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Lattice Boltzmann Modeling of Miscible Multicomponent Gas Mixtures in the Rarefied Regime

Michel Ho*, Sami Ammar, Sébastien Leclaire, Marcelo Reggio and Jean-Yves Trépanier

Departement of Mechanical Engineering, Polytechnique Montréal, 2500 Chemin de Polytechnique, Montreal H3T 1J4, Canada.

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Abstract. An extension to rarefied flow regimes of the lattice Boltzmann method-based model for miscible mixtures developed by Vienne et al. (*Physical Review E 100.2 (2019): 023309*) is presented. The model is applied to study the gas phase separation phenomenon in mixture flows that traditional macroscopic approaches fail to predict. The extension includes a wall function approach with an empirical coefficient to define an effective mean free path in solid geometries, which locally defines the kinematic viscosity and binary diffusion coefficients. The algorithm is also modified by a local multi-relaxation time collision operator and slip boundary conditions at solid walls. Gaseous mixture flow simulations are conducted through a 2D plane microchannel within the slip and early transition flow regimes. Despite a miscible gaseous phase, the mixture loses its homogeneity and independent velocity profiles for each component are observed in the rarefied regime and captured with the current modeling. In addition, the gas separation phenomenon increases with the rarefaction rate and the molecular mass ratio. The individual treatment of the species within mixture flows in the developed lattice Boltzmann model helps understanding the increasing independent behavior of the individual species within the mixture as the regime becomes more rarefied.

AMS subject classifications: 76P05

Key words: Lattice Boltzmann, gaseous mixtures, rarefied regimes.

1 Introduction

Understanding gas flow in rarefied regimes has received increasing interest over the past decades in various applications, including micro-filtering [1, 2], shale gas [3–7], or near-vacuum flows [8–12]. The Knudsen number (Kn) characterizes the rarefaction rate, and

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*Corresponding author. *Email addresses:* `michel.ho@polymtl.ca` (M. Ho), `sami.ammar@polymtl.ca` (S. Ammar), `s.leclaire@polymtl.ca` (S. Leclaire), `marcelo.reggio@polymtl.ca` (M. Reggio), `jean-yves.trepanier@polymtl.ca` (J.-Y. Trépanier)

is defined as the ratio of the gas mean free path λ to the characteristic length of the domain H, so that $\mathrm{Kn} = \lambda/H$. Fluid flow is generally classified with respect to Kn in the continuum ($\mathrm{Kn} < 0.001$), slip ($0.001 \leq \mathrm{Kn} < 0.1$), transition ($0.1 \leq \mathrm{Kn} < 10$) or free molecular ($\mathrm{Kn} \geq 10$) flow regimes [13, 14]. Continuum mechanics fail to predict the fluid flow behavior at high Kn regimes [14, 15]. Simulating without the continuum assumptions on a smaller scale is thus required to recover the fluid behavior more reliably at high Kn.

Among the different mesoscale/microscale fluid numerical models, the lattice Boltzmann method (LBM) is an appropriate tool for flow simulation in the rarefied regime thanks to its mesoscopic approach based on the Boltzmann equation. Furthermore, its computational efficiency and simple implementation have encouraged several developments to extend the LBM to rarefied regimes. Based on the kinetic theory of gases, relationships between Kn and the collision operator have been developed to account for the decrease in particle-particle interactions at high Kn [16–18]. The collision operator has also been improved by implementing a multi-relaxation time (MRT) operator to avoid non-physical slip at solid interfaces by tuning the free parameters with the additional relaxation times [19–21]. Slippage effects have also been treated by developing slip boundary conditions, such as the diffuse bounce back (DBB) [17, 19, 20, 22] or the combined bounce back and specular reflection (CBBSR) [23–25]. The resulting flow behavior has been validated against different analytical solutions and experimental data [18, 19, 24, 26–29]. At high Kn flow regimes (transition and free molecular), different wall functions were developed to correct the effective gas mean free path in a bounded domain compared to a solid-free one [21,24,28,30–32]. Numerical results indicate that the mass flow rate was in good agreement with experimental data with these wall functions, whereas it was inaccurately estimated with analytical slip flow models [24, 29, 33]. Based on these models, rarefied gas flows have been simulated through complex microstructures [21, 27] to underline the global influence of the rarefied effects on mass flow and highlight the need for a Boltzmann-equation-based numerical model to appropriately predict the fluid behavior.

Most of the LBM models in rarefied regimes have been developed by considering a single pure component flow. However, in practical applications, the gas phase is often a multicomponent gaseous mixture. For instance, the atmosphere is commonly modeled as a mixture of nitrogen and oxygen. In the continuum regime, no difference is noticeable: gaseous mixtures flow in a similar fashion as a single component flow with mixture transport properties. In the rarefied regime, gas phase separation appears: species flow independently from one another with respect to their individual properties [34, 35]. This phenomenon appears in many applications, such as micro-pumping [36, 37], microfiltration [38–40] or micro-mixing systems [41]. Few works have focused on multicomponent flow LBM modeling in the rarefied regime. Joshi et al. [42] have investigated diffusion at high Kn for ternary mixtures based on the multicomponent LBM model for the continuum regime developed by Luo et al. [43]. Kim et al. [44] have modeled diffusion slip in the rarefied regime with a higher-order LBM model and validated it against other numerical methods. Rather than modifying the boundary conditions, Ma et al. [45] added