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Comparison of relaxation phenomena in binary gas-mixtures of Maxwell molecules and hard spheres

Vinay Kumar Gupta *, Manuel Torrilhon

Center for Computational Engineering Science, Department of Mathematics, RWTH Aachen University, Schinkelstr. 2, D-52062 Aachen, Germany

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ABSTRACT

The strategy for computing the Boltzmann collision integrals for gaseous mixtures is presented and bestowed to compute the fully non-linear Boltzmann collision integrals for hard sphere gas-mixtures. The Boltzmann collision integrals associated with the first 26 moments of each constituent in a gas-mixture are presented. Moreover, the Boltzmann collision integrals are exploited to study the relaxation phenomena of diffusion velocities, stresses and heat fluxes in binary gas-mixtures of Maxwell molecules and hard spheres.

1. Introduction

The gaseous mixtures are encountered more often than a single gas in practice and the description of processes in rarefied gas-mixtures far from equilibrium is a real challenge. It is eminent that the Boltzmann equation(s) can well describe the processes in rarefied gases (for both single gas as well as gaseous mixtures) [1,2]. Nevertheless, the direct numerical solution of the Boltzmann equation – e.g., by discrete velocity method [3] or direct simulation Monte Carlo (DSMC) method [4] – are computationally very expensive, especially, in the transition regime [5]. Therefore, the proper models for describing the rarefied gas flows in the transition regime are desired.

The main source of difficulty in dealing with the Boltzmann equation is its collision term, referred to as the Boltzmann collision operator. In the context of a single gas, the Boltzmann collision operator can be approximated by the well-known Bhatnagar–Gross–Krook (BGK) model [6], which drastically simplifies the Boltzmann equation. Several authors have attempted to obtain the similar BGK model for gaseous mixtures, see e.g. [7–14], however most of these models either fail to reproduce the correct transport coefficients or do not satisfy some fundamental properties. The recent works [13,14] first consider the transport coefficients computed either by hydrodynamic limit of the Boltzmann equation or by experiments and then construct the BGK model by fitting these coefficients into the model, however both the works are restricted to obtain only correct Fick's and Newton's laws.

The alternative approaches to deal with the Boltzmann equation protrude through kinetic theory. The two well-known methods in kinetic theory to solve the Boltzmann equation approximately are the Chapman–Enskog expansion (CE) method [1,5,15,16] and Grad's moment method [17,5,15]. Both the methods have been successfully extended to the gaseous mixtures [1,18,19]. While the higher-order equations resulting from the CE method in case of a single gas are known to

* Corresponding author.
E-mail address: gupta@mathcces.rwth-aachen.de (V.K. Gupta).

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suffer from instabilities [20], the moment equations resulting from Grad's moment method are always stable [5]. Despite the success of Grad's moment method and its variants (e.g., [21]) in describing many rarefaction effects in case of a single gas [22–25], Grad's moment method for mixtures has not been exploited enough. One reason, among others, could be the computation of the production terms or the Boltzmann collision integrals, which emanate from the Boltzmann collision operator while deriving the moment equations.

In this paper, we present the strategy for computing the full non-linear production terms for gaseous mixtures of monatomic–inert–ideal gases interacting with any general interaction potential. However, due to the complex structure of the production terms for general interaction potential, we restrict ourselves to provide the production terms explicitly associated with first 26 moments in Grad's 26-moment (G26) system for each constituent only in a gaseous mixture of hard spheres (HS). The corresponding production terms for Maxwell molecules (MM) can be found in [26]. This part of the present paper can be considered as a follow up of [27], where we computed the (quasi-)linear production terms for binary gas-mixtures of hard spheres. Furthermore, we study the relaxation of diffusion velocities, stresses and heat fluxes of individual components in binary gas-mixtures using these production terms.

The structure of the paper is as follows. The Boltzmann equations for gaseous mixture, few definitions and the production terms are introduced in Section 2. The procedure for computing the production terms is detailed in Section 3. The relaxation phenomena in binary HS gas-mixtures and in binary MM gas mixtures is studied in Section 4. The conclusions are given in Section 5.

2. Boltzmann equations

The Boltzmann equation for a constituent α ($\alpha = 1, 2, \ldots, N$) in a N-component monatomic–inert–ideal gas mixture reads [1,18,15,27,26]

$$\frac{\partial f_\alpha}{\partial t} + c_i^{(\alpha)} \frac{\partial f_\alpha}{\partial x_i} + F_i^{(\alpha)} \frac{\partial f_\alpha}{\partial c_i^{(\alpha)}} = \sum_{\beta=1}^{N} \int_{\mathbb{R}^3} \int_0^{2\pi} \int_0^{\infty} \left(f'_\alpha f'_\beta - f_\alpha f_\beta\right) g_{\alpha\beta}\, b \,\mathrm{d}b \,\mathrm{d}\epsilon \,\mathrm{d}\boldsymbol{c}_\beta, \tag{1}$$

where $f_\alpha \equiv f_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t)$ is the distribution function of the α-constituent in the mixture; $\boldsymbol{F}_\alpha$ is the external force per unit mass acting on the α-species; $\boldsymbol{g}_{\alpha\beta} = \boldsymbol{c}_\alpha - \boldsymbol{c}_\beta$ is the relative velocity; b is the collision parameter; ϵ is the collision angle; $\boldsymbol{x}$, $\boldsymbol{c}_\alpha$, t denote the position, instantaneous velocity and time, respectively; the primes on distribution functions denote the distribution functions with post-collision velocities, e.g., $f'_\alpha \equiv f_\alpha(\boldsymbol{x}, \boldsymbol{c}'_\alpha, t)$; and the right-hand side (RHS) of (1) is termed as the *Boltzmann collision operator*. Hereafter, unless necessary, we shall suppress the limits over the integrations and only one integration symbol will be used in order to make the notations compact. Furthermore, the integrals over any velocity space should always be understood as the volume integrals over all the components of that velocity, each ranging from $-\infty$ to ∞.

The moment of the distribution function f_α with respect to a function $\psi_\alpha \equiv \psi_\alpha(\boldsymbol{x}, \boldsymbol{c}_\alpha, t)$ is defined as

$$\langle \psi_\alpha \rangle = \int \psi_\alpha f_\alpha \,\mathrm{d}\boldsymbol{c}_\alpha, \tag{2}$$

and the governing equation for the moment $\langle \psi_\alpha \rangle$, referred to as the moment equation for $\langle \psi_\alpha \rangle$, can be obtained by multiplying the Boltzmann equation (1) with ψ_α and integrating over the velocity space $\boldsymbol{c}_\alpha$. The derivation of moment equations is omitted here and the reader is referred to [26] for the detailed derivation of Grad's $N \times 26$ moment equations for a N-component gaseous mixture. Nevertheless, the Boltzmann collision operator on multiplying with ψ_α and integrating over the velocity space $\boldsymbol{c}_\alpha$ yields

$$\mathcal{P}(\psi_\alpha) = \sum_{\beta=1}^{N} \int \psi_\alpha \left(f'_\alpha f'_\beta - f_\alpha f_\beta\right) g_{\alpha\beta}\, b \,\mathrm{d}b \,\mathrm{d}\epsilon \,\mathrm{d}\boldsymbol{c}_\alpha \,\mathrm{d}\boldsymbol{c}_\beta, \tag{3}$$

which is referred to as the *production term* or the *Boltzmann collision integral* for ψ_α. The typical structure of ψ_α is

$$\psi_\alpha = m_\alpha C_\alpha^{2a}\, C^{(\alpha)}_{\langle i_1} \cdots C^{(\alpha)}_{i_n \rangle} \tag{4}$$

where a and n are non-negative integers, m_α is the molecular mass of α-species, $\boldsymbol{C}_\alpha = \boldsymbol{c}_\alpha - \boldsymbol{v}$ is the peculiar velocity with $\boldsymbol{v}$ being the mass-averaged velocity of the mixture defined in $(7)_2$, and angle brackets around the indices denote the symmetric trace-free tensors [5]. Therefore, the typical form of the production term is

$$\mathcal{P}^{a(\alpha)}_{i_1 \cdots i_n} = m_\alpha \sum_{\beta=1}^{N} \int \left\{ (C'_\alpha)^{2a}\, C'^{(\alpha)}_{\langle i_1} \cdots C'^{(\alpha)}_{i_n \rangle} - C_\alpha^{2a}\, C^{(\alpha)}_{\langle i_1} \cdots C^{(\alpha)}_{i_n \rangle} \right\} f_\alpha f_\beta\, g_{\alpha\beta}\, b \,\mathrm{d}b \,\mathrm{d}\epsilon \,\mathrm{d}\boldsymbol{c}_\alpha \,\mathrm{d}\boldsymbol{c}_\beta. \tag{5}$$

In writing (5), the symmetry properties of the Boltzmann collision operator [1,5] have been employed. Some of the physical quantities for the constituent α ($\alpha = 1, 2, \ldots, N$) – density $\rho_\alpha(\boldsymbol{x}, t)$, diffusion velocity $\boldsymbol{u}_\alpha(\boldsymbol{x}, t)$, temperature $T_\alpha(\boldsymbol{x}, t)$, stress