2332 (1988).

[2] F. Higuera, S. Succi, R. Benzi, "Lattice Gas Dynamics with Enhanced Collisions", Europhys. Lett. **9**, 4 (1989).

[3] F. Higuera, J. Jimenez, S. Succi, "Boltzmann approach to lattice gas simulations", Europhys. Lett, **9**, 663 (1989).

[4] H. Chen, S. Chen, W. H. Matthaeus, "Recovery of the Navier-Stokes equations using a lattice-gas Boltzmann method", Phys. Rev. A **45**, R5339 (1992).

[5] Y.H. Qian, D. D'Humieres, P. Lallemand, "Lattice BGK models for Navier-Stokes equation", Europhys. Lett. **17**, 479 (1992).

[6] X. He, L.-S. Luo, "Theory of the lattice Boltzmann method: From the Boltzmann equation to the lattice Boltzmann equation", Phys. Rev. E **56**, 6811 (1997).

[7] X. Shan, X. He, "Discretization of the velocity space in the solution of the Boltzmann equation", Phys. Rev. Lett. **80**, 65 (1998).

[8] D. Wolf-Gladrow, *Lattice-Gas Cellular Automata and Lattice Boltzmann Models*, Lecture Notes in Mathematics Vol. 1725, Springer-Verlag, Berlin (2000).

[9] S. Succi, *The Lattice Boltzmann Equation for Fluid Dynamics and Beyond*, Oxford University Press, New York (2001).

[10] G.D. Doolen, *Lattice Gas Methods for Partial Differential Equations*, Addison-Wesley, New York (1990).

[11] R. Benzi, S. Succi, M. Vergassola, Phys. Rep. **222**, 145, (1992).

[12] S. Chen, G. D. Doolen, "Lattice Boltzmann method for fluid flow", Annu. Rev. Fluid Mech. **30**, 329 (1998).

[13] B. Manz, L.F. Gladden, P.B. Warren, "Flow and dispersion in porous media: lattice-Boltzmann and NMR studies", AIChE. J. **45**, 1845 (1999).

[14] Th. Zeiser, P. Lammers, E. Klemm, Y.W. Li, J. Bernsdorf, G. Brenner, "CDF-calculartion of flow, dispersion and reaction in a catalyst filled tube by the lattice Boltzmann method", Chem. Eng. Science, **56**, 1697 (2001).

[15] K. Xu, "BGK-Based Scheme for Multicomponent Flow Calculations", J. Comput. Phys. **134**, 122 (1997).

[16] Y.S. Lian, K. Xu, "A Gas-Kinetic Scheme for Multimaterial Flows and Its Application in Chemical Reactions", J. Comput. Phys. **163**, 349 (2000).

[17] X. Shan, H. Chen, "Lattice Boltzmann model for simulating flows with multiple phases and components", Phys. Rev. E **47**, 1815 (1993).

[18] E.G. Flekkoy, "Lattice bhatnagar-gross-krook models for miscible fluids", Phys. Rev. E **47**, 4247 (1993).

[19] X. Shan, G. Doolen, "Multicomponent lattice-Boltzmann model with interparticle interaction", J. Stat. Phys. **81**, 379 (1995).

[20] X. Shan, G. Doolen, "Diffusion in a multicomponent lattice Boltzmann equation model", Phys. Rev. E **54**, 3614 (1996).

[21] E. Orlandini, W.R. Osborn, J.M. Yeomans, "A lattice Boltzmann model of binary-fluid mixtures", Europhys. Lett. **32**, 463 (1995).

[22] W.R. Osborn, E. Orlandini, M.R. Swift, J.M. Yeomans, J.R. Banavar, "Lattice Boltzmann study of hydrodynamic spinodal decomposition", Phys. Rev. Lett. **75**, 4031 (1995).

[23] M.R. Swift, E. Orlandini, W.R. Osborn, J.M. Yeomans, "Lattice Boltzmann simulations of liquid-gas and binary fluid systems", Phys. Rev. E **54**, 5041 (1996).

[24] A. Lamura, G. Gonnella, J.M. Yeomans, "A Lattice-Boltzmann model of ternary-fluid mixtures", Europhys. Lett. **45**, 314 (1999).

[25] V. Sofonea, R.F. Sekerka, "BGK models for diffusion in isothermal binary fluid systems", Physica A **299**, 494 (2001).

[26] Z. Guo, T.S. Zhao, "Discrete velocity and lattice Boltzmann models for binary mixtures of nonideal fluids", Phys. Rev. E **68**, 035302 (2003).

[27] L.-S. Luo, S.S. Girimaji, "Theory of the lattice Boltzmann method: Two-fluid model for binary mixtures", Phys. Rev. E **67**, 036302 (2003).

[28] A. Xu, "Finite-Difference Lattice Boltzmann Methods for binary fluids", arXiv:cond-mat/0406012, www.arxiv.org (2004).

[29] P.C. Fancin, P.C. Philippi, L.O.E. dos Santos, "Non-linear lattice-Boltzmann model for ideal miscible fluids", Future Generation Computer Systems J. **20**, 945 (2004).

[30] P. Asinari, "Viscous coupling based lattice Boltzmann model for binary mixtures", Phys. Fluids **17**, 067102 (2005).

[31] B.B. Hamel, "Boltzmann Equations for Binary Gas Mixtures", Ph.D. dissertation, Princeton University (1963).

[32] B.B. Hamel, "Kinetic model of binary mixtures", Phys. Fluids **8**, 418 (1965).

[33] B.B. Hamel, "Kinetic Model for Binary Gas Mixtures", Phys. Fluids **9**, 12 (1966).

[34] D. d'Humiéres, "Generalized lattice Boltzmann equations", in *Rarefied gas dynamics: theory and simulations* (ed. B. D. Shizgal & D. P. Weaver), Prog. Astronaut. Aeronaut. **159**, 450 (1992).

[35] P. Lallemand, L.-S. Luo, "Theory of the lattice Boltzmann method: Dispersion, dissipation, isotropy, Galilean invariance, and stability", Phys. Rev. E, **61**, 6546-6562 (2000).

[36] M. Junk, A. Klar, L.-S. Luo, "Asymptotic analysis of the lattice Boltzmann equation", J. Computational Physics **210**, 676-704 (2005).

[37] V. Garzò, A. Santos, J.J. Brey, "A kinetic model for multicomponent gas", Phys. Fluids A **1**(2), 380 (1989).

[38] P. Andries, K. Aoki, B. Perthame, "A consistent BGK-type model for gas mixtures", J. Stat. Phys. **106** 5/6, 993 (2002).

[39] P. Asinari, "Semi-implicit-linearized multiple-relaxation-time formulation of lattice Boltzmann schemes for mixture modeling", Phys. Rev. E **73**, to be published (2006).

[40] Y. Sone, *Kinetic Theory and Fluid Dynamics*, Birkhäuser, Boston (2002).

[41] M.E. McCracken, J. Abraham, "Lattice Boltzmann methods for binary mixtures with different molecular weights", Phys. Rev. E **71**, 046704 (2005).