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Automated Boltzmann Collision Integrals for Moment Equations

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Abstract. We present a methodology to evaluate the moments of the Boltzmann collision term, in a general automated way, using the computer algebra software Mathematica. Based on Grad's distribution function with 26-moments, we compute the non-linear production terms for a simple gas and a granular gas, and the linear production terms for a binary mixture of gases. The results can be shown for general interaction potential, but, in this paper, they are given only for hard-sphere interaction potential.

Keywords: Boltzmann Equation, Moment Equations, Grad's Method of Moments

PACS: 51.10.+y, 47.45.-n, 47.45.Ab, 05.20.Dd

INTRODUCTION

The Navier–Stokes–Fourier equations fail to fully describe the processes in rarefied regime, even though gases behave as a continuum in this regime. Therefore, one needs a more refined set of equations to describe the processes in rarefied gases. The behaviour of gases in the rarefied regime is well described by the Boltzmann equation [1–3].

To get an approximate solution of the Boltzmann equation, the two widely used methods in kinetic theory are: the Chapman–Enskog expansion [1, 3–5] and Grad's method of moments [3, 6, 7]. The Chapman–Enskog expansion works well in deriving the Navier–Stokes–Fourier equations but higher-order expansions result into the Burnett and super-Burnett equations—which are unstable [8]. On the other hand, the equations resulting from Grad's method of moments are always stable but their hyperbolic nature leads to unphysical discontinuous shocks for large Mach numbers.

Considering the desired features of the above-mentioned methods, Struchtrup and Torrilhon [9] regularized the moment equations by performing the Chapman–Enskog expansion on Grad's 13-moment equations. The resulting equations are termed as the R13 equations; these equations are stable and yield continuous shock structures for all Mach numbers.

The starting point of all the above-mentioned methods is the Boltzmann equation, but the main source of difficulty in dealing with the Boltzmann equation is the collision term (the right-hand side of the Boltzmann equation). In Grad's moment method or regularized moment method, one has to consider the moments of the Boltzmann equation, which result into moment equations. The moment equations do not form a closed system of partial differential equations because each moment equation contains a higher-order flux on the left-hand side and, of course, the unknown moment of the collision term on the right-hand side—the moments of the collision term are called the *production terms* or the *collision integrals* [10]. The system of moment equations is closed by assuming a certain approximation for the velocity distribution function. A standard choice for the approximation is given by a Hermite series and yields so-called Grad's 13- or 26-moment distribution functions [1, 4]. By approximating the distribution function and after some algebra, the unknown higher-order flux can be represented in terms of the field variables of the system of moment equations. However, it is not always easy to evaluate the production terms by hand because of their tensorial structure and the large number of terms occurring during the evaluation process. Due to the mathematical complexity involved in evaluating the production terms, the R13 equations have been derived only for the single gas, with Maxwell molecules [9] and, very recently, with hard-sphere interaction potential (HS) [11].

The main goal of this work is to present a method by which one can evaluate the production terms in a general automated way using the computer algebra software Mathematica. Based on the results of this paper, the regularized moment equations can be obtained for a single gas, a binary mixture of gases and a granular gas with Grad's 13- or 26-moment equations, even for the general interaction potential and with non-linear terms, in future. The source code to be used with Mathematica is available at [12].

We have evaluated the production terms for the above-mentioned problems with general interaction potential, but here we present the results only for HS.

FORMULATION OF THE PROBLEM

Simple Gas

Let us consider an ideal gas with molecule diameter d and molecular mass m . The *phase density* (or velocity distribution function) $f \equiv f(\mathbf{x}, \mathbf{c}, t)$ is defined in such a way that $f(\mathbf{x}, \mathbf{c}, t) d\mathbf{x} d\mathbf{c}$ gives the number of particles in an infinitesimal volume $d\mathbf{x}$ located at point \mathbf{x} whose velocities belong to an infinitesimal volume in the velocity space $d\mathbf{c}$ centred around \mathbf{c} . The hydrodynamic fields: the density $\rho(\mathbf{x}, t)$, the macroscopic velocity $\mathbf{v}(\mathbf{x}, t)$ and the temperature $T(\mathbf{x}, t)$ are defined by the relations

$$\rho = m \int f d\mathbf{c}, \quad \rho \mathbf{v} = m \int \mathbf{c} f d\mathbf{c} \quad \text{and} \quad \frac{3}{2} \rho \theta = \frac{3}{2} \rho \left(\frac{k}{m} T \right) = \frac{1}{2} m \int C^2 f d\mathbf{c}, \quad (1)$$

where k is the Boltzmann constant and $\mathbf{C} = \mathbf{c} - \mathbf{v}$ is the peculiar velocity of the particle. In eq. (1) and throughout this paper, the limits of integration over any velocity space \mathbf{c} are $-\infty$ to ∞ for $c_x, c_y,$ and c_z ; to make the notations compact, the limits are not explicitly mentioned and only one integral sign is used.

Let us introduce the trace-free part of the pressure tensor $p_{ij}(\mathbf{x}, t)$, and the heat flux $q_i(\mathbf{x}, t)$ as

$$\sigma_{ij} = p_{\langle ij \rangle} = m \int C_{\langle i} C_{j \rangle} f d\mathbf{c} \quad \text{and} \quad q_i = \frac{1}{2} m \int C^2 C_i f d\mathbf{c}. \quad (2)$$

The indices in angular brackets represent the symmetric and trace-free part of a tensor. The other higher-order moments, usually, do not have physical meaning. The higher-order–trace-free moments and the differences between the scalar moments and their equilibrium values are defined as

$$u_{i_1 \dots i_n}^a = m \int C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} f d\mathbf{c} \quad \text{and} \quad w^a = u^a - u_{|E}^a = m \int C^{2a} (f - f_0) d\mathbf{c}, \quad (3)$$

respectively. In the above equation, f_0 is the equilibrium (Maxwellian) distribution function, given by

$$f_0 = \frac{\rho}{m} \left(\frac{m}{2\pi kT} \right)^{3/2} \exp \left(-\frac{mC^2}{2kT} \right). \quad (4)$$

We start the problem with the Boltzmann equation [4]

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + F_i \frac{\partial f}{\partial c_i} = \int \int_0^{2\pi} \int_0^\infty (f' f'_1 - f f_1) g b db d\epsilon d\mathbf{c}_1, \quad (5)$$

where \mathbf{F} is the external force per unit mass and does not depend on velocity \mathbf{c} ; $f' \equiv f(\mathbf{x}, \mathbf{c}', t)$; b is the collision parameter; and the angle ϵ describes the orientation of the collision plane.

Multiplying the Boltzmann equation (5) with an arbitrary function $\psi \equiv \psi(\mathbf{x}, \mathbf{c}, t)$ and integrating over velocity space \mathbf{c} , one obtains the transfer equation [4]

$$\frac{\partial}{\partial t} \int \psi f d\mathbf{c} + \frac{\partial}{\partial x_i} \int \psi c_i f d\mathbf{c} - \int \left(\frac{\partial \psi}{\partial t} + c_i \frac{\partial \psi}{\partial x_i} + F_i \frac{\partial \psi}{\partial c_i} \right) f d\mathbf{c} = \int \int \int_0^{2\pi} \int_0^\infty (\psi' - \psi) f f_1 g b db d\epsilon d\mathbf{c} d\mathbf{c}_1. \quad (6)$$

In writing the right-hand side of eq. (6), the symmetry property of the collision integral is used.

Typically, ψ is of the tensorial form: $\psi = m C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle}$ and, thus, the general production term is given by

$$\mathcal{P}_{i_1 \dots i_n}^a = m \int \int \int_0^{2\pi} \int_0^\infty \left\{ (C')^{2a} C'_{\langle i_1} C'_{i_2} \dots C'_{i_n \rangle} - C^{2a} C_{\langle i_1} C_{i_2} \dots C_{i_n \rangle} \right\} f f_1 g b db d\epsilon d\mathbf{c} d\mathbf{c}_1. \quad (7)$$

In case of 26 field variables, we take $\psi = \{m, mc_i, \frac{1}{2}mC^2, mC_{\langle i}C_{j\rangle}, \frac{1}{2}mC^2C_i, mC_{\langle i}C_jC_k\rangle, mC^2C_{\langle i}C_{j\rangle}, mC^4\}$ to get the moment equations for the 26 field variables $\{\rho, \rho v_i, \frac{3}{2}\rho\theta, \sigma_{ij}, q_i, m_{ijk} = u_{ijk}^0, u_{ij}^1, \Delta = w^2\}$. The 26-moment system (6) is closed by approximating the phase density f with Grad's 26-moment distribution function, which reads

$$f_{|26} = f_0 \left\{ 1 + \frac{\Delta}{8\rho\theta^2} \left(1 - \frac{2}{3} \frac{C^2}{\theta} + \frac{1}{15} \frac{C^4}{\theta^2} \right) + \frac{1}{5} \frac{q_i C_i}{\rho\theta^2} \left(\frac{C^2}{\theta} - 5 \right) + \frac{\sigma_{ij}}{2\rho\theta^2} C_{\langle i}C_{j\rangle} \right. \\ \left. + \left(\frac{u_{ij}^1 - 7\theta\sigma_{ij}}{28\rho\theta^3} \right) C_{\langle i}C_{j\rangle} \left(\frac{C^2}{\theta} - 7 \right) + \frac{m_{ijk}}{6\rho\theta^3} C_{\langle i}C_jC_k \rangle \right\}. \quad (8)$$

With Grad's closure (8), one can easily write the unknown higher-order fluxes in terms of the field variables of the system; however, it is not easy to evaluate the production terms (7) by hand, even with closure (8). The procedure for evaluating the production terms, using computer algebra software Mathematica, is described in the next section.

Granular Gas

The qualitative properties of a dilute and smooth granular gas are described by the Boltzmann equation [4, 13]

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} + F_i \frac{\partial f}{\partial c_i} = \frac{d^2}{4} \int_0^{2\pi} \int_0^\pi \int_0^\pi \left(\frac{1}{e^2} f(c'') f(c_1'') - f(c) f(c_1) \right) g \sin \chi d\chi de dc_1, \quad (9)$$

where e is the coefficient of normal restitution and assumed as a constant in this paper, (c'', c_1'') are the pre-collisional velocities in an inverse collision (see [13] for details) and other symbols have same meanings as above. The general production term, in this case, reads [13]

$$\mathcal{P}_{i_1 \dots i_n}^a = \frac{m d^2}{4} \int_0^{2\pi} \int_0^\pi \int_0^\pi \left\{ (C')^{2a} C'_{\langle i_1} \dots C'_{i_n \rangle} - C^{2a} C_{\langle i_1} \dots C_{i_n \rangle} \right\} f f_1 g \sin \chi d\chi de dc dc_1. \quad (10)$$

Note that the integrand in eq. (10) still depends on e via the relation between C' and C . The system of 26-moment equations is obtained in a similar way as for a simple gas and the moment system is closed by approximating the phase density f with Grad's 26-moment distribution function (8). In the elastic limit ($e \rightarrow 1$), the equilibrium distribution function is given by eq. (4). The procedure for evaluating the production terms is described in the next section.

Binary Mixture of Gases

For the usual details of binary mixtures, the reader is referred to [4]. Here, we consider the mixture of two (inert) ideal gases—the constituents of these gases are labelled with α and β , say. Let m_i and d_i be the mass and diameter, respectively, of the molecule of gas i , where $i = \alpha, \beta$. In the mixture, there can be several velocities, namely, the instantaneous velocity of α particles c_α , the macroscopic velocity of α particles v_α , the peculiar velocity of α particles $C_\alpha = c_\alpha - v_\alpha$, the macroscopic velocity of the mixture v , peculiar velocity of α particles with respect to the velocity of the mixture $\bar{C}_\alpha = c_\alpha - v$, the diffusion velocity of α particles $u_\alpha = v_\alpha - v$ and, of course, similar velocities for β particles also. In the following, we shall mainly concentrate on the quantities with velocities \bar{C}_α and \bar{C}_β ; let us call the moments with respect to these velocities *diffusive moments*. Using the notation $f_\alpha \equiv f(c_\alpha) = f(\bar{C}_\alpha + v) = \bar{f}(\bar{C}_\alpha) \equiv \bar{f}_\alpha$, the first few diffusive moments are

$$\rho_\alpha = m_\alpha \int \bar{f}_\alpha d\bar{C}_\alpha, \quad \rho_\alpha u_i^{(\alpha)} = m_\alpha \int \bar{C}_i^{(\alpha)} \bar{f}_\alpha d\bar{C}_\alpha, \quad \frac{3}{2} \rho_\alpha \bar{\theta}_\alpha = \frac{3}{2} \rho_\alpha \left(\frac{k}{m_\alpha} \bar{T}_\alpha \right) = \frac{1}{2} m_\alpha \int \bar{C}_\alpha^2 \bar{f}_\alpha d\bar{C}_\alpha.$$

The other higher-order moments are constructed in a similar way as in the single gas (see eqs. (2) and (3)), but using velocities \bar{C}_α . Also, $\bar{f}_0^{(\alpha)}$, the equilibrium distribution function for constituent α is analogous to the equilibrium distribution function for a single gas (see eq. (4)), but based on diffusive moments and velocity \bar{C}_α .

The Boltzmann equation for a mixture of M gases can easily be written as

$$\frac{D\bar{f}_\alpha}{Dt} + \bar{C}_j^{(\alpha)} \frac{\partial \bar{f}_\alpha}{\partial x_j} + F_j \frac{\partial \bar{f}_\alpha}{\partial \bar{C}_j^{(\alpha)}} = \sum_{\beta=1}^M \int (\bar{f}'_\alpha \bar{f}'_\beta - \bar{f}_\alpha \bar{f}_\beta) \bar{g}_{\alpha\beta} b db d\epsilon d\bar{C}_\beta, \quad (11)$$

where $\frac{D}{Dt} \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$ is the material derivative and $\bar{g}_{\alpha\beta} = \bar{C}_\alpha - \bar{C}_\beta = \mathbf{c}_\alpha - \mathbf{c}_\beta = \mathbf{g}_{\alpha\beta}$. The general production term for a mixture of M gases is given by

$$\mathcal{P}_{i_1 \dots i_n}^{a(\alpha)} = m_\alpha \sum_{\beta=1}^M \int \int \int_0^{2\pi} \int_0^\infty \left\{ (\bar{C}'_\alpha)^{2a} \bar{C}'_{i_1} \dots \bar{C}'_{i_n} - \bar{C}_\alpha^{2a} \bar{C}_{i_1} \dots \bar{C}_{i_n} \right\} \bar{f}_\alpha \bar{f}_\beta \bar{g}_{\alpha\beta} b db d\epsilon d\bar{C}_\alpha d\bar{C}_\beta. \quad (12)$$

Similar to a simple gas, multiplying the Boltzmann equation (11) with $\psi = \{m_\alpha, m_\alpha \bar{C}_i^{(\alpha)}, \frac{1}{2} m_\alpha \bar{C}_\alpha^2, m_\alpha \bar{C}_{i_1}^{(\alpha)} \bar{C}_{i_2}^{(\alpha)}, \frac{1}{2} m_\alpha \bar{C}_\alpha^2 \bar{C}_i^{(\alpha)}, m_\alpha \bar{C}_{i_1}^{(\alpha)} \bar{C}_{i_2}^{(\alpha)} \bar{C}_k^{(\alpha)}, m_\alpha \bar{C}_\alpha^2 \bar{C}_{i_1}^{(\alpha)} \bar{C}_{i_2}^{(\alpha)}, m_\alpha \bar{C}_\alpha^4\}$ and integrating over \bar{C}_α , we get the moment equations for 26 field variables: $\{\rho_\alpha, \rho_\alpha u_i^{(\alpha)}, \frac{3}{2} \rho_\alpha \bar{\theta}_\alpha, \bar{\sigma}_{ij}^{(\alpha)}, \bar{q}_i^{(\alpha)}, \bar{m}_{ijk}^{(\alpha)}, \bar{u}_{ij}^{1(\alpha)}, \bar{\Delta}^{(\alpha)}\}$. Again, the system of 26-moment equations is closed by approximating the phase density \bar{f}_α with Grad's 26-moment distribution function, which reads

$$\begin{aligned} \bar{f}_{|26}^{(\alpha)} = \bar{f}_0^{(\alpha)} & \left\{ 1 + \frac{\bar{\Delta}^{(\alpha)}}{8\rho_\alpha \bar{\theta}_\alpha^2} \left(1 - \frac{2\bar{C}_\alpha^2}{3\bar{\theta}_\alpha} + \frac{1}{15} \frac{\bar{C}_\alpha^4}{\bar{\theta}_\alpha^2} \right) + \frac{1}{5} \frac{\bar{q}_i^{(\alpha)} \bar{C}_i^{(\alpha)}}{\rho_\alpha \bar{\theta}_\alpha^2} \left(\frac{\bar{C}_\alpha^2}{\bar{\theta}_\alpha} - 5 \right) - \frac{1}{2} \frac{u_i^{(\alpha)} \bar{C}_i^{(\alpha)}}{\bar{\theta}_\alpha} \left(\frac{\bar{C}_\alpha^2}{\bar{\theta}_\alpha} - 7 \right) \right. \\ & \left. + \frac{\bar{\sigma}_{ij}^{(\alpha)}}{2\rho_\alpha \bar{\theta}_\alpha^2} \bar{C}_{i_1}^{(\alpha)} \bar{C}_{i_2}^{(\alpha)} + \left(\frac{\bar{u}_{ij}^{1(\alpha)} - 7\bar{\theta}_\alpha \bar{\sigma}_{ij}^{(\alpha)}}{28\rho_\alpha \bar{\theta}_\alpha^3} \right) \bar{C}_{i_1}^{(\alpha)} \bar{C}_{i_2}^{(\alpha)} \left(\frac{\bar{C}_\alpha^2}{\bar{\theta}_\alpha} - 7 \right) + \frac{\bar{m}_{ijk}^{(\alpha)}}{6\rho_\alpha \bar{\theta}_\alpha^3} \bar{C}_{i_1}^{(\alpha)} \bar{C}_{i_2}^{(\alpha)} \bar{C}_{i_3}^{(\alpha)} \right\}. \quad (13) \end{aligned}$$

The procedure for evaluating the production terms is described in the next section.

PROCEDURE

Simple Gas

The general production term $\mathcal{P}_{i_1 \dots i_n}^a$ can easily be written in terms of $P_{i_1 \dots i_n}$, which is given by

$$P_{i_1 \dots i_n} = m \int \int \int_0^{2\pi} \int_0^\infty (C'_{i_1} C'_{i_2} \dots C'_{i_n} - C_{i_1} C_{i_2} \dots C_{i_n}) f f_1 g b db d\epsilon d\mathbf{c} d\mathbf{c}_1. \quad (14)$$

Therefore, we shall show how to evaluate $P_{i_1 \dots i_n}$ instead of $\mathcal{P}_{i_1 \dots i_n}^a$.

With the help of relation between pre-collisional and post-collisional velocities, and the definition of peculiar velocity, one can write $C'_i = C_i - k_i g \cos \Theta$, where Θ is the angle between the contact vector \mathbf{k} and the relative velocity \mathbf{g} . Thus, eq. (14) can be written as

$$P_{i_1 \dots i_n} = m \sum_{\beta=1}^n (-1)^\beta \binom{n}{\beta} \int \int \left(\int_0^{2\pi} \int_0^\infty k_{i_1} \dots k_{i_\beta} \cos^\beta \Theta g b db d\epsilon \right) g^\beta C_{i_{\beta+1}} \dots C_{i_n} f f_1 d\mathbf{C} d\mathbf{C}_1,$$

where the indices in round brackets denote the symmetric part of the tensor. The integrals over b and ϵ simplify to

$$I_{i_1 \dots i_\beta} = \int_0^{2\pi} \int_0^\infty k_{i_1} \dots k_{i_\beta} \cos^\beta \Theta g b db d\epsilon = \sum_{\gamma=0}^{\frac{\beta}{2}} a_\gamma^{(\beta)}(g) \delta_{i_1 i_2} \dots \delta_{i_{2\gamma-1} i_{2\gamma}} \frac{g_{i_{2\gamma+1}}}{g} \dots \frac{g_{i_\beta}}{g}$$

with scalar coefficients $a_\gamma^{(\beta)}$ depending only on the relative speed g . This expression finally unveils the tensorial structure of the production term. We have

$$P_{i_1 \dots i_n} = m \sum_{\beta=1}^n \sum_{\gamma=0}^{\frac{\beta}{2}} (-1)^\beta \binom{n}{\beta} \delta_{i_1 i_2} \dots \delta_{i_{2\gamma-1} i_{2\gamma}} \int \int a_\gamma^{(\beta)}(g) g^{2\gamma} g_{i_{2\gamma+1}} \dots g_{i_\beta} C_{i_{\beta+1}} \dots C_{i_n} f f_1 d\mathbf{C} d\mathbf{C}_1, \quad (15)$$

where all collision aspects are hidden in the coefficients $a_\gamma^{(\beta)}$. Eq. (15) is the starting point in the Mathematica program.

Next, the integrations over velocities \mathbf{C} and \mathbf{C}_1 are performed by transforming these velocities to the relative velocity $\mathbf{g} = \mathbf{C} - \mathbf{C}_1$ and the velocity of the center of mass $\mathbf{h} = (\mathbf{C} + \mathbf{C}_1)/2$. The specific form of Grad's distribution function (8) makes it simple to separate the integrals—one over \mathbf{g} and the other over \mathbf{h} . The precise expressions of the integrals are involved as the velocity transformation acts both on the products of C_i 's and in both the distribution functions of type (8). However, any single integral over \mathbf{h} occurring in the expression will have the following form and the integration results into a combination of delta tensors.

$$\begin{aligned} \int h^{2n} h_{i_1} \cdots h_{i_p} \exp\left(-\frac{h^2}{\theta}\right) d\mathbf{h} &= \int_0^\infty h^{2n+p+2} \exp\left(-\frac{h^2}{\theta}\right) dh \cdot \int_0^{2\pi} \int_0^\pi n_{i_1} \cdots n_{i_p} \sin \vartheta d\vartheta d\varphi \\ &= \frac{1}{2} \theta^{\frac{2n+p+3}{2}} \Gamma\left(\frac{2n+p+3}{2}\right) \cdot \frac{4\pi}{p+1} \delta_{i_1 \cdots i_p}, \end{aligned}$$

where $n_i = h_i/h = \{\sin \vartheta \cos \varphi, \sin \vartheta \sin \varphi, \cos \vartheta\}_i$ are the components of the direction vectors and $\delta_{i_1 \cdots i_p}$ is a fully symmetrized product of Kronecker deltas with in total p indices (p is even); the above integral vanishes when p is odd. The Mathematica program [12] scans through the transformed equation obtained from eq. (15), identifies the powers of h (e.g., $2n$ in h^{2n}) and the indices in the vectorial part $h_{i_1} \cdots h_{i_p}$, and replaces the integral by the expression above. In the integral over \mathbf{g} , only the vectorial part can be evaluated; the scalar part remains in the form of integral due to the unknown coefficients $a_\gamma^{(\beta)}(g)$. The coefficients $a_\gamma^{(\beta)}(g)$ will be absorbed into $\Omega^{(l,r)}$ expressions, which are defined by

$$\Omega^{(l,r)} = \int_0^\infty \int_0^\pi (1 - \cos^l \chi) \gamma^{2r+3} \exp(-\gamma^2) B(2\sqrt{\theta}\gamma, \chi) \sin \chi d\chi d\gamma, \quad (16)$$

where $\gamma = g/(2\sqrt{\theta})$ is dimensionless speed and $\chi = \pi - 2\Theta$ is the scattering angle [4]. The Mathematica program identifies the vectorial part and replaces it with a combination of delta tensors (similar as in vectorial integral over \mathbf{h}) and writes the final remaining scalar integrals over g in terms of $\Omega^{(l,r)}$ expressions. For a specific potential, e.g., for HS or for Maxwellian potential, $\Omega^{(l,r)}$ expressions are known and the integrals over g can also be performed.

The vectorial integrals introduce combinations of Kronecker deltas which contract the tensors involved in the product of moments in every term. Note that the software Mathematica does not handle tensor manipulations *per se*, instead, we provide a corresponding tensor framework in [12].

Granular Gas

The procedure to evaluate the production terms for a granular gas is also similar to that for a simple gas. The few key points to evaluate the production terms are listed below. Similar to a simple gas, we shall evaluate

$$P_{i_1 \cdots i_n} = \frac{m d^2}{4} \int_0^{2\pi} \int_0^\pi \int_0^\pi (C'_{i_1} \cdots C'_{i_n} - C_{i_1} \cdots C_{i_n}) f f_1 g \sin \chi d\chi d\epsilon d\mathbf{C} d\mathbf{C}_1 \quad (17)$$

instead of $\mathcal{P}_{i_1 \cdots i_n}^a$. The raw form of $P_{i_1 \cdots i_n}$, in this case, is

$$P_{i_1 \cdots i_n} = \frac{m d^2}{4} \sum_{\beta=1}^n w_0^\beta \binom{n}{\beta} \int \int \left(\int_0^{2\pi} \int_0^\pi k_{(i_1} \cdots k_{i_\beta} \cos^\beta \Theta g \sin \chi d\chi d\epsilon \right) g^\beta C_{i_{\beta+1}}^{(1)} \cdots C_{i_n}^{(1)} f f_1 d\mathbf{C} d\mathbf{C}_1,$$

where $w_0 = (1 + e)/2$. The rest of the procedure is same as that for a simple gas.

Binary Mixture of Gases

The procedure to evaluate the production terms for a binary mixture of gases is similar to that for a simple gas, only the notations are different. The few key points to evaluate the production terms are listed below. Similar to a simple gas, we shall evaluate

$$P_{i_1 \dots i_n}^{(\alpha)} = m_\alpha \int \int \int_0^{2\pi} \int_0^\infty \left(\overline{C}_{i_1}^{(\alpha)} \dots \overline{C}_{i_n}^{(\alpha)} - \overline{C}_{i_1}^{(\alpha)} \dots \overline{C}_{i_n}^{(\alpha)} \right) \overline{f}_\alpha \overline{f}_\beta \overline{g}_{\alpha\beta} b db d\epsilon d\overline{C}_\alpha d\overline{C}_\beta \quad (18)$$

instead of evaluating $\mathcal{P}_{i_1 \dots i_n}^{(\alpha)}$. Note that this would only give the contribution due to collision of an α particle with a β particle; the contribution due to collision between two α particles (i.e., the other term in the summation) is evaluated by replacing β with α in the finally obtained value of $P_{i_1 \dots i_n}$. The raw form of $P_{i_1 \dots i_n}$, in this case, is

$$P_{i_1 \dots i_n}^{(\alpha)} = m_\alpha \sum_{\kappa=1}^n (-1)^\kappa w_0^\kappa \binom{n}{\kappa} \int \int \left(\int_0^{2\pi} \int_0^\infty k_{i_1}^{(\alpha\beta)} \dots k_{i_\kappa}^{(\alpha\beta)} \cos^\kappa \theta_{\alpha\beta} \overline{g}_{\alpha\beta} b db d\epsilon \right) \overline{g}_{\alpha\beta}^\kappa \overline{C}_{i_{\kappa+1}}^{(\alpha)} \dots \overline{C}_{i_n}^{(\alpha)} \overline{f}_\alpha \overline{f}_\beta d\overline{C}_\alpha d\overline{C}_\beta$$

with $w_0 = 2m_\beta / (m_\alpha + m_\beta)$.

While transforming the velocities \overline{C}_α and \overline{C}_β to $\overline{g}_{\alpha\beta}$ and $\overline{h}_{\alpha\beta}$ in order to make separable integrals, in this case, $\overline{h}_{\alpha\beta}$ is defined as $\overline{h}_{\alpha\beta} = \frac{1}{2} \left(\sqrt{\frac{\theta_\beta}{\theta_\alpha}} \overline{C}_\alpha + \sqrt{\frac{\theta_\alpha}{\theta_\beta}} \overline{C}_\beta \right)$ so that $\frac{\overline{C}_\alpha^2}{2\theta_\alpha} + \frac{\overline{C}_\beta^2}{2\theta_\beta} = \frac{1}{\bar{\theta}} \left(\frac{\overline{g}_{\alpha\beta}^2}{4} + \overline{h}_{\alpha\beta}^2 \right)$ with $\bar{\theta} = \frac{\theta_\alpha + \theta_\beta}{2}$.

Since we are interested in linear production terms, each small field variable (e.g., $u_i^{(\alpha)}$, $\tilde{\sigma}_{ij}^{(\alpha)}$, $\tilde{q}_i^{(\alpha)}$, $\tilde{m}_{ijk}^{(\alpha)}$, $\tilde{u}_{ij}^{1(\alpha)}$, $\tilde{\Delta}^{(\alpha)}$) in the Grad's 26-moment distribution function (13) is multiplied with a small parameter ε before substituting the distribution function (13) into the production term. All the higher-order terms (terms of order ε^2 , ε^3 etc.) in the product $\overline{f}_\alpha \overline{f}_\beta$ and at any stage in the evaluation are neglected. The temperature difference $\overline{T}_\alpha - \overline{T}_\beta$ is also a small quantity, therefore using the relations $\bar{\theta} = \frac{\theta_\alpha + \theta_\beta}{2}$ and $\Delta\theta = \frac{m_\alpha}{m_\alpha + m_\beta} \bar{\theta}_\alpha - \frac{m_\beta}{m_\alpha + m_\beta} \bar{\theta}_\beta = \frac{k}{m_\alpha + m_\beta} (\overline{T}_\alpha - \overline{T}_\beta)$, $\bar{\theta}_\alpha$ and $\bar{\theta}_\beta$ are finally replaced by $\frac{2m_\beta}{m_\alpha + m_\beta} \bar{\theta} + \varepsilon \Delta\theta$ and $\frac{2m_\alpha}{m_\alpha + m_\beta} \bar{\theta} - \varepsilon \Delta\theta$, respectively, and the higher-order terms in ε are neglected to make the complete linearization. In the final expression, ε is replaced by 1.

RESULTS

Simple Gas

For simplicity, we shall use the abbreviations: $u_{ij}^1 - 7\theta\sigma_{ij} = R_{ij}$, $\tilde{\sigma}_{ij} = \frac{\sigma_{ij}}{\rho\theta}$, $\tilde{q}_i = \frac{q_i}{\rho\theta^{3/2}}$, $\tilde{m}_{ijk} = \frac{m_{ijk}}{\rho\theta^{3/2}}$, $\tilde{R}_{ij} = \frac{R_{ij}}{\rho\theta^2}$, $\tilde{\Delta} = \frac{\Delta}{\rho\theta^2}$, and $\frac{16}{5m} \sqrt{\pi} \rho^2 d^2 \sqrt{\theta} = \rho\nu = \bar{\nu}$. Note that ν has the dimensions of collision frequency. Thus, the non-linear production terms in the 26-moment equations for a simple gas with HS, using Mathematica, turned out to be the following, along with $\mathcal{P}^0 = \mathcal{P}_i^0 = \mathcal{P}^1 = 0$.

$$\begin{aligned} \mathcal{P}_{ij}^0 &= -\bar{\nu}\theta \left(1 - \frac{\tilde{\Delta}}{480} \right) \tilde{\sigma}_{ij} - \frac{1}{28} \bar{\nu}\theta \left(1 + \frac{\tilde{\Delta}}{160} \right) \tilde{R}_{ij} \\ &\quad - \bar{\nu}\theta \left(\frac{1}{14} \tilde{\sigma}_{k(i} \tilde{\sigma}_{j)k} + \frac{1}{100} \tilde{q}_{(i} \tilde{q}_{j)} + \frac{1}{504} \tilde{m}_{kl(i} \tilde{m}_{j)kl} + \frac{3}{10976} \tilde{R}_{k(i} \tilde{R}_{j)k} - \frac{1}{196} \tilde{\sigma}_{k(i} \tilde{R}_{j)k} + \frac{1}{140} \tilde{m}_{ijk} \tilde{q}_k \right), \\ \frac{1}{2} \mathcal{P}_i^1 &= -\frac{2}{3} \bar{\nu}\theta^{3/2} \left(1 + \frac{\tilde{\Delta}}{480} \right) \tilde{q}_i - \bar{\nu}\theta^{3/2} \left(\frac{1}{10} \tilde{q}_j \tilde{\sigma}_{ij} - \frac{1}{840} \tilde{q}_j \tilde{R}_{ij} - \frac{1}{42} \tilde{m}_{ijk} \tilde{\sigma}_{jk} + \frac{1}{588} \tilde{m}_{ijk} \tilde{R}_{jk} \right), \\ \mathcal{P}_{ijk}^0 &= -\frac{3}{2} \bar{\nu}\theta^{3/2} \left(1 - \frac{\tilde{\Delta}}{1120} \right) \tilde{m}_{ijk} + \bar{\nu}\theta^{3/2} \left(\frac{3}{140} \tilde{q}_{(i} \tilde{\sigma}_{j)k} - \frac{3}{560} \tilde{q}_{(i} \tilde{R}_{j)k} - \frac{3}{28} \tilde{\sigma}_{l(i} \tilde{m}_{j)kl} + \frac{1}{784} \tilde{R}_{l(i} \tilde{m}_{j)kl} \right), \\ \mathcal{P}_{ij}^1 &= -\frac{15}{2} \bar{\nu}\theta^2 \left(1 - \frac{\tilde{\Delta}}{21600} \right) \tilde{\sigma}_{ij} - \frac{247}{168} \bar{\nu}\theta^2 \left(1 + \frac{\tilde{\Delta}}{1824} \right) \tilde{R}_{ij} \\ &\quad - \bar{\nu}\theta^2 \left(\frac{107}{84} \tilde{\sigma}_{k(i} \tilde{\sigma}_{j)k} - \frac{47}{600} \tilde{q}_{(i} \tilde{q}_{j)} - \frac{29}{1008} \tilde{m}_{kl(i} \tilde{m}_{j)kl} - \frac{19}{65856} \tilde{R}_{k(i} \tilde{R}_{j)k} + \frac{107}{1176} \tilde{\sigma}_{k(i} \tilde{R}_{j)k} + \frac{19}{120} \tilde{m}_{ijk} \tilde{q}_k \right), \\ \mathcal{P}^2 &= -\frac{2}{3} \bar{\nu}\theta^2 \left(1 + \frac{\tilde{\Delta}}{480} \right) \tilde{\Delta} - \bar{\nu}\theta^2 \left(\frac{2}{3} \tilde{\sigma}_{ij} \tilde{\sigma}_{ij} + \frac{4}{15} \tilde{q}_i \tilde{q}_i - \frac{1}{21} \tilde{m}_{ijk} \tilde{m}_{ijk} + \frac{1}{1176} \tilde{R}_{ij} \tilde{R}_{ij} + \frac{1}{21} \tilde{\sigma}_{ij} \tilde{R}_{ij} \right). \end{aligned}$$

Granular Gas

Using the same abbreviations as in the case of a simple gas, the non-linear production terms in the 26-moment equations for a granular gas with HS, using Mathematica, turned out to be the following, along with $\mathcal{P}^0 = \mathcal{P}_i^0 = 0$.

$$\frac{1}{2}\mathcal{P}^1 = -(1-e^2)\bar{\nu}\theta\left(\frac{5}{8} + \frac{\tilde{\Delta}}{128} + \frac{\tilde{\Delta}^2}{40960} + \frac{1}{64}\tilde{\sigma}_{ij}\tilde{\sigma}_{ij} + \frac{1}{320}\tilde{q}_i\tilde{q}_i + \frac{1}{2688}\tilde{m}_{ijk}\tilde{m}_{ijk} + \frac{3}{50176}\tilde{R}_{ij}\tilde{R}_{ij} - \frac{1}{896}\tilde{\sigma}_{ij}\tilde{R}_{ij}\right),$$

$$\mathcal{P}_{ij}^0 = -\frac{(1+e)(3-e)}{4}\bar{\nu}\theta\left[\left(1 - \frac{\tilde{\Delta}}{480}\right)\tilde{\sigma}_{ij} + \frac{1}{28}\left(1 + \frac{\tilde{\Delta}}{160}\right)\tilde{R}_{ij} + \frac{1}{14}\tilde{\sigma}_{k\langle i}\tilde{\sigma}_{j\rangle k} + \frac{1}{100}\tilde{q}_{\langle i}\tilde{q}_{j\rangle} + \frac{1}{504}\tilde{m}_{kl\langle i}\tilde{m}_{j\rangle kl}\right. \\ \left. + \frac{3}{10976}\tilde{R}_{k\langle i}\tilde{R}_{j\rangle k} - \frac{1}{196}\tilde{\sigma}_{k\langle i}\tilde{R}_{j\rangle k} + \frac{1}{140}\tilde{m}_{ijk}\tilde{q}_k\right],$$

$$\frac{1}{2}\mathcal{P}_i^1 = -(1+e)\bar{\nu}\theta^{3/2}\left[\left(\frac{49-33e}{48} + \frac{(19-3e)\tilde{\Delta}}{23040}\right)\tilde{q}_i\right. \\ \left. + \left(\frac{7+e}{160}\right)\tilde{q}_j\tilde{\sigma}_{ij} + \left(\frac{13-21e}{13440}\right)\tilde{q}_j\tilde{R}_{ij} + \left(\frac{11-27e}{1344}\right)\tilde{m}_{ijk}\tilde{\sigma}_{jk} + \left(\frac{23+9e}{37632}\right)\tilde{m}_{ijk}\tilde{R}_{jk}\right],$$

$$\mathcal{P}_{ijk}^0 = -\frac{(1+e)(3-e)}{4}\bar{\nu}\theta^{3/2}\left[\frac{3}{2}\left(1 - \frac{\tilde{\Delta}}{1120}\right)\tilde{m}_{ijk} - \frac{3}{140}\tilde{q}_{\langle i}\tilde{\sigma}_{j\rangle k} + \frac{3}{560}\tilde{q}_{\langle i}\tilde{R}_{j\rangle k} + \frac{3}{28}\tilde{\sigma}_{l\langle i}\tilde{m}_{j\rangle kl} - \frac{1}{784}\tilde{R}_{l\langle i}\tilde{m}_{j\rangle kl}\right],$$

$$\mathcal{P}_{ij}^1 = -(1+e)\bar{\nu}\theta^2\left[\left(\frac{(87-54e+22e^2-10e^3)}{12} - \frac{(55-18e-66e^2+30e^3)\tilde{\Delta}}{5760}\right)\tilde{\sigma}_{ij}\right. \\ \left. + \left(\frac{(499-288e+66e^2-30e^3)}{336} + \frac{(137-36e-66e^2+30e^3)\tilde{\Delta}}{161280}\right)\tilde{R}_{ij} + \frac{(44+27e+66e^2-30e^3)}{168}\tilde{\sigma}_{k\langle i}\tilde{\sigma}_{j\rangle k}\right. \\ \left. + \frac{(4-15e-66e^2+30e^3)}{1200}\tilde{q}_{\langle i}\tilde{q}_{j\rangle} + \frac{(28-45e-22e^2+10e^3)}{2016}\tilde{m}_{kl\langle i}\tilde{m}_{j\rangle kl}\right. \\ \left. + \frac{(116-99e-66e^2+30e^3)}{131712}\tilde{R}_{k\langle i}\tilde{R}_{j\rangle k} + \frac{(44+27e+66e^2-30e^3)}{2352}\tilde{\sigma}_{k\langle i}\tilde{R}_{j\rangle k} + \frac{(169-66e^2+30e^3)}{1680}\tilde{m}_{ijk}\tilde{q}_k\right],$$

$$\mathcal{P}^2 = -(1+e)\bar{\nu}\theta^2\left[\frac{5(1-e)(9+2e^2)}{4} + \frac{(271-207e+30e^2-30e^3)}{192}\tilde{\Delta} + \frac{(137-9e-30e^2+30e^3)}{184320}\tilde{\Delta}^2\right. \\ \left. + \frac{(23+9e+30e^2-30e^3)}{96}\tilde{\sigma}_{ij}\tilde{\sigma}_{ij} + \frac{(61+3e-30e^2+30e^3)}{480}\tilde{q}_i\tilde{q}_i + \frac{(7-39e-10e^2+10e^3)}{1344}\tilde{m}_{ijk}\tilde{m}_{ijk}\right. \\ \left. + \frac{(113-81e-30e^2+30e^3)}{75264}\tilde{R}_{ij}\tilde{R}_{ij} + \frac{(23+9e+30e^2-30e^3)}{1344}\tilde{\sigma}_{ij}\tilde{R}_{ij}\right].$$

Binary Mixture of Gases

To get the moment equations for binary mixture in a nice form, we rewrite the moment equations in terms of new variables $\hat{\sigma}_{ij}^{(\alpha)} = \bar{\sigma}_{ij}^{(\alpha)}/\rho_\alpha$, $\hat{q}_i^{(\alpha)} = \bar{q}_i^{(\alpha)}/\rho_\alpha$, $\hat{m}_{ijk}^{(\alpha)} = \bar{m}_{ijk}^{(\alpha)}/\rho_\alpha$, $\hat{u}_{ij}^{1(\alpha)} = \bar{u}_{ij}^{1(\alpha)}/\rho_\alpha$ and $\hat{\Delta}^{(\alpha)} = \bar{\Delta}^{(\alpha)}/\rho_\alpha$. For simplicity, we shall use the abbreviations: $\hat{q}_i^{(\alpha)} - \frac{5}{2}\bar{\theta}_\alpha u_i^{(\alpha)} = \hat{h}_i^{(\alpha)}$, $\hat{u}_{ij}^{1(\alpha)} - 7\bar{\theta}_\alpha \hat{\sigma}_{ij}^{(\alpha)} = \hat{R}_{ij}^{(\alpha)}$, $\mu_k = m_k/(m_\alpha + m_\beta)$ for $k = \alpha, \beta$, $d_{\alpha\beta} = \frac{1}{2}(d_\alpha + d_\beta)$, $\frac{16}{5}\sqrt{\pi}m_\alpha n_\alpha^2 d_\alpha^2 \sqrt{\bar{\theta}_\alpha} = \rho_\alpha \nu_\alpha = \bar{\nu}_\alpha$ and $\frac{16}{5}\sqrt{\pi}\frac{2m_\alpha m_\beta}{m_\alpha + m_\beta} n_\alpha n_\beta d_{\alpha\beta}^2 \sqrt{\bar{\theta}} = \frac{\rho_\alpha \rho_\beta}{\rho_\alpha + \rho_\beta} \nu_{\alpha\beta} = \bar{\nu}_{\alpha\beta}$. Note that ν_α and $\nu_{\alpha\beta}$ have the dimensions of collision frequency. Thus, the corresponding linear production terms in the 26-moment equations for a binary mixture of gases with HS, using Mathematica, turned out to be the following, along with $\mathcal{P}^0 = 0$.

$$\mathcal{P}_i^{0(\alpha)} = -\bar{\nu}_{\alpha\beta}\left\{\frac{5}{6}\left(u_i^{(\alpha)} - u_i^{(\beta)}\right) + \frac{1}{12\bar{\theta}}\left(\hat{h}_i^{(\alpha)} - \hat{h}_i^{(\beta)}\right)\right\},$$

$$\frac{1}{2}\mathcal{P}^{1(\alpha)} = -\frac{1}{24\bar{\theta}}\bar{\nu}_{\alpha\beta}(\mu_\alpha - \mu_\beta)\hat{\Delta}^{(\alpha)} - \frac{1}{24\bar{\theta}}\bar{\nu}_{\alpha\beta}\mu_\beta\left(\hat{\Delta}^{(\alpha)} - \hat{\Delta}^{(\beta)}\right) - \frac{5}{2}\bar{\nu}_{\alpha\beta}(\mu_\alpha\bar{\theta}_\alpha - \mu_\beta\bar{\theta}_\beta),$$

$$\begin{aligned}\mathcal{P}_{ij}^{0(\alpha)} = & -(\bar{\nu}_\alpha + \bar{\nu}_{\alpha\beta})\left\{\hat{\sigma}_{ij}^{(\alpha)} + \frac{1}{28\bar{\theta}}\hat{R}_{ij}^{(\alpha)}\right\} - \bar{\nu}_{\alpha\beta}(\mu_\alpha - \mu_\beta)\left\{\frac{2}{3}\hat{\sigma}_{ij}^{(\alpha)} + \frac{1}{21\bar{\theta}}\hat{R}_{ij}^{(\alpha)}\right\} \\ & - \bar{\nu}_{\alpha\beta}\mu_\beta\left\{\frac{2}{3}\left(\hat{\sigma}_{ij}^{(\alpha)} - \hat{\sigma}_{ij}^{(\beta)}\right) + \frac{1}{21\bar{\theta}}\left(\hat{R}_{ij}^{(\alpha)} - \hat{R}_{ij}^{(\beta)}\right)\right\},\end{aligned}$$

$$\begin{aligned}\frac{1}{2}\mathcal{P}_i^{1(\alpha)} = & -\frac{2}{3}(\bar{\nu}_\alpha + \bar{\nu}_{\alpha\beta})\hat{h}_i^{(\alpha)} - \frac{11}{6}\bar{\nu}_{\alpha\beta}(\mu_\alpha - \mu_\beta)\hat{h}_i^{(\alpha)} \\ & - \bar{\nu}_{\alpha\beta}\mu_\beta\left\{\frac{1}{12}(5\mu_\alpha + 32\mu_\beta)\left(\hat{h}_i^{(\alpha)} - \hat{h}_i^{(\beta)}\right) + \frac{5}{6}(5\mu_\alpha + 6\mu_\beta)\bar{\theta}\left(u_i^{(\alpha)} - u_i^{(\beta)}\right)\right\},\end{aligned}$$

$$\mathcal{P}_{ijk}^{0(\alpha)} = -\frac{3}{2}(\bar{\nu}_\alpha + \bar{\nu}_{\alpha\beta})\hat{m}_{ijk}^{(\alpha)} - \bar{\nu}_{\alpha\beta}(\mu_\alpha - \mu_\beta)\hat{m}_{ijk}^{(\alpha)} - \frac{9}{14}\bar{\nu}_{\alpha\beta}\mu_\beta^2\left(\hat{m}_{ijk}^{(\alpha)} - \hat{m}_{ijk}^{(\beta)}\right),$$

$$\begin{aligned}\mathcal{P}_{ij}^{1(\alpha)} = & -(\bar{\nu}_\alpha + \bar{\nu}_{\alpha\beta})\left\{\frac{15}{2}\bar{\theta}\hat{\sigma}_{ij}^{(\alpha)} + \frac{247}{168}\hat{R}_{ij}^{(\alpha)}\right\} \\ & - \bar{\nu}_{\alpha\beta}(\mu_\alpha - \mu_\beta)\left\{-\frac{1}{6}(45\mu_\alpha^2 + 40\mu_\alpha\mu_\beta - 21\mu_\beta^2)\bar{\theta}\hat{\sigma}_{ij}^{(\alpha)} + \frac{1}{168}(313\mu_\alpha^2 + 384\mu_\alpha\mu_\beta + 551\mu_\beta^2)\hat{R}_{ij}^{(\alpha)}\right\} \\ & - \bar{\nu}_{\alpha\beta}\mu_\beta^2\left\{\frac{4}{3}(7\mu_\alpha + 9\mu_\beta)\bar{\theta}\left(\hat{\sigma}_{ij}^{(\alpha)} - \hat{\sigma}_{ij}^{(\beta)}\right) + \frac{2}{21}(7\mu_\alpha + 37\mu_\beta)\left(\hat{R}_{ij}^{(\alpha)} - \hat{R}_{ij}^{(\beta)}\right)\right\},\end{aligned}$$

$$\begin{aligned}\mathcal{P}^{2(\alpha)} = & -\frac{2}{3}(\bar{\nu}_\alpha + \bar{\nu}_{\alpha\beta})\hat{\Delta}^{(\alpha)} - \frac{1}{3}\bar{\nu}_{\alpha\beta}(\mu_\alpha - \mu_\beta)(8\mu_\alpha^2 + 15\mu_\alpha\mu_\beta + 22\mu_\beta^2)\hat{\Delta}^{(\alpha)} \\ & - \frac{5}{3}\bar{\nu}_{\alpha\beta}\mu_\beta^2(\mu_\alpha + 4\mu_\beta)\left(\hat{\Delta}^{(\alpha)} - \hat{\Delta}^{(\beta)}\right) - 20\bar{\nu}_{\alpha\beta}\mu_\beta(5\mu_\alpha + 6\mu_\beta)\bar{\theta}(\mu_\alpha\bar{\theta}_\alpha - \mu_\beta\bar{\theta}_\beta).\end{aligned}$$

CONCLUSIONS

Based on Grad's distribution function with 26 moments, we presented the non-linear production terms for a simple gas and a granular gas, and the linear production terms for a binary mixture of gases, all with HS.

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