

Hydrodynamics of binary mixtures of granular gases with stochastic coefficient of restitution

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(Received ?; revised ?; accepted ?. - To be entered by editorial office)

A hydrodynamic description of dilute binary gas mixtures comprising smooth inelastic spheres interacting by binary collisions with a random coefficient of restitution is presented. Constitutive relations are derived using the Chapman-Enskog perturbative method, associated with a computer-aided method to allow high order Sonine polynomial expansions. The transport coefficients obtained are checked against DSMC simulations. The resulting equations are applied to the analysis of a vertically vibrated system. It is shown that differences in the shape of the distributions of coefficient of restitution are sufficient to produce partial segregation.

1. Introduction

Granular materials, i.e. collections of macroscopic solid grains, are ubiquitous in Nature and of central importance in industry. They exhibit a fascinating and often counter-intuitive range of phenomena, behaving at times like solids (when at rest), liquids, or gases (Goldhirsch (2003); Jaeger *et al.* (1996)). This last regime, characterized by the fact that the grains interact by near-instantaneous binary collisions, is reminiscent of the classical picture of an atomic gas, and Kinetic Theory is expected to provide a reliable description of the kinetics and hydrodynamics of the system. This analogy is of course not complete since the grain interactions are dissipative, this property constituting the source of much of the rich phenomenology exhibited by granular gases (Goldhirsch (2003)): Breaking of scale separation, clustering (Goldhirsch & Zanetti (1993)) and collapse, just to name a few. The dissipative nature of the collisions is standardly taken into account through the introduction of a coefficient of normal restitution, relating the normal component of the relative velocities of the colliding particles at contact before and after collision. The common way of modeling granular gases is to consider them as a collection of hard spheres whose collisions are characterized by a fixed coefficient of restitution. Though detailed analysis and experiments indicate that the coefficient depend on impact velocity (Schwager & Pöschel (1998); Pöschel *et al.* (2003)), the fixed coefficient of restitution has long been recognized to provide a reliable description. An aspect that has however been seldom addressed so far is the fact that even for virtually perfect spheres like ball bearing, significant scatter is observed in experimental measurement of the coefficient of restitution (Lifshitz & Kolsky (1964); Montaine *et al.* (2011)), that can be associated with microscopic surface asperities (Hatzes *et al.* (1988); Montaine *et al.* (2011)). A natural way of taking this scatter into account theoretical is to consider a randomly

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fluctuating coefficient of restitution (Gunkelmann *et al.* (2014)). This type of model was also introduced in other contexts such as to model heating through collisions in a vertically vibrating granular system (Barrat *et al.* (2001); Barrat & Trizac (2003)), to describe a gas of one-dimensional particles accounting for internal degrees of freedom (Giese & Zippelius (1996); Aspelmeier & Zippelius (2000)) and in gases on Maxwellian molecules (Carrillo *et al.* (2009)) to investigate the high velocity tail of the distribution function. However, to our knowledge, no continuum description of such systems has been derived so far. It is the purpose of the present article to fill this gap, and derive a hydrodynamic description of a granular gas with random coefficient of restitution.

This description is achieved here for a binary mixture. In the polydisperse case (which corresponds to the typical situation encountered in Nature and industry), granular gases exhibit a host of specific effects, the most prominent being undoubtedly their tendency to spontaneously segregate under external forcing (Ottino & Khakhar (2000); Shinbrot & Muzzio (2000); Kudrolli (2004); Farkas *et al.* (2002); Rapaport (2001)), as a result of small differences in the properties of their constituents: Mass, shape, frictional (Kondic *et al.* (2003); Ulrich *et al.* (2007)) or inelastic (Serero *et al.* (2006); Brito *et al.* (2008)) properties differences may yield segregation. In the case of dilute granular gases, one of the prominent segregation mechanisms is the Soret effect (Hsiao & Hunt (1996); Schröter *et al.* (2006)) or its single-particle manifestation, thermophoresis, which drives large or massive particles to move down temperature gradients (Goldhirsch & Ronis (1983*a,b*)). Thermal diffusion in mixtures of granular gases has therefore been invoked (Arnarson & Willits (1998); Brey *et al.* (2005); Serero *et al.* (2006); Garzó (2006, 2008); Jenkins & Yoon (2002); Yoon & Jenkins (2006); Trujillo *et al.* (2003)) to obtain segregation criterion in vibrated systems under gravity, and inelasticity was shown to have a direct influence of segregation (Serero *et al.* (2006)): For near-elastic collisions particles with identical mass and size may segregate on the basis of differences in their inelastic properties alone, when subject to a temperature gradient. This was corroborated in molecular dynamics (MD) simulations of vertically vibrated granular gas mixtures (Serero *et al.* (2006); Brito *et al.* (2008)). It is yet another objective of this work to analyze some of the implications of the stochastic nature of the coefficient of restitution, and in particular a similar direct effect of the fluctuations, on the segregation properties of granular gases.

The structure of this paper is as follows. Section 2 provides a description of the system studied below, basic definitions, and provides the kinetic formulation of the problem, as well as the hydrodynamics description of the system. Section 3 describes the method employed to derive the constitutive relation, the computation of the transport coefficients, and presents the computer-aided method we employ for the analysis. In section 4 the results are checked by numerical DSMC simulations. Section 5 presents an application of the results to show the existence of a stochasticity-induced segregation. Finally, Section 6 provides concluding comments. A series of Appendices contains some technical details.

2. Formulation of the problem

Consider a mixture of smooth hard spheres, composed of species A and B , of masses m_A and m_B , and diameters d_A , and d_B . The decay of kinetic energy in a collision is characterized by a coefficient normal restitution e , assumed to be independent of the initial normal relative velocity, defined as the ratio between the postcollisional and precollisional normal relative velocity of the colliding spheres.

The transformation of velocities in a collision between a sphere A and a sphere B

reads:

$$\begin{aligned}\mathbf{v}_1 &= \mathbf{v}'_1 - (1+e)M^{BA}(\mathbf{k} \cdot \mathbf{v}'_{12})\mathbf{k} \\ \mathbf{v}_2 &= \mathbf{v}'_2 + (1+e)M^{AB}(\mathbf{k} \cdot \mathbf{v}'_{12})\mathbf{k}\end{aligned}\quad (2.1)$$

where $M^{\alpha\beta} \equiv \frac{m_\alpha}{m_\alpha+m_\beta}$ for $\{\alpha, \beta\} \in \{A, B\}$, primes denote precollisional velocities, the indices ‘1’ and ‘2’ pertain here to the species A and B , respectively, $\mathbf{v}_{12} \equiv \mathbf{v}_1 - \mathbf{v}_2$, and \mathbf{k} is a unit vector pointing from the center of sphere A to that of sphere B . The standard description of binary mixtures of inelastic gases involves three coefficients of restitution, one for each type of collisions. In the case of fluctuating coefficient of restitution, these have to be replaced by three distributions for e , denoted here $\rho_{AA}(e)$, $\rho_{AB}(e)$, and $\rho_{BB}(e)$. The kinetic description of a binary mixture of dilute gas requires two distribution functions, $f_A(\mathbf{v}, \mathbf{r}, t)$ and $f_B(\mathbf{v}, \mathbf{r}, t)$. Their dynamics is described by a set of two coupled Boltzmann equations:

$$\mathcal{D}f_\alpha \equiv \frac{\partial f_\alpha}{\partial t} + \mathbf{v}_1 \cdot \nabla f_\alpha = \mathcal{B}_{\alpha\alpha}(f_\alpha, f_\alpha, \rho_{\alpha\alpha}) + \mathcal{B}_{\alpha\beta}(f_\alpha, f_\beta, \rho_{\alpha\beta}), \quad (2.2)$$

for $\{\alpha, \beta\} \in \{A, B\}$, with $\alpha \neq \beta$. The Boltzmann operator $\mathcal{B}_{\alpha\beta}(f_\alpha, f_\beta, \rho_{\alpha\beta})$ corresponding to α - β collisions in the case of (impact velocity independent) stochastic coefficient of restitution is a generalization of that defined for mixtures of gas interacting with constant coefficients of restitution (Chapman & Cawling (1970)). Its dependence on the coefficient of restitution is modified to include a functional dependence on the distributions $\rho_{\alpha\beta}(e)$ for the coefficients of restitution, corresponding to an average over the values of e , with a weight given by $\rho_{\alpha\beta}(e)$:

$$\begin{aligned}\mathcal{B}_{\alpha\beta}(f_\alpha, f_\beta, \rho_{\alpha\beta}) &= d_{\alpha\beta}^2 \int \int \int_{\mathbf{v}_{12} \cdot \mathbf{k} > 0} \rho_{\alpha\beta}(e) \left[\frac{f_\alpha(\mathbf{v}'_1) f_\beta(\mathbf{v}'_2)}{e^2} - f_\alpha(\mathbf{v}_1) f_\beta(\mathbf{v}_2) \right] \\ &\quad \times (\mathbf{v}_{12} \cdot \mathbf{k}) \, d\mathbf{v}_2 \, d\mathbf{k} \, de,\end{aligned}\quad (2.3)$$

where $d_{\alpha\beta} \equiv \frac{d_\alpha + d_\beta}{2}$. Here \mathbf{v}_1 and \mathbf{v}'_1 pertain to species α , and \mathbf{v}_2 and \mathbf{v}'_2 pertain to β . From a hydrodynamic point of view, the system is described by a set of fields corresponding to averages of the conserved quantities in collisions, namely the two number densities n_A and n_B (or alternatively the total number density $n \equiv n_A + n_B$ and the concentration $c \equiv \frac{n_A}{n}$ of species A), the velocity \mathbf{V} (or momentum density), which is defined as a mass average of the species’ mean velocities, and the temperature field, T , defined as (twice) the mean fluctuating kinetic energy of a fluid particle. Notice that in the case of inelastic gases, the temperature is not a proper hydrodynamic field, as it corresponds to the mean kinetic energy, which is dissipated in collision. The hydrodynamic fields can be expressed in terms of the distribution function the following way: The number density for species α is given by:

$$n_\alpha = \int f_\alpha(\mathbf{v}) \, d\mathbf{v} \quad (2.4)$$

the corresponding mass density being $\rho_{m_\alpha} = m_\alpha n_\alpha$. The overall number density is $n = n_A + n_B$, and the overall mass density is $\rho_m \equiv \rho_{m_A} + \rho_{m_B}$. The mixture’s velocity field is:

$$\mathbf{V} = \frac{1}{\rho_m} (\rho_{m_A} \mathbf{V}_A + \rho_{m_B} \mathbf{V}_B). \quad (2.5)$$

where \mathbf{V}_α is the velocity field of species α , given by:

$$\mathbf{V}_\alpha = \frac{1}{n_\alpha} \int f_\alpha(\mathbf{v}) \, \mathbf{v} \, d\mathbf{v} \quad (2.6)$$

\mathbf{V}_α is not a hydrodynamic field and it needs to be expressed as a functional of the hydrodynamic fields. The granular temperature of species α is defined by:

$$T_\alpha = \frac{1}{n_\alpha} \int f_\alpha(\mathbf{v}) m_\alpha (\mathbf{v} - \mathbf{V})^2 d\mathbf{v} \quad (2.7)$$

The mixture's granular temperature (average fluctuating kinetic energy multiplied by 2) is defined by:

$$T \equiv \frac{1}{n} (n_A T_A + n_B T_B). \quad (2.8)$$

The equations of motions for the hydrodynamic fields can be readily obtained upon considering moments of the Boltzmann equations (although their validity is not restricted to the range of validity of the latter). Multiplying the Boltzmann equations by 1, $m_\alpha \mathbf{v}$, and $m_\alpha u^2$, integrating, and summing over the species provide kinetic expressions for the particle flux densities, stress tensor, and heat flux. The equation of motion for the number density, n_α , with $\alpha \in \{A, B\}$, is obtained by integrating Eq. (2.2) over velocities::

$$\frac{Dn_\alpha}{Dt} = -\text{div} \mathbf{J}_\alpha - n_\alpha \text{div} \mathbf{V} \quad (2.9)$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + \mathbf{V} \cdot \nabla$ is the material derivative and

$$\mathbf{J}_\alpha = n_\alpha (\mathbf{V}_\alpha - \mathbf{V}) \quad (2.10)$$

is the particle flux density of species α . As \mathbf{V}_α , the velocity field of species α , or equivalently, the flux, \mathbf{J}_α , is not a hydrodynamic field, it must be given by an appropriate constitutive relation. The equation of motion obeyed by the velocity field (in the absence of external force) can be written in the following standard form, obtained by multiplying Eq. (2.2) by $m_\alpha \mathbf{v}$, integrating on velocities, and summing over the two species:

$$\rho_m \frac{DV_i}{Dt} = -\frac{\partial P_{ij}}{\partial x_j} \quad (2.11)$$

The kinetic expression for the stress tensor (in the dilute case, which excludes the collisional contribution) is given by:

$$P_{ij} = m_A \int f_A(\mathbf{v}) u_i u_j d\mathbf{v} + m_B \int f_B(\mathbf{v}) u_i u_j d\mathbf{v}, \quad (2.12)$$

where $\mathbf{u} \equiv \mathbf{v} - \mathbf{V}$ is the peculiar (fluctuating) velocity. The granular temperature field obeys the equation of motion (obtained by integrating (2.2) multiplied by $m_\alpha u^2$ and summing the contributions of the two species), reads:

$$n \frac{DT}{Dt} = T \text{div} \mathbf{J} - \text{div} \mathbf{Q} - 2P_{ij} \frac{\partial V_i}{\partial x_j} - \Gamma, \quad (2.13)$$

where $\mathbf{J} \equiv \mathbf{J}_A + \mathbf{J}_B$ is the total particle flux, \mathbf{Q} the heat flux, given by:

$$\mathbf{Q} = \int f_A(\mathbf{v}) m_A u^2 \mathbf{u} d\mathbf{v} + \int f_B(\mathbf{v}) m_B u^2 \mathbf{u} d\mathbf{v} \quad (2.14)$$

and Γ is the energy sink term, which accounts for the rate of loss of energy due to the inelasticity of the collisions (and therefore vanishes in the elastic limit). It is given by:

$$\Gamma = \Gamma_A + \Gamma_B + \Gamma_{AB} \quad (2.15)$$

The contributions to Γ are:

$$\Gamma_\alpha \equiv \int \int \int \rho_{\alpha\alpha}(e) \frac{(1-e^2) m_\alpha}{8} \pi d_\alpha^2 f_\alpha(\mathbf{v}_1) f_\alpha(\mathbf{v}_2) |v_{12}|^3 d\mathbf{v}_1 d\mathbf{v}_2 de, \quad (2.16)$$

and

$$\Gamma_{AB} \equiv \int \int \int \rho_{AB}(e) \frac{(1-e^2) m_{AB} \pi d_{AB}^2}{2} f_A(\mathbf{v}_1) f_B(\mathbf{v}_2) |\mathbf{v}_{12}|^3 d\mathbf{v}_1 d\mathbf{v}_2 de. \quad (2.17)$$

where $m_{AB} \equiv \frac{m_A m_B}{m_A + m_B}$ is the reduced mass and $d_{AB} = \frac{d_A + d_B}{2}$.

3. Constitutive relations and transport coefficients

3.1. The Chapman-Enskog (CE) expansion

In order to derive the constitutive relation for the fluxes (2.10, 2.12, 2.14) and the sources (2.15), we proceed to solve Eqs. (2.2) by performing a Chapman-Enskog expansion. The latter consists in a perturbative gradient expansion of the distribution function (formally in powers of the Knudsen number) around a reference state corresponding to a homogeneous solution of the Boltzmann equation (the Maxwellian equilibrium distribution function for elastic systems, $f_\alpha^M = n_\alpha \left(\frac{\gamma_\alpha}{\pi}\right)^{\frac{3}{2}} e^{-\gamma_\alpha u^2}$, with $\gamma_\alpha \equiv \frac{3m_\alpha}{2T}$, or the distribution function corresponding to the Homogeneous Cooling State in the present case (Brey *et al.* (1998)), see below). The distribution function is thus written:

$$f_\alpha \equiv f_\alpha^M \phi_\alpha = f_\alpha^M \left(\phi_\alpha^{(0)} + \phi_\alpha^K + \phi_\alpha^{K^2} + \dots \right) \quad (3.1)$$

where ϕ_α denotes the correction to the Maxwellian elastic equilibrium distribution, and the superscripts denote the order of each term in gradient expansion. In addition to the assuming small gradients (or more precisely Knudsen numbers), the CE method relies on the assumption that the dependence of the distribution function on space and time is implicit through its functional dependence on the fields and that there is no additional space or time dependence. In the case at hand the pertinent hydrodynamic fields are n , $c \equiv \frac{n_A}{n}$ (or alternatively n_A and n_B), \mathbf{V} , and T , so that the time derivative $\mathcal{D}f$ in Eqs. (2.2) can be written:

$$\mathcal{D}f_\alpha = \phi_\alpha f_\alpha^M \left[\mathcal{D} \ln n_\alpha + 2\gamma_\alpha u_i \mathcal{D}V_i + \left(\gamma u^2 - \frac{3}{2} \right) \mathcal{D} \ln T \right] + f_\alpha^M \mathcal{D}\phi_\alpha \quad (3.2)$$

The result of the application of the operator \mathcal{D} on any functional of the hydrodynamic fields can thus be in turn expanded in powers of gradients, by making use of the hydrodynamic equations, (2.9), (2.11), (2.13): $\mathcal{D}f = \mathcal{D}^{(0)}f + \mathcal{D}^K f + \dots$, where the subscript identifies the order in expansion. Upon substituting Eq. (3.1) and the expansion of $\mathcal{D}f$ in equation (2.2), and equating the terms of the same order in expansion on both sides of the equation, one obtains a hierarchy of equations.

3.1.1. Zeroth order correction: The Homogeneous Cooling State (HCS)

The homogeneous cooling state (HCS) of a granular gas is defined as a state of vanishing velocity and homogeneous density fields. Considering normal solutions, the distribution functions are rendered ‘time independent’ by scaling the velocities by the thermal speed of the species comprising the mixture, i.e, the distribution is assumed to depend on velocity through the variable $\gamma_\alpha u^2$. Since all gradients vanish in this state, the corresponding distribution function can be taken to serve as the zeroth order in the CE expansion. Using Eqs. (2.9), (2.11) and (2.13), one has: $\mathcal{D}^{(0)} \ln n_\alpha = 0$, $\mathcal{D}^{(0)} V_i = 0$, and $\mathcal{D}^{(0)} \ln T = -\frac{\Gamma}{nT}$. The zeroth order of Eq. (3.2) therefore reads:

$$\mathcal{D}^{(0)} f_\alpha = -f_\alpha^M \left(\gamma_\alpha u^2 \left(\phi_\alpha^{(0)} - \phi_\alpha^{(0)'} \right) - \frac{3}{2} \phi_\alpha^{(0)} \right) \frac{\Gamma}{nT}$$

where prime denotes derivative with respect to $\gamma_\alpha u^2$, and the temperature dependence of $\phi^{(0)}$ through its argument $\gamma_\alpha u^2$ has been taken into account. The two coupled Boltzmann equations (2.2) reduce to the following equations for the corrections $\phi_\alpha^{(0)}$:

$$\begin{aligned} & -f_\alpha^M \left(\gamma_\alpha u^2 \left(\phi_\alpha^{(0)} - \phi_\alpha^{(0)'} \right) - \frac{3}{2} \phi_\alpha^{(0)} \right) \frac{\Gamma}{nT} \\ &= \int \mathcal{B}_{\alpha\alpha} \left(f_\alpha^M \phi_\alpha^{(0)}, f_\alpha^M \phi_\alpha^{(0)}, \rho_{\alpha\alpha}(e), e \right) de + \int \mathcal{B}_{\alpha\beta} \left(f_\alpha^M \phi_\alpha^{(0)}, f_\beta^M \phi_\beta^{(0)}, \rho_{\alpha\beta}(e), e \right) de, \end{aligned} \quad (3.3)$$

where the Boltzmann operator $\mathcal{B}_{\alpha\beta}$ is defined in Eq. (2.3). These equations need to be solved subject to the following constraints:

$$\int f_A d\mathbf{u} = n_A \quad (3.4)$$

$$\int f_B d\mathbf{u} = n_B \quad (3.5)$$

$$\int f_A m_A u^2 d\mathbf{u} + \int f_B m_B u^2 d\mathbf{u} = nT \quad (3.6)$$

which express the fact that the two number densities and the temperature field have to be given by the appropriate moment of the distribution function.

3.1.2. First order correction

Computing the transport coefficients to Navier-Stokes order requires calculating the correction ϕ_α^K corresponding to first order in gradient. Carrying out the procedure described above to first order, one obtains the following expression for ϕ_α^K (Appendix A provides details of the derivation):

$$\begin{aligned} \phi_\alpha^K &= \Phi_\alpha^{K,T} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \cdot \nabla \ln T + \Phi_\alpha^{K,n} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \cdot \nabla \ln n \\ &+ \Phi_\alpha^{K,c} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \cdot \nabla \ln c + \Phi_\alpha^{K,V} (\gamma_\alpha u^2) \gamma_\alpha^{\frac{3}{2}} \overline{\mathbf{u}\mathbf{u}} : \nabla \mathbf{V} \end{aligned} \quad (3.7)$$

where overbar denotes the traceless symmetric part of any second rank tensor, $\mathbf{A}: \overline{A_{ij}} \equiv \frac{1}{2} (A_{ij} + A_{ji} - \frac{2}{3} \delta_{ij} A_{kk})$, and the functions $\Phi_\alpha^{K,T}$, $\Phi_\alpha^{K,c}$, $\Phi_\alpha^{K,n}$ and $\Phi_\alpha^{K,V}$ are isotropic functions of the rescaled peculiar velocity $\gamma_\alpha u^2$, and obey the following set of equations: The function $\Phi_\alpha^{K,V}$ obeys:

$$\begin{aligned} & \left(L_{\alpha\alpha}^{(1)} + L_{\alpha\alpha}^{(2)} + L_{\alpha\beta}^{(1)} \right) \{ \Phi_\alpha^{K,V} (\gamma_\alpha u^2) \gamma_\alpha^{\frac{3}{2}} \overline{\mathbf{u}\mathbf{u}} \} + L_{\alpha\beta}^{(2)} \{ \Phi_\beta^{K,V} (\gamma_\beta u^2) \gamma_\beta^{\frac{3}{2}} \overline{\mathbf{u}\mathbf{u}} \} \\ & - \frac{\sqrt{6\pi}}{9} \frac{nd_{\alpha\beta}^2}{\sqrt{m_0}} \tilde{\Gamma} \sqrt{T} f_\alpha^M \left(\left(\mathcal{H} \{ \Phi_\alpha^{K,V} \} + 3 \right) \Phi_\alpha^{K,V} (\gamma_\alpha u^2) \gamma_\alpha^{\frac{3}{2}} \overline{\mathbf{u}\mathbf{u}} \right) = 2f_\alpha^M \gamma_\alpha \left(\phi_\alpha^{(0)} - \phi_\alpha^{(0)'} \right) \overline{\mathbf{u}\mathbf{u}}, \end{aligned} \quad (3.8)$$

where $m_0 \equiv m_A + m_B$, and $\tilde{\Gamma} \equiv \frac{9}{\sqrt{6\pi}} \frac{\sqrt{m_0}}{n^2 d_{AB}^2 T^{\frac{3}{2}}} \Gamma$, the function $\Phi_\alpha^{K,T}$ obeys:

$$\begin{aligned} & \left(L_{\alpha\alpha}^{(1)} + L_{\alpha\alpha}^{(2)} + L_{\alpha\beta}^{(1)} \right) \{ \Phi_\alpha^{K,T} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \} + L_{\alpha\beta}^{(2)} \{ \Phi_\beta^{K,T} (\gamma_\beta u^2) \sqrt{\gamma_\beta} \mathbf{u} \} \\ & - \frac{\sqrt{6\pi}}{9} \frac{nd_{\alpha\beta}^2}{\sqrt{m_0}} \tilde{\Gamma} \sqrt{T} f_\alpha^M \left(\left(\mathcal{H} \{ \Phi_\alpha^{K,T} \} + \frac{3}{4} \right) \Phi_\alpha^{K,T} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \right) \\ & = f_\alpha^M \left(\left(\gamma_\alpha u^2 - \frac{nm_\alpha}{\rho_m} \right) \left(\phi_\alpha^{(0)} - \phi_\alpha^{(0)'} \right) - \frac{3}{2} \phi_\alpha^{(0)} \right) \mathbf{u} \end{aligned} \quad (3.9)$$

the function $\Phi_\alpha^{K,n}$ obeys:

$$\begin{aligned} & \left(L_{\alpha\alpha}^{(1)} + L_{\alpha\alpha}^{(2)} + L_{\alpha\beta}^{(1)} \right) \{ \Phi_\alpha^{K,n} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \} + L_{\alpha\beta}^{(2)} \{ \Phi_\beta^{K,n} (\gamma_\beta u^2) \sqrt{\gamma_\beta} \mathbf{u} \} \\ & - \frac{\sqrt{6\pi}}{9} \frac{nd_{\alpha\beta}^2}{\sqrt{m_0}} \tilde{\Gamma} \sqrt{T} f_\alpha^M \left((\mathcal{H} \{ \Phi_\alpha^{K,n} \} + 2) \Phi_\alpha^{K,n} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} - \Phi_\alpha^{K,T} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \right) \\ & = f_\alpha^M \left(\phi_\alpha^{(0)} - \frac{nm_\alpha}{\rho_m} \left(\phi_\alpha^{(0)} - \phi_\alpha^{(0)'} \right) \right) \mathbf{u} \end{aligned} \quad (3.10)$$

for $\{\alpha, \beta\} \in \{A, B\}$, with $\alpha \neq \beta$. The function $\Phi_A^{K,c}$ obeys:

$$\begin{aligned} & \left(L_{AA}^{(1)} + L_{AA}^{(2)} + L_{AA}^{(1)} \right) \{ \Phi_A^{K,c} (\gamma_A u^2) \sqrt{\gamma_B} \mathbf{u} \} + L_{AB}^{(2)} \{ \Phi_B^{K,c} (\gamma_B u^2) \sqrt{\gamma_B} \mathbf{u} \} \\ & - \frac{\sqrt{6\pi}}{9} \frac{nd_{AB}^2}{\sqrt{m_0}} \tilde{\Gamma} \sqrt{T} f_A^M \\ & \times \left((\mathcal{H} \{ \Phi_A^{K,c} \} + 2) \Phi_A^{K,c} (\gamma_A u^2) \sqrt{\gamma_A} \mathbf{u} - \frac{\partial \ln \tilde{\Gamma}}{\partial c} \Phi_\alpha^{K,T} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \right) \\ & = f_A^M \left(\phi_A^{(0)} + c \frac{\partial \phi_A^{(0)}}{\partial c} \right) \mathbf{u} \end{aligned} \quad (3.11)$$

and the function $\Phi_B^{K,c}$ verifies:

$$\begin{aligned} & \left(L_{BB}^{(1)} + L_{BB}^{(2)} + L_{BA}^{(1)} \right) \{ \Phi_B^{K,c} (\gamma_B u^2) \sqrt{\gamma_B} \mathbf{u} \} + L_{BA}^{(2)} \{ \Phi_A^{K,c} (\gamma_A u^2) \sqrt{\gamma_A} \mathbf{u} \} \\ & - \frac{\sqrt{6\pi}}{9} \frac{nd_{AB}^2}{\sqrt{m_0}} \tilde{\Gamma} \sqrt{T} f_B^M \\ & \times \left((\mathcal{H} \{ \Phi_B^{K,c} \} + 2) \Phi_B^{K,c} (\gamma_B u^2) \sqrt{\gamma_B} \mathbf{u} - \frac{\partial \ln \tilde{\Gamma}}{\partial c} \Phi_B^{K,T} (\gamma_B u^2) \sqrt{\gamma_B} \mathbf{u} \right) \\ & = f_B^M \left(-\frac{c}{1-c} \phi_B^{(0)} + c \frac{\partial \phi_B^{(0)}}{\partial c} \right) \mathbf{u} \end{aligned} \quad (3.12)$$

where

$$\begin{aligned} L_{\alpha\beta}^{(1)} \phi_\alpha^K & \equiv \int \mathcal{B}_{\alpha\beta} \left(f_\alpha^M \phi_\alpha^K, f_\beta^M \phi_\beta^{(0)}, \rho_{\alpha\beta}(e), e \right) de \\ L_{\alpha\beta}^{(2)} \phi_\beta^K & \equiv \int \mathcal{B}_{\alpha\beta} \left(f_\alpha^M \phi_\beta^{(0)}, f_\beta^M \phi_\beta^K, \rho_{\alpha\beta}(e), e \right) de \end{aligned}$$

are linearized Boltzmann operators, and the operator \mathcal{H} is defined by

$$\mathcal{H} \{ \Phi \} \equiv \gamma_\alpha u^2 \left((\ln \Phi)' - 1 \right)$$

3.2. Constitutive relations

Inserting Eq. (3.7) into the definitions (2.10), (2.12), and (2.14), one obtains the constitutive relations for the number density flux, stress tensor, and heat flux. While their general form can be derived based on simple tensorial considerations, the transport coefficients are given below in terms of integrals of the corrections $\Phi_\alpha^{K,T}$, $\Phi_\alpha^{K,n}$, $\Phi_\alpha^{K,c}$, and

$\Phi_\alpha^{K,V}$. To Navier-Stokes order (linear in the gradients of the hydrodynamic fields) the number density flux \mathbf{J}_α is given by:

$$\mathbf{J}_\alpha = \frac{\sqrt{6}}{6} \frac{n_\alpha}{n} \frac{1}{d_{AB}^2} \sqrt{\frac{T}{m_\alpha}} \left(\kappa_\alpha^T \nabla \ln T + \kappa_\alpha^n \nabla \ln n + \kappa_\alpha^c \nabla \ln c \right), \quad (3.13)$$

where $n = n_A + n_B$ is the total number density of the mixture, $c = \frac{n_A}{n}$ is the concentration of A particles, and the transport coefficients κ_α^T , κ_α^n and κ_α^c depend on the parameters characterizing the particles (masses, diameters and the distributions of coefficients of restitution) and the concentration field, c . They are given by:

$$\begin{aligned} \kappa_\alpha^T &= n_\alpha d_{AB}^2 \frac{8}{3\sqrt{\pi}} \int_0^\infty e^{-u^2} \Phi_\alpha^{K,T}(u^2) u^4 du \\ \kappa_\alpha^n &= n_\alpha d_{AB}^2 \frac{8}{3\sqrt{\pi}} \int_0^\infty e^{-u^2} \Phi_\alpha^{K,n}(u^2) u^4 du \\ \kappa_\alpha^c &= n_\alpha d_{AB}^2 \frac{8}{3\sqrt{\pi}} \int_0^\infty e^{-u^2} \Phi_\alpha^{K,c}(u^2) u^4 du \end{aligned}$$

Similarly, the heat flux is given by:

$$\mathbf{Q} = \frac{5\sqrt{6}}{18} \frac{1}{d_{AB}^2} \frac{T^{3/2}}{\sqrt{m_0}} \left(\lambda^T \nabla \ln T + \lambda^n \nabla \ln n + \lambda^c \nabla \ln c \right) \quad (3.14)$$

where in terms of the first order corrections:

$$\begin{aligned} \lambda^T &= \frac{16}{15\sqrt{\pi}} n d_{AB}^2 \int_0^\infty e^{-u^2} \left(c \frac{\Phi_A^{K,T}(u^2)}{\sqrt{M_A}} + (1-c) \frac{\Phi_B^{K,T}(u^2)}{\sqrt{M_B}} \right) u^6 du \\ \lambda^n &= \frac{16}{15\sqrt{\pi}} n d_{AB}^2 \int_0^\infty e^{-u^2} \left(c \frac{\Phi_A^{K,n}(u^2)}{\sqrt{M_A}} + (1-c) \frac{\Phi_B^{K,n}(u^2)}{\sqrt{M_B}} \right) u^6 du \\ \lambda^c &= \frac{16}{15\sqrt{\pi}} n d_{AB}^2 \int_0^\infty e^{-u^2} \left(c \frac{\Phi_A^{K,c}(u^2)}{\sqrt{M_A}} + (1-c) \frac{\Phi_B^{K,c}(u^2)}{\sqrt{M_B}} \right) u^6 du \end{aligned}$$

where $M_\alpha \equiv \frac{m_\alpha}{m_0}$. Finally, the stress tensor P_{ij} to Navier-Stokes order assumes the form:

$$P_{ij} = p \delta_{ij} - \mu D_{ij} \quad (3.15)$$

where $p \equiv \frac{nT}{3}$ is the pressure,

$$D_{ij} = \frac{1}{2} \left(\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \operatorname{div} \mathbf{V} \quad (3.16)$$

is the symmetrized traceless rate of strain tensor, and μ is the shear viscosity, given by:

$$\mu = -\frac{4\pi\sqrt{6}}{45} n \sqrt{m_0 T} \int_0^\infty e^{-u^2} \left(c \sqrt{M_A} \Phi_A^{K,V}(u^2) + (1-c) \sqrt{M_B} \Phi_B^{K,V}(u^2) \right) u^6 du \quad (3.17)$$

The constitutive relations have been given here in terms of gradients of the concentration, number density, temperature, and velocity. Other gradients can naturally be employed, yielding different forms for the constitutive relations, (see e.g., Landau & Lifshitz (1959); de Groot & Mazur (1969); Garzó & Dufty (2002)), trivially related to those given above.

3.3. Transport coefficients: Sonine polynomial expansion and the generating function method

Following standard treatment, in order to solve Eqs. (3.3, 3.8, 3.9, 3.10, 3.11, 3.12), the corrections distribution $\phi_\alpha^{(0)}$, $\Phi_\alpha^{K,V}$, $\Phi_\alpha^{K,T}$, $\Phi_\alpha^{K,n}$, and $\Phi_\alpha^{K,c}$ are approximated by truncated series in Sonine polynomials. For extreme values of the parameters, such as very low values of the coefficients of restitution (or large distributions) or large mass ratios, the use of high order truncations of Sonine polynomial series is crucial, but forbiddingly tedious to carry out. To this end we employ a computer-aided method (Noskowitz *et al.* (2007); Serero *et al.* (2007)) which exploits the fact that the Sonine polynomials can be derived from their respective generating functions, $G_m(x; s) \equiv (1-s)^{-m-1} e^{-\frac{x}{1-s}} = \sum_{p=0}^{\infty} s^p S_m^p(x)$:

Defining, for any set of variables $\{x_1, \dots, x_k\}$ and integers $\{p_1, \dots, p_k\}$, $\tilde{\partial}_{x_1^{p_1}, \dots, x_k^{p_k}}$:

$$\tilde{\partial}_{x_1^{p_1}, \dots, x_k^{p_k}} \equiv \lim_{x_1, \dots, x_k \rightarrow 0} \frac{1}{p_1! \dots p_k!} \frac{\partial^{p_1 + \dots + p_k}}{\partial x_1^{p_1} \dots \partial x_k^{p_k}}, \quad (3.18)$$

one has:

$$S_m^p = \tilde{\partial}_{s^p} G_m(x; s) \quad (3.19)$$

One can therefore easily calculate a generating function for the action of a linear operator (such as the integrals required in the process of solving the hierarchy of equations resulting for the Chapman Enskog expansion) on a Sonine polynomial by evaluating its action on G_m . In addition, it turns out that most of the generating functions that are computed in the sequel can be obtained in terms of successive derivatives "super-generating" functions $J_{\alpha\beta}^{(k)}$, see Appendix C, Eq. (C 3). Increasing the order of the truncated series therefore amounts to computing higher order derivatives of known functions, which can be conveniently achieved by a symbolic manipulator.

We proceed first to the evaluation of the distribution function for the homogeneous cooling state. The function $\phi_\alpha^{(0)}$ is written in the form:

$$\phi_\alpha^{(0)} \equiv \sum_{p=0}^{N_t} h_\alpha^{(p)} S_{\frac{1}{2}}^{(p)}(\gamma_\alpha u^2) = \sum_{p=0}^{N_t} h_\alpha^{(p)} \tilde{\partial}_{s^p} G_{\frac{1}{2}}(\gamma_\alpha u^2; s) \quad (3.20)$$

where N_t is the order of truncation. Upon substituting the form (3.20) in Eq. (3.3) and projecting on the Nth order Sonine polynomial $S_{\frac{1}{2}}^N(\gamma_\alpha u_1^2) = \tilde{\partial}_{s^N} G(\gamma_\alpha u_1^2, s)$ one obtains:

$$\begin{aligned} \frac{\sqrt{\pi}}{3} \tilde{\Gamma} \sum_{p=0}^{N_t} h_A^{(p)} \tilde{\partial}_{s^p w^N} \hat{R}(s, w) &= \frac{M_A^3}{\pi^3} \frac{d_A^2}{d_{AB}^2} \frac{n_A}{n} \sum_{p,q=0}^{N_t} \tilde{\partial}_{s^p t^q w^N} \hat{B}_{AA}(w, s, t) h_A^{(p)} h_A^{(q)} \\ &+ \frac{M_B^{\frac{3}{2}} M_A^{\frac{3}{2}}}{\pi^3} \frac{n_B}{n} \sum_{p,q=0}^{N_t} \tilde{\partial}_{s^p t^q w^N} \hat{B}_{AB}(w, s, t) h_A^{(p)} h_B^{(q)} \quad (3.21) \end{aligned}$$

$$\begin{aligned} \frac{\sqrt{\pi}}{3} \tilde{\Gamma} \sum_{p=0}^{N_t} h_B^{(p)} \tilde{\partial}_{s^p w^N} \hat{R}(s, w) &= \frac{M_B^3}{\pi^3} \frac{d_B^2}{d_{AB}^2} \frac{n_B}{n} \sum_{p,q=0}^{N_t} \tilde{\partial}_{s^p t^q w^N} \hat{B}_{BB}(w, s, t) h_B^{(p)} h_B^{(q)} \\ &+ \frac{M_A^{\frac{3}{2}} M_B^{\frac{3}{2}}}{\pi^3} \frac{n_A}{n} \sum_{p,q=0}^{N_t} \tilde{\partial}_{s^p t^q w^N} \hat{B}_{BA}(w, s, t) h_B^{(p)} h_A^{(q)} \quad (3.22) \end{aligned}$$

where the generating function, $\hat{R}(s, w)$, which corresponds to the left hand side of Eqs.

(3.3) is:

$$\begin{aligned}\hat{R}(s, w) &\equiv \frac{1}{\pi^{\frac{3}{2}}} \int e^{-u^2} G_{\frac{1}{2}}(u^2, w) \left[\frac{3}{2} G_{\frac{1}{2}}(u^2, s) - u^2 \left(G_{\frac{1}{2}}(u^2, s) - \frac{\partial}{\partial u^2} G_{\frac{1}{2}}(u^2, s) \right) \right] d\mathbf{u} \\ &= \frac{3}{2} \frac{(1-s)w}{(1-ws)^{\frac{5}{2}}}\end{aligned}\quad (3.23)$$

The generating function $\hat{B}_{\alpha\beta}(w, s, t)$ corresponds to the Boltzmann operator, and can be written in terms of the ‘‘super-generating’’ functions defined in Eq. (C3):

$$\begin{aligned}\hat{B}_{\alpha\beta}(w, s, t) &\equiv \int \rho_{\alpha\beta}(e) \int G_{\frac{1}{2}}^N(M_\alpha u_1^2, w) \int \int_{\mathbf{u}_{12} \cdot \mathbf{k} > 0} \left[\frac{e^{-M_\alpha u_1'^2 - M_\beta u_2'^2}}{e^2} G_{\frac{1}{2}}(M_\alpha u_1'^2, s) \right. \\ &\quad \left. \times G_{\frac{1}{2}}(M_\beta u_2'^2, t) - e^{-M_\alpha u_1^2 - M_\beta u_2^2} G_{\frac{1}{2}}(M_\alpha u_1^2, s) G_{\frac{1}{2}}(M_\beta u_2^2, t) \right] (\mathbf{u}_{12} \cdot \mathbf{k}) d\mathbf{u}_1 d\mathbf{u}_2 d\mathbf{k} de \\ &= \frac{1}{(1-s)^{\frac{3}{2}} (1-t)^{\frac{3}{2}} (1-w)^{\frac{3}{2}}} \\ &\quad \times \left[J_{\alpha\beta}^{(1)} \left(\frac{M_\alpha w}{1-w}, 0, \left(\frac{1}{1-s} \right) M_\alpha, \left(\frac{1}{1-t} \right) M_\beta, 0, 0, 0 \right) \right. \\ &\quad \left. - J_{\alpha\beta}^{(0)} \left(M_\alpha \left(\frac{w}{1-w} + \frac{1}{1-s} \right), \left(\frac{1}{1-t} \right) M_\beta, 0, 0, 0 \right) \right]\end{aligned}\quad (3.24)$$

The non-dimensionalized sink term can be expressed in terms of the coefficients $\{h_A^{(p)}, h_B^{(p)}\}$ to complete the system (3.21,3.22), by using the expression (3.20) in Eqs. (2.16) and (2.17):

$$\begin{aligned}\tilde{\Gamma} &= (1 - \langle e^2 \rangle_{AA}) \frac{n_A^2}{n^2} \frac{d_A^2}{d_{AB}^2} M_A^4 \sum_{p,q=0}^{\infty} \tilde{\partial}_{s^p t^q} \hat{G}_{AA}^\Gamma(s, t) h_A^{(p)} h_A^{(q)} \\ &\quad + 4(1 - \langle e^2 \rangle_{AB}) \frac{n_A n_B}{n^2} M_A^{\frac{5}{2}} M_B^{\frac{5}{2}} \sum_{p,q=0}^{\infty} \tilde{\partial}_{s^p t^q} \hat{G}_{AB}^\Gamma(s, t) h_A^{(p)} h_B^{(q)} \\ &\quad + (1 - \langle e^2 \rangle_{BB}) \frac{n_B^2}{n^2} \frac{d_B^2}{d_{AB}^2} M_B^4 \sum_{p,q=0}^{\infty} \tilde{\partial}_{s^p t^q} \hat{G}_{BB}^\Gamma(s, t) h_B^{(p)} h_B^{(q)}\end{aligned}\quad (3.25)$$

where for any function $\psi(e)$ of the coefficient of restitution, $\langle \psi \rangle_{\alpha\beta} \equiv \int \rho_{\alpha\beta}(e) \psi(e) de$, and the generating function $\hat{G}_{\alpha\beta}^\Gamma(s, t)$ is given by:

$$\begin{aligned}\hat{G}_{\alpha\beta}^\Gamma(s, t) &\equiv \int \int e^{-M_\alpha u_1^2} e^{-M_\beta u_2^2} G_{\frac{1}{2}}(M_\alpha u_1^2, s) G_{\frac{1}{2}}(M_\beta u_2^2, t) |u_{12}|^3 d\mathbf{u}_1 d\mathbf{u}_2 \\ &= \frac{((1-t)M_\alpha + (1-s)M_\beta)^{\frac{3}{2}}}{M_\alpha^3 M_\beta^3}\end{aligned}\quad (3.26)$$

The system of equations (3.21,3.22,3.25) for the coefficients $\{h_A^{(p)}, h_B^{(p)}, \tilde{\Gamma}\}$ is to be solved in conjunction with the requirements (3.4), (3.5) and (3.6) that imposes, using (3.20): $h_A^{(0)} = 1$, $h_B^{(0)} = 1$, $\frac{n_A}{n} h_A^{(1)} + \frac{n_B}{n} h_B^{(1)} = 0$. Fig. (1) shows a comparison between theoretical and (DSMC) simulations values for the coefficient $h_\alpha^{(2)}$ of a monodisperse system obtained within a fifth order truncation of the polynomial expansion, for Laplace distributed coefficients of restitution (c.f Section 4).

The equations corresponding to the gradient-induced corrections of the distribution

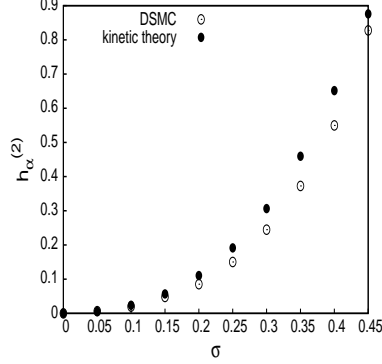


FIGURE 1. Plot of the second Sonine polynomial expansion coefficient, $h_\alpha^{(2)}$, for a monodisperse system with Laplace distributed coefficients of restitution around mean value $\langle e \rangle = 0.9$, as a function of the width of the distribution σ . The theoretical results for a 5th order polynomial expansion (filled circles) are plotted together with DSMC simulation results (empty circles), cf section 4.

functions, Eqs. (3.8-3.12), are solved by proceeding as for the homogeneous inelastic corrections $\phi_\alpha^{(0)}$ to the Maxwellian distribution. The isotropic functions $\Phi_\alpha^{K,X}$, $X \in \{T, c, n, V\}$ are expressed as truncated series of Sonine polynomials:

$$\Phi_\alpha^{K,T} = \sum_{p=0}^{N_t} \frac{k_\alpha^{T,(p)}}{nd_{AB}^2} S_{\frac{3}{2}}^p(\gamma_\alpha u^2) = \sum_{p=0}^{N_t} \frac{k_\alpha^{T,(p)}}{nd_{AB}^2} \tilde{\partial}_{t^p} G_{\frac{3}{2}}(t, \gamma_\alpha u^2) \quad (3.27)$$

$$\Phi_\alpha^{K,n} = \sum_{p=0}^{N_t} \frac{k_\alpha^{n,(p)}}{nd_{AB}^2} S_{\frac{3}{2}}^p(\gamma_\alpha u^2) = \sum_{p=0}^{N_t} \frac{k_\alpha^{n,(p)}}{nd_{AB}^2} \tilde{\partial}_{t^p} G_{\frac{3}{2}}(t, \gamma_\alpha u^2) \quad (3.28)$$

$$\Phi_\alpha^{K,c} = \sum_{p=0}^{N_t} \frac{k_\alpha^{c,(p)}}{nd_{AB}^2} S_{\frac{3}{2}}^p(\gamma_\alpha u^2) = \sum_{p=0}^{N_t} \frac{k_\alpha^{c,(p)}}{nd_{AB}^2} \tilde{\partial}_{t^p} G_{\frac{3}{2}}(t, \gamma_\alpha u^2) \quad (3.29)$$

$$\Phi_\alpha^{K,V} = \sum_{p=0}^{N_t} \frac{k_\alpha^{V,(p)}}{nd_{AB}^2} S_{\frac{5}{2}}^p(\gamma_\alpha u^2) = \sum_{p=0}^{N_t} \frac{k_\alpha^{V,(p)}}{nd_{AB}^2} \tilde{\partial}_{t^p} G_{\frac{5}{2}}(t, \gamma_\alpha u^2) \quad (3.30)$$

which are substituted in Eqs. (3.8-3.12). The resulting set of equations is then projected on

$$S_{\frac{3}{2}}^N(\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} = \tilde{\partial}_{w^N} G_{\frac{3}{2}}(w, \gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u},$$

for $X \in \{T, c, n\}$, and

$$S_{\frac{5}{2}}^N(\gamma_\alpha u^2) \gamma_\alpha^{3/2} \overline{\mathbf{u}\mathbf{u}} = \tilde{\partial}_{w^N} G_{\frac{5}{2}}(w, \gamma_\alpha u^2) \gamma_\alpha^{3/2} \overline{\mathbf{u}\mathbf{u}},$$

for $X = V$. One then obtains a linear system of equations for the coefficients $k_\alpha^{X,(p)}$:

$$\underline{\underline{\mathbf{M}}}^K \underline{\mathbf{k}} = \underline{\mathbf{R}}^K \quad (3.31)$$

where $\underline{\mathbf{k}}$ is the column vector defined by: $\underline{\mathbf{k}} \equiv \left(k_A^{T,(0)}, \dots, k_A^{T,(N)}, k_B^{T,(0)}, \dots, k_B^{T,(N)}, k_A^{n,(0)}, \dots, k_A^{n,(N)}, k_B^{n,(0)}, \dots, k_B^{n,(N)}, k_A^{c,(0)}, \dots, k_A^{c,(N)}, k_B^{c,(0)}, \dots, k_B^{c,(N)}, k_A^{V,(0)}, \dots, k_A^{V,(N)}, k_B^{V,(0)}, \dots, k_B^{V,(N)} \right)^t$, the superscript t , standing here for “transpose”. The matrix elements, M_{ij}^K and R_j^K defined in Eq. (3.31), and their generating functions, are given in Appendix B. In addition,

the constraints (3.4), (3.5), (3.6), yield, for $X \in \{T, n, c\}$:

$$\frac{n_A}{n} \sqrt{m_A} k_A^{X,(0)} + \frac{n_B}{n} \sqrt{m_B} k_B^{X,(0)} = 0$$

Using the forms (3.7), (3.27-3.30), in conjunction with the solution $\{k_\alpha^{X,(q)}\}$, where $0 \leq q \leq N_t$, of the system (3.31), in the definitions of the diffusion velocity, heat flux and stress tensor, one obtains the constitutive relations. The resulting transport coefficients (like the coefficients $\{k_\alpha^{X,(q)}\}$), are non-trivial functions of the mass and size ratios, concentration, and of the characteristics of the distributions $\rho_{\alpha\beta}(e)$ for the coefficient of restitution. The pressure p is given by:

$$p = \frac{nT}{3}, \quad (3.32)$$

The shear viscosity is given by:

$$\mu = -\frac{\sqrt{6}}{24} \frac{\sqrt{Tm_0}}{d_{AB}^2} \left(\frac{n_A}{n} \sqrt{M_A} k_A^{V,(0)} + \frac{n_B}{n} \sqrt{M_B} k_B^{V,(0)} \right) \quad (3.33)$$

The transport coefficients for the diffusion flux are given by:

$$\kappa_A^X = k_A^{X,(0)} \quad (3.34)$$

and the transport coefficients for the heat flux are:

$$\lambda^X = \frac{n_A}{n\sqrt{M_A}} \left(k_A^{X,(0)} - k_A^{X,(1)} \right) + \frac{n_B}{n\sqrt{M_B}} \left(k_B^{X,(0)} - k_B^{X,(1)} \right) \quad (3.35)$$

Notice that while the transport coefficients are expressed only in terms of the first two Sonine expansion coefficients, their values, as that of the expansion coefficients, actually depend on the order of truncation of the whole series in Sonine polynomials.

4. Comparison with DSMC simulations

To check the reliability of the calculation of the transport coefficients presented above, we numerically solved the Boltzmann equation by means of the DSMC method (Bird (1976)), using the particle simulator Dynamo (Bannerman *et al.* (2011)). For binary mixtures the velocity distribution is estimated by:

$$f_\alpha(v, t) = \frac{1}{N_\alpha} \sum_{i=1}^{N_\alpha} \delta(\mathbf{v} - \mathbf{v}_{(i)}(t)) \quad (4.1)$$

where N_α is the number of particles in species α , and the indices between comma indicate a given particle label.

Considering first the influence of the stochastic behavior on the reduced velocity distribution function of a homogeneous monodisperse granular gas, we performed a DSMC simulation of a system with $N \equiv N_A + N_B = 5 \times 10^5$ particles, recorded the velocities of the particles after 10^5 collisions and evaluated the Sonine polynomial expansion coefficients of the distribution function. The latter are related to the velocity moments

$$c^{2k} \equiv \frac{1}{N} \sum_{i=1}^N \left(\frac{\mathbf{v}_{(i)} \mathbf{v}_{(i)}}{2T} \right)^k \quad (4.2)$$

through (Chapman & Cawling (1970)):

$$c^{2k} = \frac{(2k+1)!!}{2^k} \left(1 + \sum_p (-1)^p \frac{k!}{(k-p)!p!} h_\alpha^{(p)} \right) \quad (4.3)$$

Figure 1 shows theoretical predictions for $h_\alpha^{(2)}$ (corresponding to a fifth order truncation of the polynomial series) together with DSMC results. Guided by recent experimental, numerical and theoretical results (Montaine *et al.* (2011); Gunkelmann *et al.* (2014)) concerning the distribution of coefficients of restitution, we considered here the case of Laplace distributed coefficients:

$$\rho_{\alpha\beta}(e) = \frac{1}{2\sigma_{\alpha\beta}} e^{-\frac{|e-\langle e \rangle_{\alpha\beta}|}{\sigma_{\alpha\beta}}} \quad (4.4)$$

The average value of the coefficient of restitution was taken to be $\langle e \rangle \equiv \langle e \rangle_{AA} = \langle e \rangle_{AB} = \langle e \rangle_{BB} = 0.9$, and we varied the width $\sigma \equiv \sigma_{AA} = \sigma_{AB} = \sigma_{BB}$ of its probability density. For the smaller standard deviations σ , DSMC and theory are in fairly good agreement, while as σ increases, discrepancies between simulation and theoretical predictions become larger, illustrating the need for high order truncation in the polynomial expansions.

We considered next the diffusion of impurities, described by the tracer limit ($c \rightarrow 0$) of the diffusion coefficient κ_A^c . In this limit, the coefficient can be measured from the mean-square displacement of the tracer particles in a the homogeneous cooling state:

$$\kappa_A^c(t) = \frac{n_B}{6\delta t} \frac{1}{N_B} \sum_{i=1}^{N_B} \left[|\mathbf{r}_{(i)}(t+\delta t) - \mathbf{r}_{(i)}(0)|^2 - |\mathbf{r}_{(i)}(t) - \mathbf{r}_{(i)}(0)|^2 \right] \quad (4.5)$$

where δt denotes a time interval, n_B is the number density of the gas in excess, and the above sum is carried out over B particles. The tracer limit (of species A) is realized in simulations by ignoring $A-A$ collisions, and by imposing that the tracer particles have no influence on the dynamics of the surrounding gas, i.e in a $A-B$ collision, only the velocity of A (tracer) particle is modified. A small number of A particle is therefore not required (Garzo & Montanero (2004)). In order to get rid of the time dependence of the diffusion coefficient that occurs through its dependence on the (decreasing in time) temperature, we consider a reduced diffusion coefficient κ_A^{c*} :

$$\kappa_A^{c*}(t) = \frac{\kappa_A^c(t)}{\sqrt{T(t)}} \quad (4.6)$$

The above rescaling allows to eliminate the time dependence of κ_A^{c*} , as can be seen in Fig. (2). The latter shows the time behaviour of κ_A^{c*} obtained in a simulation of a mixture of 13500 particles (half of which belonging to the impurity species A), having identical sizes and mass ratio $\frac{m_A}{m_B} = 4$, performing 10^5 collisions, with coefficients of restitution distributed according to Laplace laws (4.4) with identical averages and variances $\langle e \rangle = \langle e \rangle_{AA} = \langle e \rangle_{AB} = \langle e \rangle_{BB}$, and $\sigma = \sigma_{AA} = \sigma_{AB} = \sigma_{BB}$. After a transient regime, the value of the coefficient κ_A^{c*} reaches a constant value. A comparison of the corresponding value of the diffusion coefficient, normalized by its elastic counterpart, with theoretical predictions for $\langle e \rangle = 0.95$ and various values of σ is shown in Fig. (3).

5. Stochasticity-induced segregation

As has been illustrated in the previous section, taking into account the stochastic nature of the coefficient of restitution can have a quantitative influence on the values of

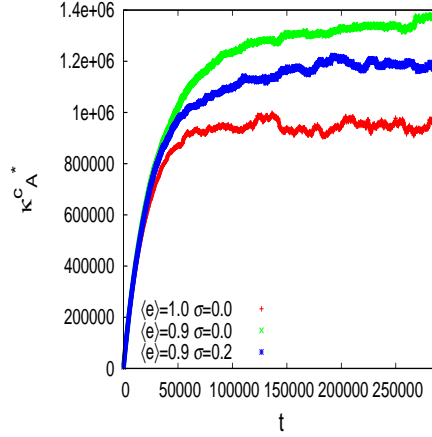


FIGURE 2. Plot of the reduced mutual diffusion coefficient as a function of time for different parameters of the Laplace distributed coefficient of restitution.

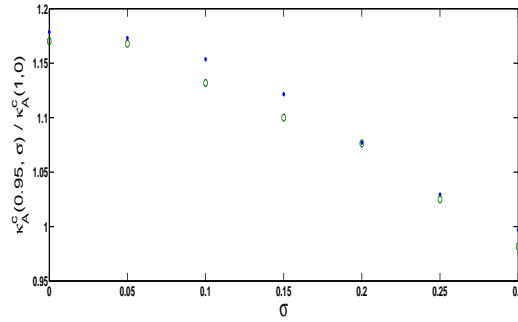


FIGURE 3. Comparison between theoretical (empty circles) and DSMC results (filled circles) for the normalized diffusion coefficient $\kappa_c^A(\langle e \rangle, \sigma) / \kappa_c^A(1, 0)$ computed in the tracer limit $\frac{n_A}{n} \rightarrow 0$, for a mass ratio $m_A/m_B = 4$, and a restitution coefficient distributed according to a Laplace law around $\langle e \rangle = 0.95$. The values are plotted as a function of the width σ of the Laplace distribution for the coefficients of restitution.

the transport coefficient. The importance of this effect depends of course on the actual shape of the distribution, and in particular its width. This section is devoted to the study of a *qualitative* signature of the stochasticity, namely the fact that the shape of the distribution influences segregation in mixtures of otherwise identical particles. More specifically, we study the temperature and gravity driven diffusion in a mixture of grains with same mass, size and mean coefficient of restitution, but different standard deviations for the (three) different types of restitution coefficient. Thermal segregation in granular mixtures has been identified as one of the main factors of the Brazil Nut effect (Hsiau & Hunt (1996); Schröter *et al.* (2006)) in the case of granular gases, and its dependence on the particle properties has been studied in the past (Arnason & Willits (1998); Jenkins & Yoon (2002); Brey *et al.* (2005); Garzó (2008)). In particular, it was predicted (Serero *et al.* (2006)) and observed in molecular dynamic simulations (Serero *et al.* (2009, 2011); Brito *et al.* (2008); Brito & Soto (2009)) that the species in a binary mixture may segregate even when they differ only in their respective coefficients of restitution, demonstrating a direct influence of inelasticity on the properties of binary granular gas mixtures. Here we proceed to a similar analysis by considering particles of same mass,

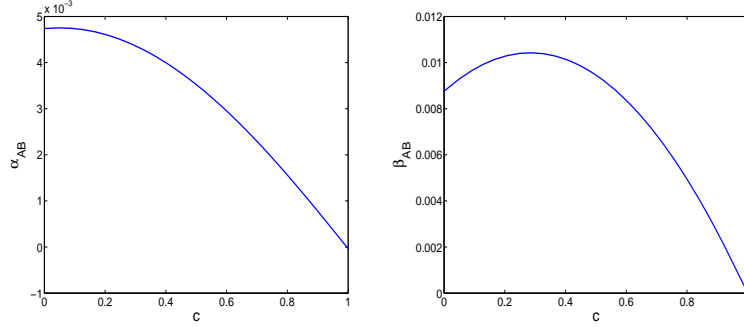


FIGURE 4. Plots of the thermal coefficients α_{AB} and β_{AB} , see Eqs. (5.4)-(5.5), as a function of the concentration, $c \equiv \frac{n_A}{n}$, for a mixture of particles whose collisions are characterized by coefficients of restitution distributed according to Laplace laws. The distributions have the same average coefficients of restitution $\langle e \rangle = \sqrt{0.8}$, and different standard deviations for the three type of collisions: $\sigma_{AA} = 0.2$, $\sigma_{AB} = 0.1$, and $\sigma_{BB} = 0.01$. The particles are otherwise identical, i.e. $m_A = m_B$, $d_A = d_B$.

size and average coefficient of restitution, and Laplacian distributions for the three types of coefficient of restitution, with different standard deviations. The momentum balance equation describing the non-convecting ($\mathbf{V} = 0$) steady state of a mixture reads, using Eqs. (2.11) (after adding $\rho_m \mathbf{g}$ on the left hand side, to account for gravity), and (3.15):

$$\nabla p = -\rho_m \mathbf{g} \quad (5.1)$$

which can be rewritten, using the equation of state $p = \frac{nT}{3}$:

$$\nabla \ln n = -\nabla \ln T - \frac{3}{T} ((m_A - m_B)c + m_B) \mathbf{g}. \quad (5.2)$$

Now substituting Eq. (5.2) in Eq. (3.13), and using the fact that the diffusive fluxes vanish ($\mathbf{J}_A = 0$), one obtains the following relation between the temperature and concentration gradients, when the temperature and concentration vary only along the vertical (z) direction:

$$\frac{\partial \ln c}{\partial \xi} = \alpha_{AB} \frac{\partial \ln T}{\partial \xi} + \beta_{AB} \quad (5.3)$$

where $\xi = \int_0^z \frac{(m_A + m_B)g}{T(z')} dz'$, is a rescaled length scale,

$$\alpha_{AB} \equiv \frac{\kappa_A^n - \kappa_A^T}{\kappa_A^c} \quad (5.4)$$

describes the effects of the temperature gradient on the gradient of concentration, and

$$\beta_{AB} = 3 \frac{\kappa_A^n}{\kappa_A^c} ((M_A - M_B)c + M_B) \quad (5.5)$$

accounts for the effects of gravity. In particular, the sign of α_{AB} determines the direction of segregation: when $\alpha_{AB} > 0$ the A particles tends to concentrate in the hotter regions. Similarly, when $\beta_{AB} > 0$ the particles A tends to concentrate near the top of the system. As mentioned, in order to emphasize the effect of the random nature of the coefficient of restitution on the segregation properties of the system, we consider here the case $m_A = m_B$, $d_A = d_B$, and $\langle e \rangle_{AA} = \langle e \rangle_{AB} = \langle e \rangle_{BB} = \sqrt{0.8}$, i.e. we study a mixture of particles differing only by the *shape* of the distribution of the coefficient of restitution characterizing the collisions they are subjected to. More specifically, we considered a set

of Laplacian distributions, with three different widths $\sigma_{AA} = 0.2$, $\sigma_{AB} = 0.1$ and $\sigma_{BB} = 0.01$. The corresponding values for the coefficients α_{AB} and β_{AB} are plotted in Fig. (4) as functions of the concentration, c , of A particles. The sign of α_{AB} indicates that the particles with the broader distribution tend to concentrate in the hotter regions. The sign of β_{AB} (Fig. 4, Right) indicates that gravity drives the particles with broader distribution upward. If those results are associated with the fact that in a vertically vibrated system of such mixtures, a minimum in the temperature profile is expected (Brey *et al.* (2001); Brey & Ruiz-Montero (2004)), as a consequence of the density gradient correction to the Fourier law, one may expect a pattern formation in the form of a three layers arrangement in vertically vibrated systems, with the particles colliding with the narrower distribution concentrating in the area situated below the minimum of temperature, as a result of the competition between the effect of the temperature gradient and gravity. For other sets of values of the widths of the distributions, or other types of distributions, one may find that the signs of the coefficients α_{AB} and β_{AB} depend on the concentration, yielding more complex interplay between the effect of gravity and temperature gradients, and resulting in different profiles of concentration.

6. Concluding remarks

A complete hydrodynamic description of a dilute binary mixture of granular gas interacting by collisions characterized by stochastic coefficients of restitution has been derived. A technique for obtaining accurate transport coefficients, limited only by computer capacity, has been presented as well. The method has been illustrated by considering the case of Laplacian distributions, which can be used to model energy transfer to integral degrees of freedom due to surface asperities, as has been recently shown in experiments and simulations. The results were compared to DSMC simulations with good agreement. The stochasticity has been shown to yield quantitative differences with respect to the non fluctuating case. Of course the discrepancies depend strongly on the actual shape of the employed distribution function: Typically, wider distributions yield stronger discrepancies. The hydrodynamic description has been employed to study the segregation in a mixture subjected to a temperature gradient under gravity. In particular, by considering a mixture of two species having the same mass and size, and interacting with the same coefficient of restitution on average, it was shown that fluctuation of the coefficient of restitution alone was sufficient to yield partial segregation. Particles whose collisions are characterized by wider distributions for the coefficient of restitution were found to tend to be driven toward the hotter regions, while gravity was found to drive those particles upward. While we considered as an illustration a particular type of distribution, the hydrodynamic description presented here, together with the described method for obtaining the transport coefficients could be applied to the effective description of the relevant degrees of freedom of other dissipative collisional systems, provided a probability distribution for the exchange of energy with the remaining degrees of freedom can be devised. Those possibly comprise, e.g., complex shaped particles or some classes of active particles.

Acknowledgments

This work was supported by the German Science Foundation (DFG) through the Cluster of Excellence “Engineering of Advance Materials”.

Appendix A. Equations for ϕ_α^K

Calculating the transport coefficients to Navier-Stokes order requires to carry out the Chapman-Enskog expansion to first order in gradients of the hydrodynamic fields. The corresponding two coupled Boltzmann equations for the corrections, ϕ_α^K , read:

$$\mathcal{D}^K f_A = \left(L_{AA}^{(1)} + L_{AA}^{(2)} + L_{AB}^{(1)} \right) \phi_A^K + L_{AB}^{(2)} \phi_B^K \quad (\text{A } 1)$$

$$\mathcal{D}^K f_B = L_{BA}^{(2)} \phi_A^K + \left(L_{BB}^{(1)} + L_{BB}^{(2)} + L_{BA}^{(1)} \right) \phi_B^K \quad (\text{A } 2)$$

where

$$L_{\alpha\beta}^{(1)} \phi_\alpha^K \equiv \int \mathcal{B}_{\alpha\beta} \left(f_\alpha^M \phi_\alpha^K, f_\beta^{(HCS)}, \rho_{\alpha\beta}(e), e \right) de$$

$$L_{\alpha\beta}^{(2)} \phi_\beta^K \equiv \int \mathcal{B}_{\alpha\beta} \left(f_\alpha^{(HCS)}, f_\beta^M \phi_\beta^K, \rho_{\alpha\beta}(e), e \right) de$$

are linearized Boltzmann operators, and $\mathcal{D}^K f_\alpha$ denotes the first order term in the expansion of $\mathcal{D} f_\alpha$, where recall that $\mathcal{D} \equiv \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla$. Following the CE approach:

$$\begin{aligned} \mathcal{D} f_\alpha = & f_\alpha^M \left[\phi_\alpha \mathcal{D} \ln n_\alpha + 2\gamma_\alpha u_i (\phi_\alpha - \phi'_\alpha) \mathcal{D} V_i + \left(\gamma_\alpha u^2 (\phi_\alpha - \phi'_\alpha) - \frac{3}{2} \phi_\alpha \right) \mathcal{D} \ln T \right. \\ & \left. + c \frac{\partial \phi_\alpha}{\partial c} \mathcal{D} \ln c \right] + f_\alpha^M \mathcal{D} \Phi_\alpha^K + \Phi_\alpha^K f_\alpha^M \left[\mathcal{D} \ln n_\alpha + 2\gamma_\alpha u_i \mathcal{D} V_i + \left(\gamma_\alpha u^2 - \frac{3}{2} \right) \mathcal{D} \ln T \right] \end{aligned}$$

Straightforward tensorial considerations can be used to determine the general form of the functions, ϕ_α^K :

$$\begin{aligned} \phi_\alpha^K = & \Phi_\alpha^{K,T} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \cdot \nabla \ln T + \Phi_\alpha^{K,n} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \cdot \nabla \ln n \\ & + \Phi_\alpha^{K,c} (\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} \cdot \nabla \ln c + \Phi_\alpha^{K,V} (\gamma_\alpha u^2) \gamma_\alpha^{\frac{3}{2}} \overline{\mathbf{u}\mathbf{u}} : \nabla \mathbf{V} + \Phi_\alpha^0 \text{div} \mathbf{V} \end{aligned}$$

where the functions $\Phi_\alpha^{K,T}, \Phi_\alpha^{K,c}, \Phi_\alpha^{K,n}, \Phi_\alpha^{K,V}$ and Φ_α^0 are isotropic functions of the rescaled peculiar velocity $\gamma_\alpha u^2$. It turns out that the Φ_α^0 vanishes. $\mathcal{D}^K f_A$ is given, using Eqs. (2.9), (2.11) and (2.13), by:

$$\begin{aligned} \mathcal{D}^K f_A = & \frac{\Gamma}{nT} f_A^M \left[\left(\gamma_A u^2 (\Phi_A^{K,c})' - (\gamma_A u^2 - 2) \Phi_A^{K,c} - c \frac{\partial \ln \tilde{\Gamma}}{\partial c} \Phi_A^{K,T} \right) \sqrt{\gamma_A} u_j \frac{\partial \ln c}{\partial x_j} \right. \\ & + \left(\gamma_A u^2 (\Phi_A^{K,n})' - (\gamma_A u^2 - 2) \Phi_A^{K,n} - \Phi_A^{K,T} \right) \sqrt{\gamma_A} u_j \frac{\partial \ln n}{\partial x_j} \\ & + \left(\gamma_A u^2 (\Phi_A^{K,T})' - (\gamma_A u^2 - 2) \Phi_A^{K,T} - \frac{1}{2} \Phi_A^{K,T} \right) \sqrt{\gamma_A} u_j \frac{\partial \ln T}{\partial x_j} \\ & + \left. \left(\gamma_A u^2 (\Phi_A^{K,V})' - (\gamma_A u^2 - 3) \Phi_A^{K,V} \right) \gamma_A^{\frac{3}{2}} \overline{u_i u_j} \frac{\partial V_i}{\partial x_j} \right] \\ & + f_A^M \left[2\gamma_A (\phi_A - \phi'_A) \overline{u_i u_j} \frac{\partial V_i}{\partial x_j} + \left(\phi_A - \frac{nm_A}{\rho} (\phi_A - \phi'_A) \right) u_i \frac{\partial \ln n}{\partial x_i} \right. \\ & + \left. \left(\left(\gamma_A u^2 - \frac{nm_A}{\rho} \right) (\phi_A - \phi'_A) - \frac{3}{2} \phi_A \right) u_i \frac{\partial \ln T}{\partial x_i} \right. \\ & \left. + \left(\phi_A + c \frac{\partial \phi_A}{\partial c} \right) u_j \frac{\partial \ln c}{\partial x_j} \right] \quad (\text{A } 3) \end{aligned}$$

A similar expression for $\mathcal{D}^K f_B$ can be obtained by inverting labels A and B (and changing c for $(1-c)$) in the above equation. Combining Eq. (A 3) and its B species counterpart with Eqs. (A 1)-(A 2) yields Eqs. (3.8)-(3.12).

Appendix B. Matrix elements

This appendix provides the matrix elements needed to solve the linear system Eq. (3.31), corresponding to a truncation of the Sonine polynomial expansion at order N . The matrix elements $M_{i,j}^K$ for $1 \leq i \leq 6N+6$, $1 \leq j \leq 6N+6$ are calculated by substituting the expressions (3.27-3.29) into the left hand side of equations (3.9-3.11), multiplying by the functions

$$S_{\frac{3}{2}}^i(\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} = \tilde{\partial}_{w^i} G_{\frac{3}{2}}(w, \gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u},$$

and integrating over the velocities. The matrix elements $M_{i,j}^K$ for $6N+7 \leq i \leq 8N+8$, $6N+7 \leq j \leq 8N+8$ are calculated by substituting the expressions (3.30) into the left hand side of equation (3.8), multiplying by the functions $S_{\frac{3}{2}}^i(\gamma_\alpha u^2) \gamma_\alpha^{3/2} \overline{\mathbf{u}} = \tilde{\partial}_{w^i} G_{\frac{3}{2}}(w, \gamma_\alpha u^2) \gamma_\alpha^{3/2} \overline{\mathbf{u}}$ and integrating over the velocities. The results are expressed below in terms of derivatives of the generating functions $\hat{L}_{\alpha\beta}^{(i,j)}(w, s, r)$ given in Eqs. (B 4-B 7), and the generating functions $\hat{H}^V(w, t)$, $\hat{H}(w, t)$, and $\hat{Z}(w, t)$ given in Eqs. (B 1-B 3). For $1 \leq i \leq N+1$, $1 \leq j \leq N+1$, the non zero elements of the $(8N+8) \times (8N+8)$ matrix $\underline{\underline{M}}^K$ are:

$$\begin{aligned} M_{i,j}^K &= \left(\frac{n_A}{n} \frac{d_A^2}{d_{AB}^2} M_A^4 \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \left(\hat{L}_{AA}^{(1,1)}(w, s, r) + \hat{L}_{AA}^{(1,2)}(w, s, r) \right) \right. \\ &\quad + \frac{n_B}{n} M_A^{\frac{5}{2}} M_B^{\frac{3}{2}} \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{AB}^{(1,1)}(w, s, r) \\ &\quad \left. - \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} \left(\tilde{\partial}_{w^i t^j} \hat{H}(w, t) + \frac{3}{2} \tilde{\partial}_{w^i t^j} \hat{Z}(w, t) \right) \right) \end{aligned}$$

$$M_{i, j+(N+1)}^K = \frac{n_B}{n} M_A^2 M_B^2 \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{AB}^{(1,2)}(w, s, r)$$

$$M_{i+(N+1), j}^K = \frac{n_A}{n} M_B^2 M_A^2 \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{BA}^{(1,2)}(w, s, r)$$

$$\begin{aligned} M_{i+(N+1), j+(N+1)}^K &= \frac{n_B}{n} \frac{d_B^2}{d_{AB}^2} M_B^4 \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \left(\hat{L}_{BB}^{(1,1)}(w, s, r) + \hat{L}_{BB}^{(1,2)}(w, s, r) \right) \\ &\quad + \frac{n_A}{n} M_B^{\frac{5}{2}} M_A^{\frac{3}{2}} \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{BA}^{(1,1)}(w, s, r) \\ &\quad - \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} \left(\tilde{\partial}_{w^i t^j} \hat{H}(w, t) + \frac{3}{2} \tilde{\partial}_{w^i, t^j} \hat{Z}(w, t) \right) \end{aligned}$$

$$M_{i+(2N+2), j}^K = \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} \sum_q \tilde{\partial}_{w^i, t^j} \hat{Z}(w, t)$$

$$\begin{aligned}
 M_{i+(2N+2),j+(2N+2)}^K &= \left(\frac{n_A}{n} \frac{d_A^2}{d_{AB}^2} M_A^4 \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \left(\hat{L}_{AA}^{(1,1)}(w, s, r) + \hat{L}_{AA}^{(1,2)}(w, s, r) \right) \right. \\
 &\quad + \frac{n_B}{n} M_A^{\frac{5}{2}} M_B^{\frac{3}{2}} \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{AB}^{(1,1)}(w, s, r) \\
 &\quad \left. - \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} \left(\tilde{\partial}_{w^i, t^j} \hat{H}(w, t) + 2\tilde{\partial}_{w^i t^j} \hat{Z}(w, t) \right) \right)
 \end{aligned}$$

$$M_{i+(2N+2),j+(3N+3)}^K = \frac{n_B}{n} M_A^2 M_B^2 \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{AB}^{(1,2)}(w, s, r)$$

$$M_{i+(3N+3),j+(N+1)}^K = \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} \sum_q \tilde{\partial}_{w^i t^j} \hat{Z}(w, t)$$

$$M_{i+(3N+3),j+(2N+2)}^K = \frac{n_A}{n} M_B^2 M_A^2 \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{BA}^{(1,2)}(w, s, r)$$

$$\begin{aligned}
 M_{i+(3N+3),j+(3N+3)}^K &= \frac{n_B}{n} \frac{d_B^2}{d_{AB}^2} M_B^4 \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \left(\hat{L}_{BB}^{(1,1)}(w, s, r) + \hat{L}_{BB}^{(1,2)}(w, s, r) \right) \\
 &\quad + \frac{n_A}{n} M_B^{\frac{5}{2}} M_A^{\frac{3}{2}} \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{BA}^{(1,1)} \\
 &\quad - \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} \left(\tilde{\partial}_{w^i, t^j} \hat{H}(w, t) + 2\tilde{\partial}_{w^i, t^j} \hat{Z}(w, t) \right)
 \end{aligned}$$

$$M_{i+(4N+4),j}^K = \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} c \frac{\partial \ln \tilde{\Gamma}}{\partial c} \sum_q \tilde{\partial}_{w^i, t^j} \hat{Z}(w, t)$$

$$\begin{aligned}
 M_{i+(4N+4),j+(4N+4)}^K &= \frac{n_A}{n} \frac{d_A^2}{d_{AB}^2} M_A^4 \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \left(\hat{L}_{AA}^{(1,1)}(w, s, r) + \hat{L}_{AA}^{(1,2)}(w, s, r) \right) \\
 &\quad + \frac{n_B}{n} M_A^{\frac{5}{2}} M_B^{\frac{3}{2}} \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{AB}^{(1,1)}(w, s, r) \\
 &\quad - \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} \left(\tilde{\partial}_{w^i, t^j} \hat{H}(w, t) + 2\tilde{\partial}_{w^i, t^j} \hat{Z}(w, t) \right)
 \end{aligned}$$

$$M_{i+(4N+4),j+(5N+5)}^K = \frac{n_B}{n} M_A^2 M_B^2 \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{AB}^{(1,2)}(w, s, r)$$

$$M_{i+(5N+5),j+(N+1)}^K = \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} c \frac{\partial \ln \tilde{\Gamma}}{\partial c} \sum_q \tilde{\partial}_{w^i, t^j} \hat{Z}(w, t)$$

$$M_{i+(5N+5),j+(4N+4)}^K = \frac{n_A}{n} M_B^2 M_A^2 \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{BA}^{(1,2)}(w, s, r)$$

$$\begin{aligned}
M_{i+(5N+5),j+(5N+5)}^K &= \frac{n_B}{n} \frac{d_B^2}{d_{AB}^2} M_B^4 \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \left(\hat{L}_{BB}^{(1,1)}(w, s, r) + \hat{L}_{BB}^{(1,2)}(w, s, r) \right) \\
&\quad + \frac{n_A}{n} M_B^{\frac{5}{2}} M_A^{\frac{3}{2}} \sum_p h_A^{(p)} \tilde{\partial}_{w^N, s^p, r^q} \hat{L}_{BA}^{(1,1)}(w, s, r) \\
&\quad - \frac{\pi^{\frac{7}{2}}}{3} \tilde{\Gamma} \left(\tilde{\partial}_{w^i, t^j} \hat{H}(w, t) + 2\tilde{\partial}_{w^i, t^j} \hat{Z}(w, t) \right)
\end{aligned}$$

$$\begin{aligned}
M_{i+(6N+6),j+(6N+6)}^K &= \frac{n_A}{n} \frac{d_A^2}{d_{AB}^2} M_A^5 \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \left(\hat{L}_{AA}^{(2,1)}(w, s, r) + \hat{L}_{AA}^{(2,2)}(w, s, r) \right) \\
&\quad + \frac{n_B}{n} M_A^{\frac{7}{2}} M_B^{\frac{3}{2}} \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{AB}^{(2,1)}(w, s, r) - \frac{5\pi^{\frac{7}{2}}}{6} \tilde{\Gamma} \tilde{\partial}_{w^i, t^j} \hat{H}^V(w, t)
\end{aligned}$$

$$M_{i+(6N+6),j+(7N+7)}^K = \frac{n_B}{n} M_A^2 M_B^3 \sum_p h_A^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{AB}^{(2,2)}(w, s, r)$$

$$M_{i+(7N+7),j+(6N+6)}^K = \frac{n_A}{n} M_B^2 M_A^3 \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p, r^j} \hat{L}_{BA}^{(2,2)}(w, s, r)$$

$$\begin{aligned}
M_{i+(7N+7),j+(7N+7)}^K &= \frac{n_B}{n} \frac{d_B^2}{d_{AB}^2} M_B^5 \sum_p h_B^{(p)} \tilde{\partial}_{w^N, s^p, r^q} \left(\hat{L}_{BB}^{(2,1)}(w, s, r) + \hat{L}_{BB}^{(2,2)}(w, s, r) \right) \\
&\quad + \frac{n_A}{n} M_B^{\frac{7}{2}} M_A^{\frac{3}{2}} \sum_p h_A^{(p)} \tilde{\partial}_{w^N, s^p, r^q} \hat{L}_{BA}^{(2,2)}(w, s, r) - \frac{5\pi^{\frac{7}{2}}}{6} \tilde{\Gamma} \tilde{\partial}_{w^i, t^j} \hat{H}^V(w, t),
\end{aligned}$$

where the generating functions \hat{H}^V , \hat{H} , and \hat{Z} are given by:

$$\hat{H}^V(w; t) = \frac{\left(-\frac{7}{2} \frac{(1-w)}{(1-wt)} + 3 \right)}{(1-wt)^{\frac{7}{2}}} \quad (\text{B1})$$

$$\hat{H}(w; t) = -\frac{15}{4} \frac{(1-w)t}{(1-wt)^{\frac{7}{2}}} \quad (\text{B2})$$

$$\hat{Z}(w; t) = \frac{3}{2} \frac{1}{(1-wt)^{\frac{5}{2}}}, \quad (\text{B3})$$

and the generating functions $\hat{L}_{\alpha\beta}^{(i,j)}(w; s, r)$ can be computed by taking derivatives of the "super-generating" functions $J_{\alpha\beta}^{(0)}$ and $J_{\alpha\beta}^{(1)}$ (c.f Eq. (C3) in Appendix C):

$$\begin{aligned}
\hat{L}_{\alpha\beta}^{(1,1)}(w; s, r) &= \frac{1}{(1-w)^{\frac{5}{2}} (1-r)^{\frac{5}{2}} (1-s)^{\frac{3}{2}}} \\
&\quad \times \left[\delta x J_{\alpha\beta}^{(1)} \left(\frac{w}{1-w} M_\alpha, 0, M_\alpha + \frac{r}{1-r} M_\alpha, M_\beta + \frac{s}{1-s} M_\beta, 0, 0, 0 \right) \right. \\
&\quad \left. - \delta a J_{\alpha\beta}^{(0)} \left(\frac{w}{1-w} M_\alpha + M_\alpha + \frac{r}{1-r} M_\alpha, M_\beta + \frac{s}{1-s} M_\beta, 0, 0, 0, 0, 0 \right) \right] \quad (\text{B4})
\end{aligned}$$

$$\begin{aligned}
 \hat{L}_{\alpha\beta}^{(1,2)}(w; s, r) &= \frac{1}{(1-w)^{\frac{5}{2}}(1-r)^{\frac{5}{2}}(1-s)^{\frac{3}{2}}} \\
 &\times \left[\delta y J_{\alpha\beta}^{(1)} \left(\frac{w}{1-w} M_\alpha, 0, M_\alpha + \frac{s}{1-s} M_\alpha, M_\beta + \frac{r}{1-r} M_\beta, 0, 0, 0 \right) \right. \\
 &\left. - \delta z J_{\alpha\beta}^{(0)} \left(\frac{w}{1-w} M_\alpha + M_\alpha + \frac{s}{1-s} M_\alpha, M_\beta + \frac{r}{1-r} M_\beta, 0, 0, 0, 0 \right) \right] \quad (\text{B5})
 \end{aligned}$$

$$\begin{aligned}
 \hat{L}_{\alpha\beta}^{(2,1)}(w; s, r) &= \frac{1}{(1-w)^{\frac{5}{2}}(1-r)^{\frac{5}{2}}(1-s)^{\frac{3}{2}}} \\
 &\times \left[\left(\delta^2 x - \frac{1}{3} \delta a \delta c \right) J_{\alpha\beta}^{(1)} \left(\frac{w}{1-w} M_\alpha, 0, M_\alpha + \frac{r}{1-r} M_\alpha, M_\beta + \frac{s}{1-s} M_\beta, 0, 0, 0 \right) \right. \\
 &\left. - \frac{2}{3} \delta^2 a J_{\alpha\beta}^{(0)} \left(\frac{w}{1-w} M_\alpha + M_\alpha + \frac{r}{1-r} M_\alpha, M_\beta + \frac{s}{1-s} M_\beta, 0, 0, 0, 0 \right) \right] \quad (\text{B6})
 \end{aligned}$$

$$\begin{aligned}
 \hat{L}_{\alpha\beta}^{(2,2)}(w; s, r) &= \frac{1}{(1-w)^{\frac{5}{2}}(1-r)^{\frac{5}{2}}(1-s)^{\frac{3}{2}}} \\
 &\times \left[\left(\delta^2 y - \frac{1}{3} \delta a \delta d \right) J_{\alpha\beta}^{(1)} \left(\frac{w}{1-w} M_\alpha, 0, M_\alpha + \frac{s}{1-s} M_\alpha, M_\beta + \frac{r}{1-r} M_\beta, 0, 0, 0 \right) \right. \\
 &\left. - \frac{2}{3} \left(\delta^2 z - \frac{1}{3} \delta a \delta b \right) J_{\alpha\beta}^{(0)} \left(\frac{w}{1-w} M_\alpha + M_\alpha + \frac{s}{1-s} M_\alpha, M_\alpha + \frac{r}{1-r} M_\beta, 0, 0, 0, 0 \right) \right] \quad (\text{B7})
 \end{aligned}$$

where $\delta a \equiv -\frac{\partial}{\partial a}$; $\delta b \equiv -\frac{\partial}{\partial b}$; $\delta c \equiv -\frac{\partial}{\partial c}$; $\delta d \equiv -\frac{\partial}{\partial d}$; $\delta x \equiv -\frac{\partial}{\partial x} + \frac{1}{2} \delta a + \frac{1}{2} \delta c$; $\delta y \equiv -\frac{\partial}{\partial y} + \frac{1}{2} \delta a + \frac{1}{2} \delta d$; $\delta z \equiv -\frac{\partial}{\partial z} + \frac{1}{2} \delta a + \frac{1}{2} \delta b$, and it is understood that the derivatives operators δ are applied before the substitution of the respective arguments. The vector elements, R_i^K , for $1 \leq i \leq 6N + 6$ are calculated by substituting the expressions (3.27-3.29) into the right hand side of equation (3.9-3.11), multiplying by the functions $S_{\frac{3}{2}}^i(\gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u} = \tilde{\partial}_{w^i} G_{\frac{3}{2}}(w, \gamma_\alpha u^2) \sqrt{\gamma_\alpha} \mathbf{u}$, and integrating over the velocities. The vector elements R_i^K for $6N + 7 \leq i \leq 8N + 8$ are calculated by substituting the expressions (3.30) into the right hand side of equation (3.8), multiplying by the functions $S_{\frac{3}{2}}^i(\gamma_\alpha u^2) \gamma_\alpha^{3/2} \overline{\mathbf{u}\mathbf{u}} = \tilde{\partial}_{w^i} G_{\frac{3}{2}}(w, \gamma_\alpha u^2) \gamma_\alpha^{3/2} \overline{\mathbf{u}\mathbf{u}}$ and integrating over the velocities. The

results, for $1 \leq i \leq N+1$, are:

$$\begin{aligned}
R_i^K &= \frac{\pi^3}{\sqrt{M_A}} \frac{n_A}{\sqrt{\gamma_A}} \sum_p h_A^p \tilde{\partial}_{w^i, s^p} \hat{R}_A^T(w; s) \\
R_{i+(N+1)}^K &= \frac{\pi^3}{\sqrt{M_B}} \frac{n_B}{\sqrt{\gamma_B}} \sum_p h_B^p \tilde{\partial}_{w^{N+1}, s^p} \hat{R}_B^T(w; s) \\
R_{i+(2N+2)}^K &= \frac{\pi^3}{\sqrt{M_A}} \frac{n_A}{\sqrt{\gamma_A}} \sum_p h_A^p \tilde{\partial}_{w^i, s^p} \hat{R}_A^n(w; s) \\
R_{i+(3N+3)}^K &= \frac{\pi^3}{\sqrt{M_B}} \frac{n_B}{\sqrt{\gamma_B}} \sum_p h_B^p \tilde{\partial}_{w^i, s^p} \hat{R}_B^n(w; s) \\
R_{i+(4N+4)}^K &= \frac{\pi^3}{\sqrt{M_A}} \sum_p \left(h_A^p + c \frac{\partial h_A^{(p)}}{\partial c} \right) \tilde{\partial}_{w^i, s^p} \hat{R}_A^c(w; s) \\
R_{i+(5N+5)}^K &= \frac{\pi^3}{\sqrt{M_B}} \sum_p \left(-\frac{c}{1-c} h_B^p + c \frac{\partial h_B^p}{\partial c} \right) \tilde{\partial}_{w^i, s^p} \hat{R}_B^c(w; s) \\
R_{i+(6N+6)}^K &= \frac{5\pi^3}{\sqrt{M_A}} \sum_p h_A^p \tilde{\partial}_{w^i, s^p} \hat{R}_A^V(w, s) \\
R_{i+(7N+7)}^K &= \frac{5\pi^3}{\sqrt{M_B}} \sum_p h_B^{(p)} \tilde{\partial}_{w^i, s^p} \hat{R}_B^V(w, s)
\end{aligned}$$

where the generating functions \hat{R}_α^V , \hat{R}_α^T , \hat{R}_α^n , and \hat{R}_α^c are given by:

$$\hat{R}_\alpha^c(w; s) = \frac{3}{2} \frac{(1-s)}{(1-ws)^{\frac{5}{2}}} \quad (\text{B 8})$$

$$\hat{R}_\alpha^n(w; s) = \left(1 - \frac{nm_0}{\rho} M_\alpha \frac{1}{1-s} \right) \hat{R}_\alpha^c(w; s) \quad (\text{B 9})$$

$$\hat{R}_\alpha^T(w; s) = -\frac{5}{2} \left(1 - \frac{\left(\frac{1}{1-s} \right)}{\left(\frac{w}{1-w} + \frac{s}{1-s} + 1 \right)} \right) \hat{R}_\alpha^c(w; s) + \hat{R}_\alpha^n(w; s) \quad (\text{B 10})$$

$$\hat{R}_\alpha^V(w; s) = \frac{(1-s)}{(1-ws)^{\frac{7}{2}}} \quad (\text{B 11})$$

Appendix C. The super generating function

Most of the generating functions necessary to derive the constitutive relations can be expressed in terms of derivatives of “super-generating” functions, $J_{\alpha\beta}^{(k)}$ defined by:

$$J_{\alpha\beta}^{(k)}(a, b, c, d, x, y, z) \equiv \int \frac{\rho_{\alpha\beta}(e)}{e^{2k}} \int_{\mathbf{u}_{12} \cdot \hat{\mathbf{k}} > 0} d\mathbf{u}_1 d\mathbf{u}_2 d\hat{\mathbf{k}} (\mathbf{k} \cdot \mathbf{u}_{12}) e^{-F} de \quad (\text{C 1})$$

where $\hat{\mathbf{k}}$ is a unit vector,

$$F \equiv au_1^2 + bu_2^2 + cu_1'^2 + du_2'^2 + \frac{x}{2} (\mathbf{u}_1 + \mathbf{u}_1')^2 + \frac{y}{2} (\mathbf{u}_1 + \mathbf{u}_2')^2 + \frac{z}{2} (\mathbf{u}_1 + \mathbf{u}_2)^2, \quad (\text{C 2})$$

primed vectors denote precollisional velocities, unprimed vectors denotes postcollisional velocities, and the collision law relating the two is given in Eq. (2.1). The indices α and β denote the species' identities as explained in the text following Eq. (2.1). Calculation yields:

$$J_{\alpha\beta}^{(k)} = \frac{2\pi^{\frac{7}{2}}}{\lambda^{\frac{3}{2}}} \int \frac{\rho_{\alpha\beta}(e)}{e^{2k}} \frac{1}{\mu_{\alpha\beta}(\nu_{\alpha\beta} + \mu_{\alpha\beta})} de \quad (\text{C } 3)$$

where $\lambda = a + b + c + d + 2x + 2y + 2z$ and:

$$\begin{aligned} \mu_{\alpha\beta} &= R_{\alpha\beta} - \frac{K_{\alpha\beta}^2}{\lambda} \\ \nu_{\alpha\beta} &= S_{\alpha\beta}^2 - \frac{(1+e)}{\lambda e} ((d+y) M^{\alpha\beta} - (c+x) M^{\beta\alpha}) \\ &\quad \times \left(2K_{\alpha\beta} + \frac{1+e}{e} ((d+y) M^{\alpha\beta} - (c+x) M^{\beta\alpha}) \right) \end{aligned}$$

with

$$\begin{aligned} R_{\alpha\beta} &= (a + c + 2x) (M^{\beta\alpha})^2 + (b + d) (M^{\alpha\beta})^2 \\ &\quad + \frac{1}{2} (M^{\alpha\beta} - M^{\beta\alpha})^2 (y + z) \\ S_{\alpha\beta} &= \frac{1+e}{2e} \left[\left(\frac{1+e}{e} - 2 \right) \left((2c+x) (M^{\beta\alpha})^2 \right. \right. \\ &\quad \left. \left. + (M^{\alpha\beta})^2 (2d+y) \right) + 2M^{\alpha\beta} M^{\beta\alpha} y - 2(M^{\beta\alpha})^2 x \right] \\ K_{\alpha\beta} &= (M^{\beta\alpha} (a + c + 2x + y + z) - M^{\alpha\beta} (b + d + y + z)). \end{aligned}$$

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