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Exact solution of the Gross–Krook kinetic model for a multicomponent gas in steady Couette flow

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Abstract

The Gross–Krook (GK) kinetic model of the Boltzmann equation for a multicomponent mixture is exactly solved in a steady state with velocity and temperature gradients (Couette flow). The hydrodynamic fields, heat and momentum fluxes, and the velocity distribution functions are determined explicitly in terms of the shear rate and the thermal gradient. The description applies for conditions arbitrarily far from equilibrium and is not restricted to specific values of the mechanical parameters of the mixture. This work completes a previous study (Physica A 289 (2001) 37) based on a formal series representation of the velocity distribution function. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Exact solutions in kinetic theory for spatially inhomogeneous states are exceedingly rare, see for instance, Ref. [1]. The difficulties increase considerably in the case of multicomponent systems since not only is the number of transport coefficients higher than for a single gas, but also new parameters (such as the mass ratios, molar fractions and size ratios) must be taken into account. This complexity leads us to consider tractable situations for which a complete description can be given. In the context of the low-density multicomponent mixtures, and to the best of our knowledge, the only two exact solutions to the Boltzmann equation correspond to the so-called color

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conductivity problem [2] and the uniform shear flow state [3]. These solutions apply to far from equilibrium conditions and have only two limitations: first, they are restricted to Maxwell molecules (r^{-5} intermolecular force), and second, they do not provide the explicit expression of the velocity distribution functions. These limitations can be overcome analytically by using convenient model kinetic equations [4,5]. In general, the predictions of these models present a quite good agreement with those found in the Boltzmann equation, even when the strength of the gradients are not small. This fact indicates again the reliability of the kinetic models in computing *nonlinear* transport properties in a multicomponent mixture.

A much more complicated nonequilibrium problem is the steady Couette planar flow. It corresponds to a fluid mixture between parallel plates in relative motion and kept, in general, at different temperatures. These boundary conditions lead to combined heat and momentum transport and the hydrodynamic balance equations become

$$\frac{\partial}{\partial y} P_{xy} = \frac{\partial}{\partial y} P_{yy} = 0, \quad (1)$$

$$\frac{\partial}{\partial y} q_y = -P_{xy} \frac{\partial}{\partial y} u_x, \quad (2)$$

where \mathbf{P} is the pressure tensor, \mathbf{q} is the heat flux, \mathbf{u} is the flow velocity, the x -axis is parallel to the direction of motion while the y -axis is orthogonal to the plates. In the above equations we have assumed that there is no diffusion in the mixture and the gradients are only directed along the y -axis. The balance Eqs. (1) and (2) do not constitute a closed set. Nevertheless, when the strength of the gradients is weak, the fluxes are well described by the Navier–Stokes (NS) relations, i.e., [6]

$$P_{xx} = P_{yy} = P_{zz} = p, \quad P_{xy} = -\eta_{NS} \frac{\partial u_x}{\partial y}, \quad (3)$$

$$q_x = 0, \quad q_y = -\lambda_{NS} \frac{\partial T}{\partial y}, \quad (4)$$

where p is the hydrostatic pressure, and η_{NS} and λ_{NS} are the NS shear viscosity and thermal conductivity, respectively.

On the other hand, when the hydrodynamic gradients are not small, the NS constitutive equations are not expected to hold and the transport must be described by nonlinear equations. In order to characterize the deviations from the NS relations, it is usual to introduce *generalized* transport coefficients, namely, a generalized shear viscosity η , the viscometric functions $\Psi_{1,2}$ (measuring normal stress differences), the generalized thermal conductivity λ , and a coefficient Φ measuring cross effects. These nonlinear transport coefficients are defined as

$$P_{xy} = -\eta \frac{\partial u_x}{\partial y}, \quad (5)$$

$$P_{yy} - P_{xx} = \Psi_1 \left(\frac{\partial u_x}{\partial y} \right)^2, \quad (6)$$

$$P_{zz} - P_{yy} = \Psi_2 \left(\frac{\partial u_x}{\partial y} \right)^2, \quad (7)$$

$$q_y = -\lambda \frac{\partial T}{\partial y}, \quad (8)$$

$$q_x = -\Phi \frac{\partial T}{\partial y}. \quad (9)$$

In general, these coefficients are nonlinear functions of the velocity and temperature gradients as well as of the mechanical parameters of the mixture. When the gradients are small, the NS equations are recovered, i.e., $\eta \rightarrow \eta_{NS}$, $\Psi_1 \rightarrow 0$, $\Psi_2 \rightarrow 0$, $\lambda \rightarrow \lambda_{NS}$, and $\Phi \rightarrow 0$.

Recently, the above generalized coefficients have been evaluated from the Gross–Krook (GK) kinetic model of the Boltzmann equation for Maxwell molecules [7]. Explicit expressions for the heat and momentum fluxes were obtained [8] from properties of a formal series representation of the velocity distribution functions, although the distribution functions themselves were not explicitly constructed. The objective here is to remove this formal element of Ref. [8] by giving explicitly the exact distribution functions and determining from them the generalized transport coefficients. In addition, given that the results derived in Ref. [8] were restricted to Maxwell molecules, we will also consider a generalization of the GK model [9] for a binary mixture where the effective collision frequencies depend on the partial *temperatures* of each species. This allows for the consideration of general repulsive intermolecular forces.

The paper is organized as follows. In Section 2, we introduce the GK model for an N -component mixture and the steady Couette flow is briefly described. Based on the formal solution obtained previously [8], we propose a solution characterized by constant pressure and linear velocity and parabolic temperature profiles with respect to a scaled variable. To confirm that this self-consistent ansatz for the hydrodynamic fields is correct, an exact solution to the GK model for this state is explicitly constructed in Section 3. This exact (normal) solution is obtained by exploiting the symmetry of the problem to guess the appropriate hydrodynamic fields. Then, we compute the generalized transport coefficients defined through Eqs. (5)–(9) from the explicit form of the generating function of the velocity distribution functions. Only the main results are quoted in this section since the details of the calculations are provided in Appendices A and B. The results obtained here for the hydrodynamic fields and the transport coefficients agree with and justify those of the previous formal analysis [8]. The simple case of a binary mixture is considered in Section 4 where the dependence of the transport coefficients and the distribution functions on the shear rate and the thermal gradient is illustrated for different values of the parameters of the mixture. Finally, the results are summarized and discussed in Section 5.

2. The kinetic model and the problem

The physical system considered is an N -component mixture in the low-density regime in steady Couette flow. The mixture of gases is enclosed between two parallel plates at $y = \pm L$ in relative motion along the x -axis and kept, in general, at different temperatures.

The resulting flow velocity is along the x -axis and, from symmetry, it is expected that the hydrodynamic fields vary only in the y direction. Since the molar fraction of species are constant (absence of mutual diffusion), the transport of momentum and energy are the relevant transport phenomena occurring in the system. Our goal is to provide an exact description of such state in terms of the imposed gradients and the mechanical parameters of the mixture (masses, concentrations, and sizes).

An appropriate theoretical description can be offered by means of the set of N coupled Boltzmann equations [10] for the distribution of velocities at each position $f_i(y, \mathbf{v})$ ($i = 1, \dots, N$). However, the intricacy of the Boltzmann collision operators hinders an exact analysis of the *nonlinear* Couette flow problem, even for a single gas. This prompts the use of a kinetic model which preserves the most important qualitative features of macroscopic transport. Specifically, we consider a generalization of the well-known Gross–Krook (GK) model [7] (proposed for Maxwell molecules) to repulsive intermolecular forces of the form $\mathbf{F}_{ij} = \kappa_{ij} r^{-\ell} \hat{\mathbf{r}}$ ($\ell = 5, \dots, \infty$). In the geometry of the Couette flow, the GK model reads

$$v_y \frac{\partial}{\partial y} f_i = -v_{ii}(f_i - f_{ii}) - \sum_{j \neq i} v_{ij}(f_i - f_{ij}), \quad (10)$$

where the reference distribution functions f_{ij} are given by

$$f_{ij} = n_i \left(\frac{m_i}{2\pi k_B T_{ij}} \right)^{3/2} \exp \left[-\frac{m_i}{2k_B T_{ij}} (\mathbf{v} - \mathbf{u}_{ij})^2 \right], \quad (11)$$

with

$$\mathbf{u}_{ij} = \frac{m_i \mathbf{u}_i + m_j \mathbf{u}_j}{m_i + m_j}, \quad (12)$$

$$T_{ij} = T_i + 2 \frac{m_i m_j}{(m_i + m_j)^2} \left[(T_j - T_i) + \frac{m_i}{6k_B} (\mathbf{u}_i - \mathbf{u}_j)^2 \right]. \quad (13)$$

The influence of the interaction law enters through the effective collision frequencies v_{ij} characterizing collisions between particles of species i with particles of species j :

$$v_{ij} = A(\delta) n_j \left(\kappa_{ij} \frac{m_i + m_j}{m_i m_j} \right)^{(1-\delta)/2} \left(\frac{2k_B T_i}{m_i} + \frac{2k_B T_j}{m_j} \right)^{\delta/2}, \quad (14)$$

$\delta = (\ell - 5)/(\ell - 1)$ and $A(\delta)$ is a (tabulated) constant for a given interparticle potential [11]. This dependence of the effective collision frequencies on the temperature of each species is the key difference between our generalized GK-type model and the familiar GK model for Maxwell molecules. The quantities \mathbf{u}_{ij} , T_{ij} , and v_{ij} are determined by imposing that the total momentum and energy are conserved and that the first five collisional moments as computed with the right-hand side of Eq. (10) be the same as those computed with the exact Boltzmann collision integrals. In the above equations, we have introduced the local number density n_i , mean velocity \mathbf{u}_i , and partial temperature

T_i of species i defined as

$$\{n_i, n_i \mathbf{u}_i, 3n_i k_B T_i\} = \int d\mathbf{v} \{1, \mathbf{v}, m_i (\mathbf{v} - \mathbf{u}_i)^2\} f_i. \tag{15}$$

From these partial quantities, one can define the total number density $n = \sum_i n_i$, the flow velocity

$$\mathbf{u} = \frac{\sum_i m_i n_i \mathbf{u}_i}{\sum_i m_i n_i}, \tag{16}$$

and the temperature T of the mixture (which is the relevant one at a hydrodynamic level)

$$n k_B T = \sum_{i=1}^N \left[n_i k_B T_i + \frac{1}{3} m_i n_i (\mathbf{u}_i - \mathbf{u})^2 \right]. \tag{17}$$

Apart from the densities of conserved quantities, one can define the pressure tensor (related to the transport of momentum)

$$\mathbf{P} = \sum_{i=1}^N \mathbf{P}_i = \sum_{i=1}^N \int d\mathbf{v} m_i \mathbf{V} \mathbf{V} f_i, \tag{18}$$

and the heat flux (related to the transport of energy)

$$\mathbf{q} = \sum_{i=1}^N \mathbf{q}_i = \sum_{i=1}^N \int d\mathbf{v} m_i V^2 \mathbf{V} f_i. \tag{19}$$

Here, $\mathbf{V} = \mathbf{v} - \mathbf{u}$ is the peculiar velocity.

Although simple in structure, the set of Eqs. (10) are highly nonlinear due to the coupling between f_{ij} and the hydrodynamic fields and, in general, it is necessary to employ numerical methods. However, here the simplicity of steady Couette flow suggests that it may be possible to *guess* the form of n_i , \mathbf{u}_i , and T_i . With these known, the GK model (10) becomes a linear problem whose solution is easy. This was the procedure followed in Ref. [8]. Here, we will also follow the same route although we will verify the consistency of the guess from an exact solution of the GK model instead of an asymptotic expansion. As in Ref. [8], we look for a normal solution, i.e., one for which the dependence of $f_i(y, \mathbf{v})$ on y occurs only through n_i , \mathbf{u} , and T . Therefore, it seems physically reasonable that the steady Couette flow for the mixture is characterized by (a) constant molar fractions $x_i = n_i/n$, (b) the absence of mutual diffusion, i.e., $\mathbf{u}_i = \mathbf{u}$, and (c) constant temperature ratios $\gamma_i \equiv T_i/T$. In addition, we assume that the partial pressure $p_i = n_i k_B T_i$ is uniform and the velocity $u_{i,x} = u_x$ and the partial temperature T_i have the forms:

$$\frac{1}{v_i(y)} \frac{\partial}{\partial y} u_{i,x} = a_i = \text{const.}, \tag{20}$$

$$\left[\frac{1}{v_i(y)} \frac{\partial}{\partial y} \right]^2 T_i = -\frac{2m_i}{k_B} \gamma_i(a_i) = \text{const.}, \tag{21}$$

where

$$v_i = \sum_{j=1}^N v_{ij} = v_{ii} + \sum_{j \neq i} v_{ij} \tag{22}$$

is the total collision frequency for a particle of species i . The conditions $\mathbf{u}_i = \mathbf{u}$ and $\chi_i = \text{const.}$ imply, respectively, that

$$v_i a_i = v_j a_j, \tag{23}$$

$$\frac{m_i \gamma_i v_i^2}{\chi_i} = \frac{m_j \gamma_j v_j^2}{\chi_j}, \tag{24}$$

where use has been made of the fact that the ratios v_i/v_j are constant. According to Eqs. (23) and (24), only one of the shear rates a_i and only one of the parameters γ_i ($i = 1, \dots, N$) is independent. The temperature ratios χ_i depend on the shear rate and the parameters of the mixture. Obviously, $\chi_i = 1$ if (i) the mixture is at equilibrium or (ii) the particles are mechanically equivalent ($m_i = m$ and $\kappa_{ij} = \kappa$).

In the next section the above hydrodynamic profiles are confirmed by an exact solution to the GK kinetic equation. In addition, this solution provides explicit expressions for the generalized transport coefficients η , $\Psi_{1,2}$, λ , and Φ as functions of the strength of the gradients and the parameters of the mixture.

3. Exact solution and transport coefficients

In order to solve the GK equations (10) it is convenient to reduce all the hydrodynamic fields with respect to a common collision frequency independent of the species considered. Since our description applies for arbitrary values of the mechanical parameters of the mixture, we choose for simplicity the collision frequency

$$v = \frac{1}{N(N-1)} \sum_{i=1}^N \sum_{j \neq i} \frac{n}{n_j} v_{ij}, \tag{25}$$

and introduce a space scaled variable s defined by $ds = v(y) dy$. Thus, the parameter

$$a = \frac{\partial u_x}{\partial s} = \text{const.} \tag{26}$$

is the dimensionless shear rate and is the relevant nonequilibrium parameter of the problem. Obviously, $a_i = (v/v_i)a$ and

$$\frac{\partial^2}{\partial s^2} T = - \frac{2m_i}{k_B} \frac{v_i^2 \gamma_i}{v^2 \chi_i} = \text{const.} \tag{27}$$

In terms of the variable s , the GK model becomes

$$\left(1 + v_y \frac{v}{v_i} \frac{\partial}{\partial s} \right) f_i = \sum_{j=1}^N \frac{v_{ij}}{v_i} f_{ij}. \tag{28}$$

The general solution to Eq. (28) is

$$f_i(s, \mathbf{v}) = f_{i,B}(s, \mathbf{v}) + \sum_{j=1}^N \frac{v_{ij}}{v} \int_0^\infty dt e^{-v_i t/v} e^{-w_y \hat{\sigma}_s} f_{ij}(s, \mathbf{v}). \quad (29)$$

The first term of the right-hand side of (29), $f_{i,B}$, is a solution to the homogeneous kinetic equation obtained from (28) by setting $f_{ij} \rightarrow 0$. The detailed form of this contribution is determined by the chosen boundary conditions. The physical boundary conditions are specified in terms of the half distributions for velocities directed away from the walls at $y = \pm L$, given explicitly or implicitly through the distributions for velocities directed at the walls. One possibility in the Couette flow problem is to use diffuse boundary conditions in which the distributions for velocities away from the walls are given by Maxwellians parametrized by the temperatures T_\pm and velocities U_\pm of the walls at $y = \pm L$. The distribution $f_{i,B}$ is responsible for the “boundary layers” effects near the wall while, the second term in the right-hand side of (29) corresponds to a *normal* solution where all its dependence on s appears only through the hydrodynamic fields. Here, we want to get rid of boundary effects and consider idealized boundary conditions to eliminate boundary layers. In the same way as in the simple gas problem [12], these idealized conditions correspond to the limit $T_\pm \rightarrow 0$, i.e., very cold walls. In this case it is easy to show that $f_{i,B} \rightarrow 0$. Thus, henceforth, we will only consider the second term in the right-hand side of Eq. (29).

It still remains to prove that the distribution (29) with this idealized boundary condition admits an exact solution for the steady Couette flow characterized by a constant partial pressure and by the profiles (20) and (21) (or (26) and (27)). The consistency conditions are

$$\int d\mathbf{v} \{1, \mathbf{V}, V^2\} f_i = \left\{ n_i, 0, 3 \frac{P_i}{m_i} \right\}. \quad (30)$$

These conditions are verified in Appendix A confirming that the distribution function (29) is an exact solution of the GK model in the steady Couette flow. The verification of the consistency of the solution provides the functional dependence of γ_i on the parameters of the problem. The details of the analysis are given in Appendix A, leading to the following implicit equation:

$$1 = \frac{4}{3\sqrt{\pi}} \sum_{j=1}^N \frac{v_{ij}}{v_i} \chi_{ij} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-t} [1 + (1 + a_i^2 t^2) u^2] (1 + 2\gamma_{ij} w^2)^{-1}, \quad (31)$$

where $w = ut$. In addition, $\gamma_{ij} = \chi_{ij} \gamma_i$, with

$$\chi_{ij} = \frac{T_{ij}}{T_i} = 1 + 2 \frac{m_i m_j}{(m_i + m_j)^2} \left(\frac{\chi_j}{\chi_i} - 1 \right). \quad (32)$$

The solution to the set of N coupled equations (31) must be subjected to the constraints (24) and

$$\sum_{i=1}^N x_i \chi_i = 1. \quad (33)$$

Therefore, we have N -independent equations (31) for a set of N unknowns, say for instance $\{\gamma_1, \chi_1, \dots, \chi_{N-1}\}$. The solution of these implicit equations provides the dependence of the curvature parameters γ_i and the temperature ratios χ_i on the shear rate and the mechanical parameters of the mixture.

The explicit expressions of the pressure tensor and the heat flux are also given in Appendix A. From them one can identify the generalized transport coefficients $\eta(a)$, $\Psi_1(a)$, $\Psi_2(a)$, $\lambda(a)$, and $\Phi(a)$ defined in Eqs. (5)–(9), respectively. The non-linear shear viscosity coefficient is

$$\eta(a) = \frac{4}{\sqrt{\pi}} nk_B T \sum_{i=1}^N \frac{x_i \chi_i}{v_i^2} \sum_{j=1}^N v_{ij} \chi_{ij} \int_0^\infty du e^{-u^2} u^2 \int_0^\infty dt e^{-t} t (1 + 2\gamma_{ij} w^2)^{-1}. \quad (34)$$

The viscometric functions characterizing normal stresses are

$$\begin{aligned} \Psi_1(a) = & -\frac{2}{\sqrt{\pi}} \frac{nk_B T}{v^2 a^2} \sum_{i=1}^N \frac{x_i \chi_i}{v_i} \sum_{j=1}^N v_{ij} \chi_{ij} \int_0^\infty du e^{-u^2} \\ & \times \int_0^\infty dt e^{-t} [1 - 2(1 + a_i^2 t^2) u^2] (1 + 2\gamma_{ij} w^2)^{-1}, \end{aligned} \quad (35)$$

$$\begin{aligned} \Psi_2(a) = & \frac{2}{\sqrt{\pi}} \frac{nk_B T}{v^2 a^2} \sum_{i=1}^N \frac{x_i \chi_i}{v_i} \sum_{j=1}^N v_{ij} \chi_{ij} \int_0^\infty du e^{-u^2} (1 - 2u^2) \\ & \times \int_0^\infty dt e^{-t} (1 + 2\gamma_{ij} w^2)^{-1}. \end{aligned} \quad (36)$$

The generalized thermal conductivity coefficient $\lambda(a)$ is

$$\begin{aligned} \lambda(a) = & \frac{4}{\sqrt{\pi}} nk_B^2 T \sum_{i=1}^N \frac{x_i \chi_i^2}{m_i v_i^2} \sum_{j=1}^N v_{ij} \chi_{ij}^2 \int_0^\infty du e^{-u^2} u \\ & \times \int_0^\infty dt e^{-t} w [1 + (1 + a_i^2 t^2) u^2] (1 + 2\gamma_{ij} w^2)^{-2}. \end{aligned} \quad (37)$$

Finally, the expression for the cross coefficient $\Phi(a)$ in the heat flux is

$$\begin{aligned} \Phi(a) = & -\frac{4}{\sqrt{\pi}} nk_B^2 T v a \sum_{i=1}^N \frac{x_i \chi_i^2}{m_i v_i^3} \sum_{j=1}^N v_{ij} \chi_{ij}^2 \int_0^\infty du e^{-u^2} u \\ & \times \int_0^\infty dt e^{-t} w t [2 + (1 + a_i^2 t^2) u^2] (1 + 2\gamma_{ij} w^2)^{-2}. \end{aligned} \quad (38)$$

An interesting and simple case corresponds to the limit of mechanically equivalent particles. In this case, $m_i = m$, $\kappa_{ij} = \kappa$, $v \propto nT^{\delta/2}$, $\gamma_i = \gamma$, and $\chi_i = 1$, so that the GK model reduces to the well-known Bathnagar–Gross–Krook (BGK) model for a single gas. Thus, Eqs. (34)–(38) reduce, respectively, to

$$\eta(a) = \frac{4}{\sqrt{\pi}} \frac{nk_B T}{v} \int_0^\infty du e^{-u^2} u^2 \int_0^\infty dt e^{-t} t (1 + 2\gamma w^2)^{-1}, \tag{39}$$

$$\Psi_1(a) = -\frac{2}{\sqrt{\pi}} \frac{nk_B T}{v^2 a^2} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-t} [1 - 2(1 - a^2 t^2)u^2] (1 + 2\gamma w^2)^{-1}, \tag{40}$$

$$\Psi_2(a) = \frac{2}{\sqrt{\pi}} \frac{nk_B T}{v^2 a^2} \int_0^\infty du e^{-u^2} (1 - 2u^2) \int_0^\infty dt e^{-t} (1 + 2\gamma w^2)^{-1}, \tag{41}$$

$$\lambda(a) = \frac{4}{\sqrt{\pi}} \frac{nk_B^2 T}{mv} \int_0^\infty du e^{-u^2} u \int_0^\infty dt e^{-t} w [1 + (1 + a^2 t^2)u^2] (1 + 2\gamma w^2)^{-2}, \tag{42}$$

$$\Phi(a) = -\frac{4}{\sqrt{\pi}} \frac{nk_B^2 T}{mv} a \int_0^\infty du e^{-u^2} u \int_0^\infty dt e^{-t} w t [2 + (1 + a^2 t^2)u^2] (1 + 2\gamma w^2)^{-2}. \tag{43}$$

These expressions coincide with those previously derived from an exact solution of the BGK model [12].

Apart from evaluating the transport properties, the use of the GK model allows one to explicitly get the velocity distribution functions f_i . These quantities provide all the complete information on the nonequilibrium state of the mixture. Taking into account the hydrodynamic (bulk) profiles (26) and (27), the distributions f_i can be written as (see the details in Appendix B)

$$f_i(s; \mathbf{V}) = \sum_{j=1}^N \frac{v_{ij}}{v} \Psi_{ij}(s; \mathbf{V}), \tag{44}$$

where

$$\begin{aligned} \Psi_{ij}(s; \mathbf{V}) = & f_i^{LE}(s, \mathbf{V}) e^{\xi_i^2} (\chi_i \chi_{ij})^{-3/2} \frac{2\alpha(1 + \alpha)^{3/2}}{\varepsilon_i |\xi_{i,y}|} \int_{w_0}^{w_1} dw [2w - (1 - \alpha)w^2]^{-5/2} \\ & \times \exp \left[-\frac{2\alpha}{1 + \alpha} \frac{v_i}{v} \frac{1 - w}{\varepsilon_i \xi_{i,y}} \right] \exp \left\{ -\frac{1 + \alpha}{2w - (1 - \alpha)w^2} (\chi_i \chi_{ij})^{-1} \right. \\ & \left. \times \left[\left(\xi_{i,x} + \frac{2\alpha}{1 + \alpha} \frac{1 - w}{\varepsilon_i} \right)^2 + \xi_{i,y}^2 + \xi_{i,z}^2 \right] \right\}. \end{aligned} \tag{45}$$

Here, $(w_0, w_1) = (0, 1)$ if $\xi_{i,y} > 0$ and $(w_0, w_1) = [1, 2/(1 - \alpha)]$ if $\xi_{i,y} < 0$. Furthermore, $\xi_i = (m_i/2k_B T)^{1/2} \mathbf{V}$,

$$f_i^{LE} = n_i \left(\frac{m_i}{2\pi k_B T} \right)^{3/2} \exp\left(-\frac{m_i}{2k_B T} V^2 \right), \quad (46)$$

is a local equilibrium distribution function of species i ,

$$\varepsilon_i = \sqrt{\frac{2k_B}{m_i T} \frac{\partial T}{\partial s}}, \quad (47)$$

is a reduced thermal gradient and

$$\alpha = \frac{\varepsilon_i}{\sqrt{\varepsilon_i^2 + 8\lambda_i}}, \quad (48)$$

with $\lambda_i = v_i^2 \gamma_i / v^2 \chi_i$.

In summary, the velocity distribution functions, hydrodynamic fields, and generalized transport coefficients for the steady Couette flow have been determined exactly in terms of the shear rate a , the thermal gradients ε_i , and the mechanical parameters characterizing the mixture. The final results are still given implicitly, but the problem has been reduced to quadratures. A numerical evaluation of these expressions will be done in the next section for the simple case of a binary mixture. Finally, let us mention that in Appendix C we show that all the above results are equivalent to those previously obtained by using a formal series representation [8]. This proves the consistency of our results.

4. A binary mixture

In this section we will numerically evaluate the expressions (31), (34)–(38), and (45) in the simple case of a binary mixture ($N = 2$). In this case, the (independent) parameters of the system are the mass ratio $\mu \equiv m_1/m_2$, the molar fraction x_1 , the size ratios $\omega_{11} \equiv \kappa_{11}/\kappa_{12}$ and $\omega_{22} \equiv \kappa_{22}/\kappa_{21}$, and the interaction parameter δ . First, we are interested in analyzing the shear-rate dependence of the temperature ratio T_1/T_2 and the transport coefficients η , $\Psi_{1,2}$, λ , and Φ for several values of the parameters of the mixture. For the sake of concreteness, we will consider the case $x_1 = 5/6$, $\omega_{11} = \omega_{22} = 1$, and two different values of the mass ratio: $\mu = 0.1$ and $\mu = 10$. We also consider the two extreme cases of Maxwell molecules ($\delta = 0$) and hard spheres ($\delta = 1$).

At a kinetic level, an interesting quantity is the temperature ratio. It measures the lack of equipartition of the total energy between both species. In Fig. 1 we plot T_1/T_2 as a function of the shear rate. We see how the traditional equipartition theorem fails in far from equilibrium situations. The deviations from the energy equipartition can be weak or strong depending on the strength of the shear rate as well as on the mechanical differences between the species. Thus, for finite shear rates, $T_1 \neq T_2$ even for not very disparate masses. This justifies the use of the so-called two-temperature theory [13]. With respect to the influence of the interaction potential, we see that the temperature ratio is practically independent of the scattering law considered.

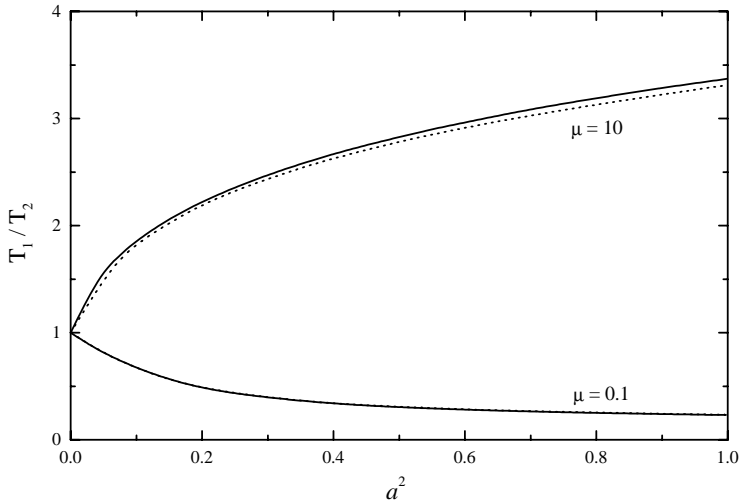


Fig. 1. Shear-rate dependence of the temperature ratio T_1/T_2 for $w_{11} = w_{22} = 1$, $x_1 = 5/6$, and two values of the mass ratio μ : $\mu = 10$, and $\mu = 0.1$. The solid lines correspond to Maxwell molecules ($\delta = 0$) while the dashed lines refer to hard spheres ($\delta = 1$).

Once the temperature ratio has been computed, one can study the shear-rate dependence of the generalized transport coefficients. Perhaps, the most important quantity in a sheared flow problem is the generalized shear viscosity $\eta(a)$. In Fig. 2 we plot the reduced shear viscosity $\eta(a)/\eta(0)$ where

$$\eta(0) = nk_B T \sum_{i=1}^2 \frac{x_i}{v_i} \tag{49}$$

is the Navier–Stokes shear viscosity coefficient. We observe that $\eta(a)$ decreases as a increases (shear thinning) whatever the interaction potential considered is. Concerning the dependence on the mass ratio we see that, at a given value of the shear rate, the generalized shear viscosity increases as the mass ratio m_1/m_2 decreases when $n_1/n_2 > 1$. In addition, for a given value of a , η increases (decreases) as the potential becomes harder when the excess component is heavier (lighter) than the defect component. In Figs. 3–6 we plot the remaining reduced transport coefficients $\Psi_1(a)/\Psi_1(0)$, $\Psi_2(a)/\Psi_2(0)$, $\lambda(a)/\lambda(0)$, and $\Phi(a)/\Phi(0)$, respectively. Here,

$$\Psi_1(0) = -2 \frac{nk_B T}{v^2} \sum_{i=1}^2 \frac{x_i}{v_i} \sum_{j=1}^2 v_{ij} \left(\frac{v^2}{v_i^2} + 2\gamma_{ij}^{(0)} \right), \tag{50}$$

$$\Psi_2(0) = 4 \frac{nk_B T}{v^2} \sum_{i=1}^2 \frac{x_i}{v_i} \sum_{j=1}^2 v_{ij} \gamma_{ij}^{(0)}, \tag{51}$$

$$\lambda(0) = \frac{5}{2} nk_B^2 T \sum_{i=1}^2 \frac{x_i}{m_i v_i}, \tag{52}$$

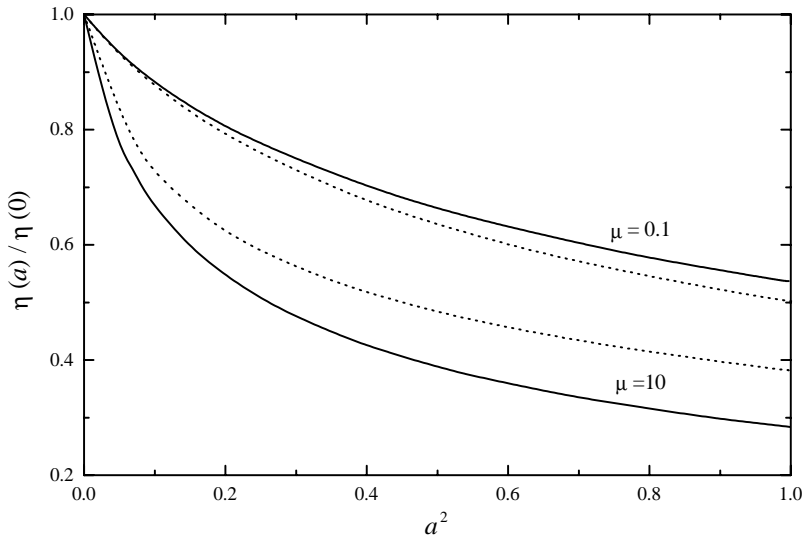


Fig. 2. Shear-rate dependence of the reduced shear viscosity $\eta(a)/\eta(0)$ for $w_{11} = w_{22} = 1$, $x_1 = 5/6$, and two values of the mass ratio μ : $\mu = 10$, and $\mu = 0.1$. The solid lines correspond to Maxwell molecules ($\delta = 0$) while the dashed lines refer to hard spheres ($\delta = 1$).

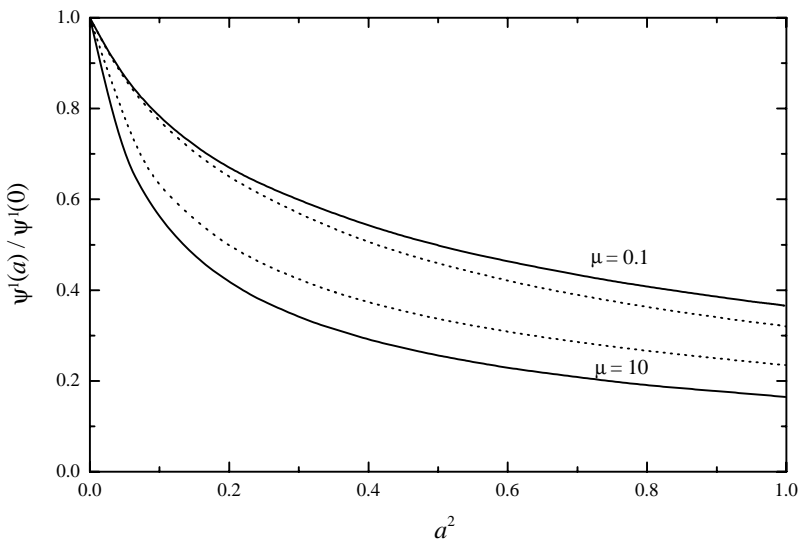


Fig. 3. Shear-rate dependence of the reduced first viscometric function $\Psi_1(a)/\Psi_1(0)$ for $w_{11} = w_{22} = 1$, $x_1 = 5/6$, and two values of the mass ratio μ : $\mu = 10$, and $\mu = 0.1$. The solid lines correspond to Maxwell molecules ($\delta = 0$) while the dashed lines refer to hard spheres ($\delta = 1$).

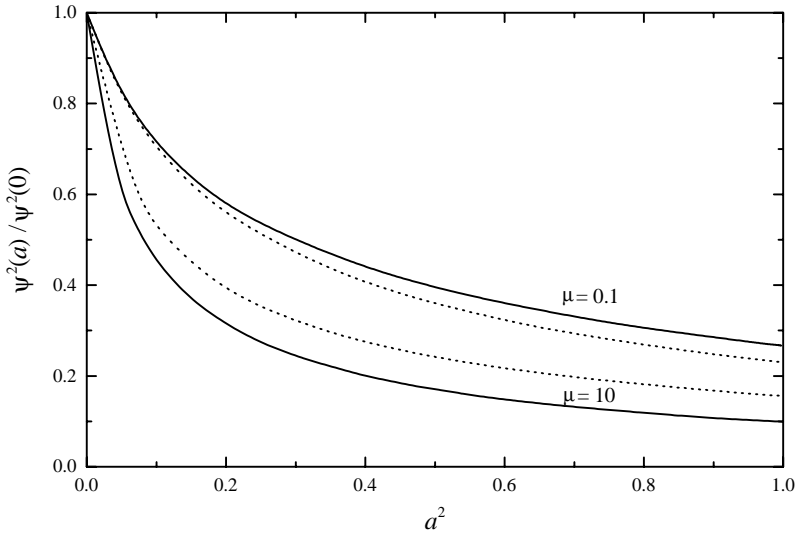


Fig. 4. Shear-rate dependence of the reduced second viscometric function $\Psi_2(a)/\Psi_2(0)$ for $w_{11} = w_{22} = 1$, $x_1 = 5/6$, and two values of the mass ratio μ : $\mu = 10$, and $\mu = 0.1$. The solid lines correspond to Maxwell molecules ($\delta = 0$) while the dashed lines refer to hard spheres ($\delta = 1$).

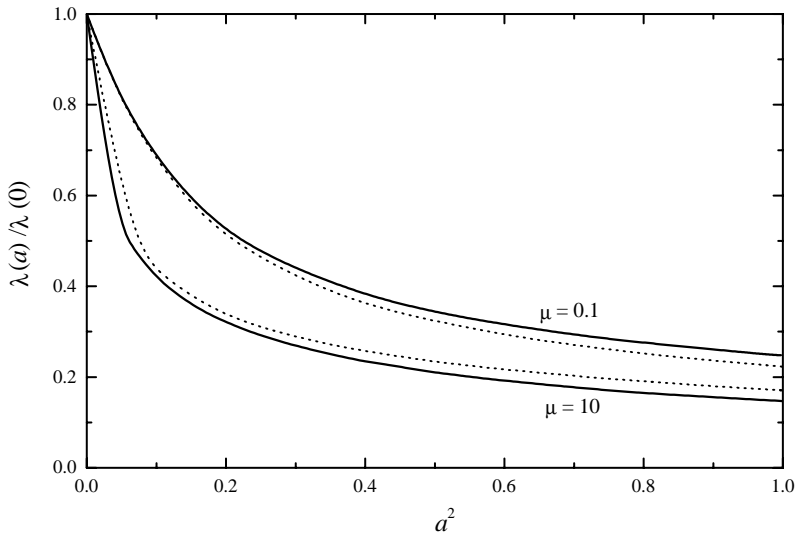


Fig. 5. Shear-rate dependence of the reduced thermal conductivity $\lambda(a)/\lambda(0)$ for $w_{11} = w_{22} = 1$, $x_1 = 5/6$, and two values of the mass ratio μ : $\mu = 10$, and $\mu = 0.1$. The solid lines correspond to Maxwell molecules ($\delta = 0$) while the dashed lines refer to hard spheres ($\delta = 1$).

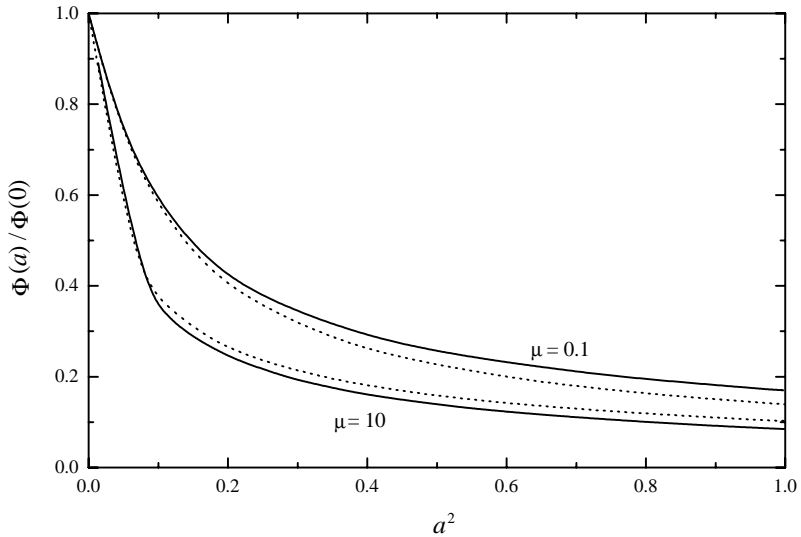


Fig. 6. Shear-rate dependence of the reduced cross coefficient $\Phi(a)/\Phi(0)$ for $w_{11} = w_{22} = 1$, $x_1 = 5/6$, and two values of the mass ratio μ : $\mu = 10$, and $\mu = 0.1$. The solid lines correspond to Maxwell molecules ($\delta = 0$) while the dashed lines refer to hard spheres ($\delta = 1$).

$$\Phi(0) = -7nk_B^2 T a v \sum_{i=1}^2 \frac{x_i}{m_i v_i^2}, \tag{53}$$

with

$$\gamma_{11}^{(0)} = \gamma_{12}^{(0)} = \frac{1}{5} \left(\frac{v}{v_1} \right)^2 \frac{v_1 v_{12} + v_2 v_{21}}{\mu v_1 v_{12} + v_2 v_{21}}, \tag{54}$$

and $\gamma_{22}^{(0)} = \gamma_{21}^{(0)} = (v_1^2/v_2^2)\mu\gamma_{11}^{(0)}$. In general, we observe that the dependence of these reduced coefficients on the shear rate is very similar to the one found for the shear viscosity, namely, the corresponding transport property decreases as a increases.

Since the velocity distribution function depends on the three components of ξ_i , it is useful to define the marginal distribution

$$R_{1,y}(\xi_{1,y}) = \frac{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_{1,x} d\xi_{1,z} f_1}{\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} d\xi_{1,x} d\xi_{1,z} f_1^{LE}}. \tag{55}$$

Figs. 7 and 8 show the shape of this distribution when the (reduced) shear rate $a = 1$ and the (reduced) thermal gradient $\varepsilon_1 = 1$. Further, $w_{11} = w_2 = 1$, $x_1 = 5/6$, $\mu = 0.1$, and $\mu = 10$ in the cases of Maxwell molecules and hard spheres. In general, the distortion from local equilibrium ($R_{1,y} = 1$) is quite important for the two mass ratios considered. We also observe that the qualitative differences between Maxwell molecules and hard spheres are more significant when the mass of the defect particles is smaller than that of the excess component, especially in the high-velocity region.

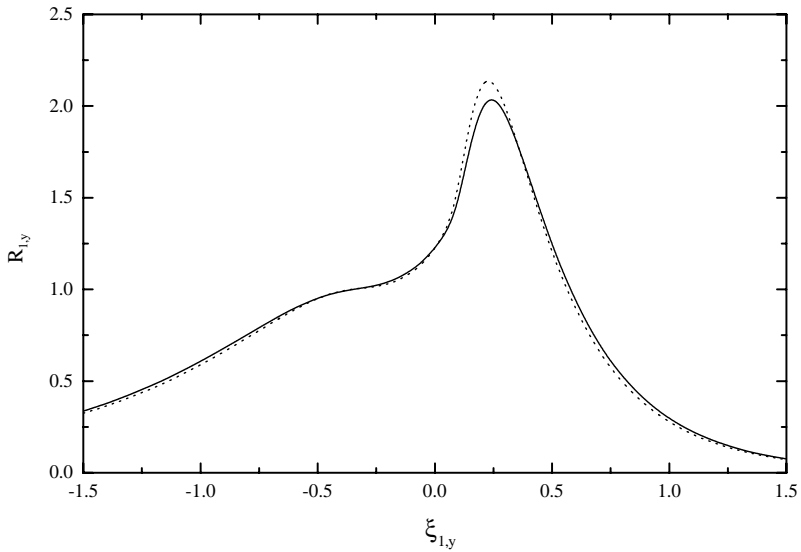


Fig. 7. Marginal distribution $R_{1,y}(\xi_{1,y})$ versus $\xi_{1,y}$ for $a = 1$ and $\epsilon_1 = 1$. The parameters characterizing the mixture are $w_{11} = w_{22} = 1$, $x_1 = 5/6$, and $\mu = 0.1$. The solid line refers to Maxwell molecules while the dotted line refers to hard spheres.

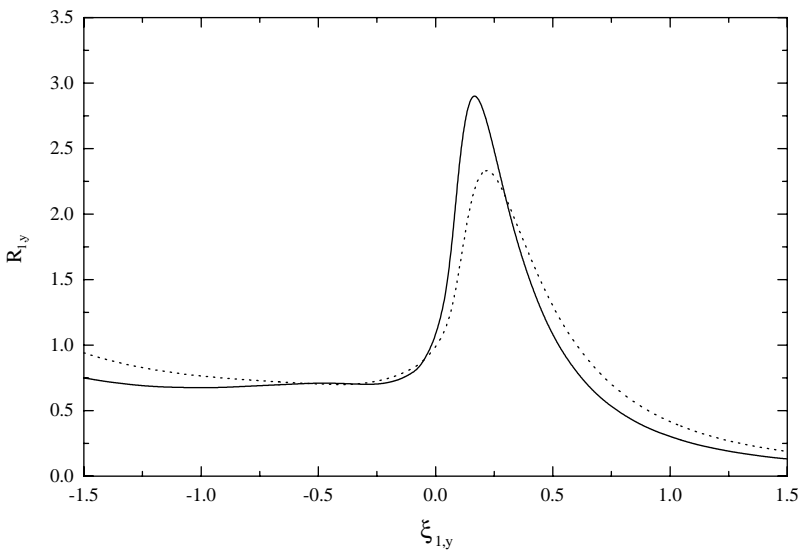


Fig. 8. Marginal distribution $R_{1,y}(\xi_{1,y})$ versus $\xi_{1,y}$ for $a = 1$ and $\epsilon_1 = 1$. The parameters characterizing the mixture are $w_{11} = w_{22} = 1$, $x_1 = 5/6$, and $\mu = 10$. The solid line refers to Maxwell molecules while the dotted line refers to hard spheres.

5. Discussion

An exact solution of the GK kinetic model of the Boltzmann equation for a multi-component mixture with repulsive intermolecular forces describing combined heat and momentum transport has been obtained. This nonequilibrium state is usually referred to as the steady Couette flow. The macroscopic state is characterized by constant partial pressures, no diffusion, and linear velocity and parabolic temperature profiles with respect to a given scaled variable (distance times the local collision frequency). Consequently, there are two parameters measuring the departure of the mixture from equilibrium: the shear rate and the thermal gradient. The main motivation of our work has been to get the transport properties and the velocity distribution functions for arbitrary values of the velocity and temperature gradients. In addition, no restriction to specific values of the parameters of the mixture (mass ratios, concentration ratios, and size ratios) is considered in our solution. This makes the analysis of this nonequilibrium problem more complicated than others, say for instance the case of uniform shear flow [3]. Progress has been possible here due to a previous analysis [8] based on a formal series solution of the GK model.

In Section 2, specific forms for the hydrodynamic fields have been postulated to hold for Couette flow. Then, in Section 3 an exact solution to the GK model kinetic equation has been constructed and the assumed forms for the densities, velocity and temperature have been consistently obtained from the corresponding distribution functions. In particular, the parameters γ_i (which measure the curvature of the parabolic temperature profiles) and the temperature ratios χ_i have been determined from the numerical solution of a set of N transcendent equations, Eqs. (31). Since we are interested in describing transport properties in the bulk of the system, we have considered idealized boundary conditions such that boundary layer complications are avoided and *simple* profiles are possible in the appropriate variables.

Once the temperature ratios are determined, the generalized transport coefficients η , Ψ_1 , Ψ_2 , λ , and Φ are explicitly obtained. Their expressions are given by Eqs. (34), (35), (36), (37), and (38), respectively. In general, these coefficients present a very complex dependence on the gradients as well as on the parameters of the mixture. The influence of the interaction potential considered appears through the effective collision frequencies v_{ij} , which depend on the temperature of each species. Apart from the transport properties, one of the main motivations of this paper has been to get the explicit form of the distribution functions f_i . Their expressions are given by Eqs. (44) and (45). Such distributions can be considered as *normal* solutions since all space dependence occurs entirely through the hydrodynamic fields.

To illustrate the dependence of the transport coefficients and the distributions on the parameters of the problem, the special case of a binary mixture is considered in Section 4. In general, we observe that the magnitude of the generalized transport coefficients decreases as the shear rate increases so that the main effect of the shear flow is to inhibit the transport of momentum and energy across the system. This inhibition is more significant when the defect component is lighter than the excess component, with independence of the model interaction considered. Concerning the influence of the interaction potential, the results for the main transport properties show that, by

a convenient scaling of the physical quantities, the reduced transport coefficients are rather insensitive to the choice of the interaction law. This influence is more significant as the mechanical differences between the two species and/or the strengths of gradients increase. With respect to the distribution functions, we observe that they are strongly distorted from their equilibrium values. This fact could be anticipated on the basis of the highly nonlinear dependence of the transport coefficients on the shear rate and the parameters of the mixture.

As a final comment, it is apparent that the results found here can also be of relevance in connection with computer simulations. As we have indicated in previous works, in the context of the Boltzmann equation, the so-called direct simulation Monte Carlo method [14] is an efficient tool to analyze nonlinear transport properties in a low-density fluid. We hope that this paper may stimulate the performance of Monte Carlo simulations to test the accuracy of the GK predictions. In the case of a single gas, recent computer simulations [15] have shown the reliability of the BGK kinetic model to study nonlinear transport in the Couette flow state.

Acknowledgements

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Appendix A. Consistency conditions and the fluxes

A.1. Generating function

The verification of the consistency conditions (30) requires the explicit form of the velocity distribution function f_i in terms of the hydrodynamic fields. To do this, it is convenient to refer the velocities of the particles to a local Lagrangian frame $\mathbf{V} = \mathbf{v} - \mathbf{u}$, so that f_i with the idealized boundary conditions is given by

$$f_i(s; \mathbf{V}) = \sum_{j=1}^N \frac{v_{ij}}{v} \int_0^\infty dt e^{-v_i t/v} e^{-tV_y \partial_s} e^{atV_y \partial_{v_x}} f_{ij}(s, \mathbf{V}). \quad (\text{A.1})$$

In this equation, the derivative ∂_s is taken at constant \mathbf{V} and the distribution f_{ij} is

$$f_{ij}(s; \mathbf{V}) = \Theta(T(s)) \frac{2p_{ij}}{m_i} \pi^{-3/2} v_{0,ij}^{-5}(s) \exp[-(V/v_{0,ij}(s))^2]. \quad (\text{A.2})$$

Here, $p_{ij} = n_i k_B T_{ij} \equiv \text{const.}$, $v_{0,ij}^2 = 2k_B T_{ij}(s)/m_i$ is the thermal velocity corresponding to the “temperature” T_{ij} and Θ is the Heaviside function. In terms of the variable s , the temperature profile becomes simply

$$T(s) = T_0 - \frac{m_i}{k_B} \lambda_i(a) s^2 = \frac{m_i \lambda_i}{k_B} (s_0^2 - s^2), \quad (\text{A.3})$$

where $\lambda_i = v_i^2 \gamma_i / v^2 \chi_i$ and $s_0 \equiv (k_B T_0 / m_i \lambda_i)^{1/2}$. Notice that, according to Eq. (24), $m_i \lambda_i = m_j \lambda_j$. Since the ratio T_{ij} / T is uniform, the dependence of T_{ij} on the scaled space variable s can be written as

$$T_{ij}(s) = \frac{m_i \lambda_{ij}}{k_B} (s_0^2 - s^2), \tag{A.4}$$

where $\lambda_{ij} = (v_i^2 / v^2) \gamma_{ij}$, with $\gamma_{ij} = \chi_{ij} \gamma_i$.

The velocity integrals for the consistency conditions and for the fluxes are the low-order moments of the distribution f_i . They can be obtained from appropriate derivatives of its corresponding generating function

$$\begin{aligned} G_i(s, \mathbf{k}) &= \int d\mathbf{V} e^{i\mathbf{k} \cdot \mathbf{V}} f_i(s, \mathbf{V}) \\ &= \sum_{j=1}^N \frac{v_{ij}}{v} \int_0^\infty dt e^{-v_i t / v} \int d\mathbf{V} e^{i\mathbf{k} \cdot \mathbf{V}} e^{-t V_y \partial_s} e^{at V_y \partial_{V_x}} f_{ij}(s, \mathbf{V}) \\ &\equiv \sum_{j=1}^N \frac{v_{ij}}{v} G_{ij}(s, \mathbf{k}), \end{aligned} \tag{A.5}$$

where the corresponding generating function G_{ij} can be easily identified from Eq. (A.5). Our goal now is to get the explicit expression of $G_{ij}(s, \mathbf{k})$. This function is given by

$$G_{ij}(s, \mathbf{V}) = \int_0^\infty dt e^{-v_i t / v} \int d\mathbf{V} e^{i\mathbf{k}'(t) \cdot \mathbf{V}} e^{-t V_y \partial_s} f_{ij}(s, \mathbf{V}), \tag{A.6}$$

where

$$\mathbf{k}'(t) = e^{-at k_x \partial_{k_y}} \mathbf{k}, \tag{A.7}$$

and in the last step we have made use of the identity

$$\int d\mathbf{V} F_1(\mathbf{V}) e^{at V_y \partial_{V_x}} F_2(\mathbf{V}) = \int d\mathbf{V} F_2(\mathbf{V}) e^{-at V_y \partial_{V_x}} F_1(\mathbf{V}). \tag{A.8}$$

Integration over $\mathbf{V}_\perp \equiv \mathbf{V} - V_y \hat{\mathbf{y}}$ leads to

$$G_{ij}(s, \mathbf{k}) = G_{ij}^{(+)}(s, \mathbf{k}) + G_{ij}^{(-)}(s, \mathbf{k}), \tag{A.9}$$

where

$$G_{ij}^{(\pm)}(s, \mathbf{k}) = \int_0^\infty dt e^{-v_i t / v} \int_0^\infty dV_y e^{\pm i k'_y(t) V_y} e^{\mp t V_y \partial_s} e^{-V_y^2 / v_{0,ij}^2(s)} F_{ij}(s, \mathbf{k}'_\perp), \tag{A.10}$$

with

$$F_{ij}(s; \mathbf{k}'_\perp) = \Theta(T(s)) \frac{2P_{ij}}{m_i} \pi^{-1/2} v_{0,ij}^{-3}(s) \exp \left[-\frac{1}{4} k'^2_\perp(t) v_{0,ij}^2(s) \right]. \tag{A.11}$$

We will focus on our attention in the calculation of $G_{ij}^{(+)}$ since $G_{ij}^{(+)}(s, \mathbf{k}) = G_{ij}^{(-)}(-s, -\mathbf{k})$.

Next, we consider the change of variables in the t integration, $z = V_y t$, and take into account the action of the shift operator

$$e^{-z\partial_s} f(s) = f(s - z). \tag{A.12}$$

The function $G_{ij}^{(+)}$ becomes

$$\begin{aligned} G_{ij}^{(+)}(s, \mathbf{k}) &= \int_0^\infty dz \int_0^\infty dV_y V_y^{-1} e^{-v_i z/v V_y} \\ &\times \exp \left[ik'_y(t) V_y - \frac{V_y^2}{v_{0,ij}^2(s-z)} \right] F_{ij}(s-z, \mathbf{k}'_\perp(t)) \\ &= \int_0^\infty dz \int_0^\infty du u^{-1} e^{-u^2} \\ &\times \exp \left[-\frac{v_i z}{v u v_{0,ij}(s-z)} + ik'_y(t) u v_{0,ij}(s-z) \right] F_{ij}(s-z, \mathbf{k}'_\perp(t)) \end{aligned} \tag{A.13}$$

where a change of variables in the V_y integral has been made, $V_y \rightarrow uv_{0,ij}(s-z)$. In this way, the variable t becomes: $t \rightarrow z/uv_{0,ij}(s-z)$. Next, for the z integral change variables to $w = z/v_{0,ij}(s-z)$. As a consequence, z as a function of w is $z = z_+(s, w)$, where $z_+(s, w)$ is the positive root of the quadratic equation

$$(1 + 2\lambda_{ij} w^2) z^2 - 4w^2 \lambda_{ij} s z - w^2 v_{0,ij}^2(s) = 0, \tag{A.14}$$

where use has been made of the relationship

$$\frac{v_{0,ij}^2(s-z)}{v_{0,ij}^2(s)} = 1 + \frac{2sz - z^2}{s_0^2 - s^2} = 1 + \frac{2\lambda_{ij}}{v_{0,ij}^2(s)} (2sz - z^2). \tag{A.15}$$

It can be shown that

$$\begin{aligned} \frac{dw}{dz} &= v_{0,ij}^{-1}(s-z) - z v_{0,ij}^{-2}(s-z) \frac{d}{dz} v_{0,ij}(s-z) \\ &= v_{0,ij}^{-1}(s-z) - z v_{0,ij}^2(s) v_{0,ij}^{-3}(s-z) \frac{s-z}{s_0^2 - s^2} \\ &= \left(\frac{w}{z_+} \right)^3 v_{0,ij}^2(s) \left(1 + \frac{s z_+}{s_0^2 - s^2} \right) \\ &= \left(\frac{w}{z_+} \right)^3 v_{0,ij}^2(s) \left[1 - \frac{z_+}{2} \partial_s \ln T_{ij}(s) \right]. \end{aligned} \tag{A.16}$$

Thus, the generating function $G_{ij}^{(+)}$ can be written as

$$\begin{aligned} G_{ij}^{(+)}(s, \mathbf{k}) &= \frac{2p_{ij}}{m_i v_{0,ij}^2(s) \pi^{1/2}} \int_0^\infty du u^{-1} e^{-u^2} \int_0^\infty dw e^{-v_i w/v u} \\ &\times \exp \left[ik'_y(t) \frac{uz_+}{w} - \frac{1}{4} k'^2_\perp(t) \frac{z_+^2}{w^2} \right] \left[1 - \frac{z_+}{2} \partial_s \ln T_{ij}(s) \right]^{-1}. \end{aligned} \tag{A.17}$$

Finally, change variables in the w integration to $t \rightarrow w/u$ leads to the explicit result

$$G_{ij}^{(+)}(s, \mathbf{k}) = \frac{P_{ij}}{\pi^{1/2}k_B T_{ij}} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-v_i t/v} A_{ij}^{(+)}(s, \mathbf{k}, u, t), \tag{A.18}$$

where

$$A_{ij}^{(+)}(s, \mathbf{k}, u, t) = \left[1 - \frac{z_+(s, w)}{2} \partial_s \ln T_{ij}(s) \right]^{-1} \times \exp \left[i(k_y - atk_x) \frac{z_+(s, w)}{t} - \frac{1}{4} k_\perp^2 \frac{z_+^2(s, w)}{u^2 t^2} \right]. \tag{A.19}$$

The function $G_{ij}^{(-)}(s, \mathbf{k}) = G_{ij}^{(+)}(-s, -\mathbf{k})$ is given by

$$G_{ij}^{(-)}(s, \mathbf{k}) = \frac{P_{ij}}{\pi^{1/2}k_B T_{ij}} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-v_i t/v} A_{ij}^{(-)}(s, \mathbf{k}, u, t), \tag{A.20}$$

where

$$A_{ij}^{(-)}(s, \mathbf{k}, u, t) = \left[1 - \frac{z_-(s, w)}{2} \partial_s \ln T_{ij}(s) \right]^{-1} \times \exp \left[i(k_y - atk_x) \frac{z_-(s, w)}{t} - \frac{1}{4} k_\perp^2 \frac{z_-^2(s, w)}{u^2 t^2} \right], \tag{A.21}$$

with $z_-(s, w) = -z_+(-s, w)$ being the negative root of the quadratic equation (A.14).

A.2. Consistency conditions

The consistency for the density is

$$\begin{aligned} \int d\mathbf{v} f_i &= G_i(s, \mathbf{k} = \mathbf{0}) = \sum_{j=1}^N \frac{v_{ij}}{v} G_{ij}(s, \mathbf{k} = \mathbf{0}) \\ &= \sum_{j=1}^N \frac{v_{ij}}{v} \frac{P_{ij}}{\pi^{1/2}k_B T_{ij}} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-v_i t/v} \\ &\quad \times \left\{ \left[1 - \frac{z_+}{2} \partial_s \ln T_{ij}(s) \right]^{-1} + \left[1 - \frac{z_-}{2} \partial_s \ln T_{ij}(s) \right]^{-1} \right\} \\ &= 2 \sum_{j=1}^N \frac{v_{ij}}{v_i} \frac{P_{ij}}{\pi^{1/2}k_B T_{ij}} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-t} \\ &= \frac{n_i}{v_i} \sum_{j=1}^N v_{ij} = n_i(s). \end{aligned} \tag{A.22}$$

Use has been made of the identity

$$\left[1 - \frac{z_+}{2} \partial_s \ln T_{ij}(s)\right]^{-1} + \left[1 - \frac{z_-}{2} \partial_s \ln T_{ij}(s)\right]^{-1} = 2, \tag{A.23}$$

which follows from the explicit form of the roots of (A.14). The result (A.23) is consistent with the definition of the partial density n_i .

The conditions for the flow velocity components are satisfied with independence of the values of λ_{ij} . The consistency condition for the partial temperature T_i is

$$\begin{aligned} 3n_i(s)k_B T_i(s) &= m_i \int d\mathbf{v} V^2 f_i = -m_i [\partial_{\mathbf{k}}^2 G_i(s, \mathbf{k})]_{\mathbf{k}=\mathbf{0}} = -m_i \sum_{j=1}^N \frac{v_{ij}}{v} [\partial_{\mathbf{k}}^2 G_{ij}(s, \mathbf{k})]_{\mathbf{k}=\mathbf{0}} \\ &= m_i \sum_{j=1}^N \frac{v_{ij}}{v} \frac{p_{ij}}{\pi^{1/2} k_B T_{ij}} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-v_i t/v} [1 + (1 + a^2 t^2) u^2] w^{-2} \\ &\quad \times \left\{ z_+^2 \left[1 - \frac{z_+}{2} \partial_s \ln T_{ij}(s)\right]^{-1} + z_-^2 \left[1 - \frac{z_-}{2} \partial_s \ln T_{ij}(s)\right]^{-1} \right\}. \end{aligned} \tag{A.24}$$

Using the identity

$$\begin{aligned} z_+^2 \left[1 - \frac{z_+}{2} \partial_s \ln T_{ij}(s)\right]^{-1} + z_-^2 \left[1 - \frac{z_-}{2} \partial_s \ln T_{ij}(s)\right]^{-1} \\ = \frac{4k_B T_{ij}(s)}{m_i} \frac{w^2}{1 + 2\lambda_{ij} w^2}, \end{aligned} \tag{A.25}$$

one gets the result

$$\begin{aligned} 3n_i k_B T_i \\ = \frac{4}{\sqrt{\pi}} \sum_{j=1}^N \frac{v_{ij}}{v} p_{ij} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-v_i t/v} [1 + (1 + a^2 t^2) u^2] (1 + 2\lambda_{ij} w^2)^{-1} \\ = \frac{4}{\sqrt{\pi}} \sum_{j=1}^N \frac{v_{ij}}{v_i} p_{ij} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-t} [1 + (1 + a_i^2 t^2) u^2] (1 + 2\gamma_{ij} w^2)^{-1}, \end{aligned} \tag{A.26}$$

where $a_i = va/v_i$. Eq. (A.26) can be finally written as

$$1 = \frac{4}{3\sqrt{\pi}} \sum_{j=1}^N \frac{v_{ij}}{v_i} \chi_{ij} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-t} [1 + (1 + a_i^2 t^2) u^2] (1 + 2\gamma_{ij} w^2)^{-1}. \tag{A.27}$$

This completes confirmation of the consistency conditions for the hydrodynamic fields.

A.3. Momentum and heat fluxes

The momentum and heat fluxes can also be obtained from the generating function as

$$P_{i,\alpha\beta} = \int d\mathbf{v} m_i V_\alpha V_\beta f_i = -m_i \sum_{j=1}^N \frac{v_{ij}}{v} [\partial_{k_\alpha} \partial_{k_\beta} G_{ij}(s, \mathbf{k})]_{\mathbf{k}=\mathbf{0}}, \tag{A.28}$$

$$q_{i,\alpha} = \int d\mathbf{v} \frac{1}{2} m_i V^2 V_\alpha f_i = i \frac{m_i}{2} \sum_{j=1}^N \frac{v_{ij}}{v} [\partial_{k_\alpha} \partial_{k^2} G_{ij}(s, \mathbf{k})]_{\mathbf{k}=\mathbf{0}}. \tag{A.29}$$

Following similar mathematical steps as those made in the consistency condition for the temperature, the nonzero elements of the partial pressure tensor can be evaluated. They are given by

$$P_{i,xx} = \frac{2}{\sqrt{\pi}} n_i k_B T_i \sum_{j=1}^N \frac{v_{ij}}{v_i} \chi_{ij} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-t} [1 + 2(a_i t u)^2] (1 + 2\gamma_{ij} w^2)^{-1}, \tag{A.30}$$

$$P_{i,yy} = \frac{4}{\sqrt{\pi}} n_i k_B T_i \sum_{j=1}^N \frac{v_{ij}}{v_i} \chi_{ij} \int_0^\infty du e^{-u^2} u^2 \int_0^\infty dt e^{-t} (1 + 2\gamma_{ij} w^2)^{-1}, \tag{A.31}$$

$$P_{i,zz} = \frac{2}{\sqrt{\pi}} n_i k_B T_i \sum_{j=1}^N \frac{v_{ij}}{v_i} \chi_{ij} \int_0^\infty du e^{-u^2} \int_0^\infty dt e^{-t} (1 + 2\gamma_{ij} w^2)^{-1}, \tag{A.32}$$

$$P_{i,xy} = -\frac{4}{\sqrt{\pi}} n_i k_B T_i a_i \sum_{j=1}^N \frac{v_{ij}}{v_i} \chi_{ij} \int_0^\infty du e^{-u^2} u^2 \int_0^\infty dt e^{-t} t (1 + 2\gamma_{ij} w^2)^{-1}. \tag{A.33}$$

It can be verified that these expressions satisfy $3n_i k_B T_i = P_{i,xx} + P_{i,yy} + P_{i,zz}$, which is consistent with the third condition in (30).

The nonzero components of the heat flux are $q_{i,x}$ and $q_{i,y}$. They are given by

$$q_{i,y} = -\frac{4}{\sqrt{\pi}} \frac{n_i k_B^2 T_i}{m_i v_i^2} v \sum_{j=1}^N v_{ij} \chi_{ij} \int_0^\infty du e^{-u^2} u \times \int_0^\infty dt e^{-t} [1 + (1 + a_i^2 t^2) u^2] w (1 + 2\gamma_{ij} w^2)^{-2} \partial_s T_{ij}(s), \tag{A.34}$$

$$q_{i,x} = \frac{4}{\sqrt{\pi}} \frac{n_i k_B^2 T_i}{m_i v_i^2} v \sum_{j=1}^N v_{ij} a_i \chi_{ij} \int_0^\infty du e^{-u^2} u \times \int_0^\infty dt e^{-t} t w [2 + (1 + a_i^2 t^2) u^2] (1 + 2\gamma_{ij} w^2)^{-2} \partial_s T_{ij}(s), \tag{A.35}$$

where use has been made of the identity

$$\begin{aligned}
 & z_+^3 \left[1 - \frac{z_+}{2} \partial_s \ln T_{ij}(s) \right]^{-1} + z_-^3 \left[1 - \frac{z_-}{2} \partial_s \ln T_{ij}(s) \right]^{-1} \\
 &= 16\lambda_{ij}s \frac{k_B T_{ij}(s)}{m_i} \frac{w^4}{(1 + 2\lambda_{ij}w^2)^2}.
 \end{aligned}
 \tag{A.36}$$

Appendix B. Velocity distribution function

In this appendix we derive the explicit expression of the velocity distribution function f_i given by Eqs. (44) and (45). First, the normal solution to the GK equation in the Couette flow problem is given by Eq. (A.1) so that the functions Ψ_{ij} appearing in Eq. (44) are given by

$$\Psi_{ij}(s; \mathbf{V}) = \int_0^\infty dt e^{-v_i t/v} e^{-tV_y \partial_s} e^{atV_y \partial_{V_x}} f_{ij}(s, \mathbf{V}).
 \tag{B.1}$$

Now, we assume the temperature profile (A.3) and introduce it in the form of the distribution (B.1). To do that, it is convenient to take into account the action of the exponential operator:

$$\exp[-tV_y \partial_s + atV_y \partial_{V_x}] f_{ij}(s, \mathbf{V}) = f_{ij}(s - tV_y, \mathbf{V} + ta \cdot \mathbf{V}),
 \tag{B.2}$$

where a is the matrix with elements $a_{ij} = a\delta_{ix}\delta_{jy}$. In terms of the reduced velocity $\xi_i = \mathbf{V}/\sqrt{2k_B T(s)/m_i}$ and using the property (B.2), Eq. (B.1) can be written as

$$\begin{aligned}
 \Psi_{ij}(s; \mathbf{V}) &= f_i^{LE}(s, \mathbf{V}) e^{\xi_i^2} (\chi_i \chi_{ij})^{-3/2} \int_0^\infty dt e^{-v_i t/v} [\theta(s^*, t\xi_{i,y})]^{-5/2} \Theta(\theta(s^*, t\xi_{i,y})) \\
 &\quad \times \exp\{-[\chi_i \chi_{ij} \theta(s^*, t\xi_{i,y})]^{-1} [(\xi_{i,x} + at\xi_{i,y})^2 + \xi_{i,y}^2 + \xi_{i,z}^2]\},
 \end{aligned}
 \tag{B.3}$$

where $s^* = s/\sqrt{k_B T_0/m_i}$,

$$f_i^{LE}(s; \mathbf{V}) = n_i \left(\frac{m_i}{2\pi k_B T(s)} \right)^{3/2} \exp\left(-\frac{m_i}{2k_B T(s)} V^2\right),
 \tag{B.4}$$

and

$$\theta(s^*, t\xi_{i,y}) \equiv \frac{T(s - tV_y)}{T(s)} = 1 + 2\sqrt{2}\lambda_i t \xi_{i,y} \frac{s^*}{\sqrt{1 - \lambda_i s^{*2}}} - 2\lambda_i t^2 \xi_{i,y}^2.
 \tag{B.5}$$

We decompose $\Psi_{ij}(s^*, \mathbf{V}) = \Psi_{ij}^{(+)}(s^*, \mathbf{V}) + \Psi_{ij}^{(-)}(s^*, \mathbf{V})$, with $\Psi_{ij}^{(\pm)}(s^*, \mathbf{V}) = \Theta(\pm \xi_{i,y}) \times \Psi_{ij}(s^*, \mathbf{V})$. Note that $\Psi_{ij}^{(+)}(-s^*) = \Psi_{ij}^{(-)}(s^*)$. We introduce the reduced local thermal gradient ε_i defined as

$$\begin{aligned}
 \varepsilon_i(s) &= \sqrt{\frac{2k_B}{m_i T(s)}} \frac{\partial T}{\partial s} \\
 &= -\frac{2\sqrt{2}\lambda_i s^*}{\sqrt{1 - s^{*2}}},
 \end{aligned}
 \tag{B.6}$$

where in the last step use has been made of the explicit form of the temperature profile. In terms of the variable $u = t_{\xi_{i,y}}^{\zeta}$, $\Psi_{ij}^{(+)}$ can be written as

$$\begin{aligned} \Psi_{ij}^{(+)}(s; \mathbf{V}) &= f_i^{LE}(s, \mathbf{V}) \frac{e_i^{\zeta_i^2}}{\xi_{i,y}^{\zeta}} (\chi_i \chi_{ij})^{-3/2} \\ &\times \int_0^\infty du e^{-v_i u / v \xi_{i,y}} (1 - \varepsilon_i u - 2\lambda_i u^2)^{-5/2} \Theta(1 - \varepsilon_i u - 2\lambda_i u^2) \\ &\times \exp \left\{ -(1 - \varepsilon_i u - 2\lambda_i u^2)^{-1} \frac{(\xi_{i,x} + au)^2 + \zeta_{i,y}^2 + \zeta_{i,z}^2}{\chi_i \chi_{ij}} \right\}. \end{aligned} \tag{B.7}$$

Due to the Heaviside function, $u < \beta_i$ where

$$\begin{aligned} \beta_i &= \frac{\sqrt{\varepsilon_i^2 + 8\lambda_i} - \varepsilon_i}{4\lambda_i} \\ &= \frac{1}{\varepsilon_i} \frac{2\alpha}{1 + \alpha} \end{aligned} \tag{B.8}$$

is the positive root of the quadratic equation $1 - \varepsilon_i u - 2\lambda_i u^2 = 0$. Here,

$$\alpha = \frac{\varepsilon_i}{\sqrt{\varepsilon_i^2 + 8\lambda_i}}, \tag{B.9}$$

which is independent of the species considered. Let us make the change of variables:

$$u = \frac{2\alpha}{1 + \alpha} \frac{1 - w}{\varepsilon_i} = \beta_i (1 - w). \tag{B.10}$$

Consequently,

$$\begin{aligned} 1 - \varepsilon_i \beta_i (1 - w) - 2\lambda_i \beta_i^2 (1 - w)^2 &= 1 - \varepsilon_i \beta_i - 2\lambda_i \beta_i^2 (1 + w^2) + w(\varepsilon_i \beta_i + 4\lambda_i \beta_i^2) \\ &= \frac{2w}{1 + \alpha} - \frac{1 - \alpha}{1 + \alpha} w^2, \end{aligned} \tag{B.11}$$

where use has been made of the identities:

$$\varepsilon_i \beta_i + 4\lambda_i \beta_i^2 = \varepsilon_i \beta_i + 2 - 2\varepsilon_i \beta_i = 2/(1 + \alpha), \tag{B.12}$$

$$2\lambda_i \beta_i^2 = 1 - \varepsilon_i \beta_i = (1 - \alpha)/(1 + \alpha). \tag{B.13}$$

In summary, Eq. (B.7) can be finally written as

$$\begin{aligned} \Psi_{ij}^{(+)}(s; \mathbf{V}) &= f_i^{LE}(s, \mathbf{V}) e_i^{\zeta_i^2} (\chi_i \chi_{ij})^{-3/2} \frac{2\alpha(1 + \alpha)^{3/2}}{\varepsilon_i \xi_{i,y}} \int_0^1 dw [2w - (1 - \alpha)w^2]^{-5/2} \\ &\times \exp \left[-\frac{2\alpha}{1 + \alpha} \frac{v_i}{v} \frac{1 - w}{\varepsilon_i \xi_{i,y}} \right] \exp \left\{ -\frac{1 + \alpha}{2w - (1 - \alpha)w^2} (\chi_i \chi_{ij})^{-1} \right. \\ &\times \left. \left[\left(\xi_{i,x} + \frac{2\alpha\alpha}{1 + \alpha} \frac{1 - w}{\varepsilon_i} \right)^2 + \zeta_{i,y}^2 + \zeta_{i,z}^2 \right] \right\}. \end{aligned} \tag{B.14}$$

The other half-distribution $\Psi_{ij}^{(-)}$ can be easily obtained from $\Psi_{ij}^{(+)}$ when one takes into account the symmetry property

$$\Psi_{ij}^{(-)}(a, \varepsilon_i; \mathbf{V}) = \Psi_{ij}^{(+)}(a, -\varepsilon_i; -\mathbf{V}). \tag{B.15}$$

Therefore, one gets

$$\begin{aligned} \Psi_{ij}^{(-)}(s; \mathbf{V}) &= f_i^{LE}(s, \mathbf{V}) e^{\zeta_i^2} (\chi_i \chi_{ij})^{-3/2} \frac{2\alpha(1+\alpha)^{3/2}}{\varepsilon_i |\zeta_{i,y}|} \int_1^{2/(1-\alpha)} dw [2w - (1-\alpha)w^2]^{-5/2} \\ &\quad \times \exp \left[-\frac{2\alpha}{1+\alpha} \frac{v_i}{v} \frac{1-w}{\varepsilon_i \zeta_{i,y}} \right] \exp \left\{ -\frac{1+\alpha}{2w - (1-\alpha)w^2} (\chi_i \chi_{ij})^{-1} \right. \\ &\quad \left. \times \left[\left(\zeta_{i,x} + \frac{2\alpha}{1+\alpha} \frac{1-w}{\varepsilon_i} \right)^2 + \zeta_{i,y}^2 + \zeta_{i,z}^2 \right] \right\}, \end{aligned} \tag{B.16}$$

where the change of variable $w \rightarrow [2 - (1 + \alpha)t]/(1 - \alpha)$ has been performed.

Appendix C. Equivalence with formal series solution

The results obtained in Ref. [8] from the formal series representation are expressed in terms of the functions

$$F_r(x) = \left(\frac{d}{dx} x \right)^r F_0(x), \tag{C.1}$$

where

$$\begin{aligned} F_0(x) &= \int_0^\infty dt t \int_0^\infty du u e^{-t^2 u^2 x/2} e^{-(t+u)} \\ &= \frac{2}{x} \int_0^\infty dt t e^{-t^2/2} K_0(2x^{-1/4} t^{1/2}), \end{aligned} \tag{C.2}$$

K_0 being the zeroth-order modified Bessel function. In terms of these functions, the momentum and heat fluxes can be written as¹

$$P_{i,xx} = \frac{n_i k_B T_i}{v_i} \sum_{j=1}^N v_{ij} \chi_{ij} [1 + 2F_1(\gamma_{ij})(a_i^2 - \gamma_{ij})], \tag{C.3}$$

$$P_{i,yy} = \frac{n_i k_B T_i}{v_i} \sum_{j=1}^N v_{ij} \chi_{ij} \{1 - 2\gamma_{ij}[F_1(\gamma_{ij}) + 2F_2(\gamma_{ij})]\}, \tag{C.4}$$

$$P_{i,zz} = \frac{n_i k_B T_i}{v_i} \sum_{j=1}^N v_{ij} \chi_{ij} [1 - 2\gamma_{ij} F_1(\gamma_{ij})], \tag{C.5}$$

¹ While working on this paper, we have found some errors in the expression of the xx element of the pressure tensor, namely Eqs. (32) and (45) of Ref. [8]. Their corresponding correct expressions are given here in the Appendix C. These errors do not alter the qualitative behavior and the conclusions made in Ref. [8] on the first viscometric function Ψ_1 .

$$P_{i,xy} = -\frac{n_i k_B T_i}{v_i} \sum_{j=1}^N v_{ij} \chi_{ij} F_0(\gamma_{ij}) a_i, \tag{C.6}$$

$$q_{i,y} = -\frac{1}{2} \frac{n_i k_B^2 T_i}{m_i v_i} \frac{v}{v_i} \sum_{j=1}^N v_{ij} \chi_{ij} \{3F_1(\gamma_{ij}) + 2F_2(\gamma_{ij}) + 2a_i^2 [4F_4(\gamma_{ij}) + 4F_3(\gamma_{ij}) + F_2(\gamma_{ij})]\} \partial_s T_{ij}(s), \tag{C.7}$$

$$q_{i,x} = \frac{n_i k_B^2 T_i}{m_i v_i} \frac{v}{v_i} a_i \sum_{j=1}^N v_{ij} \chi_{ij} \{5F_2(\gamma_{ij}) + 2F_3(\gamma_{ij}) + 2a_i^2 [4F_5(\gamma_{ij}) + 8F_4(\gamma_{ij}) + 5F_3(\gamma_{ij}) + F_2(\gamma_{ij})]\} \partial_s T_{ij}(s). \tag{C.8}$$

Let us show, for instance, that the expressions of the nonzero elements of the pressure tensor P_i given by Eqs. (A.30)–(A.33) are the same as those found in Ref. [8], Eqs. (C.3)–(C.6). First, taking into account the integral representation of K_0 [16], the function $F_0(\gamma_{ij})$ can be rewritten as

$$F_0(\gamma_{ij}) = \int_0^\infty dt t \int_0^\infty du e^{-t^2 u^2 \gamma_{ij}/2} e^{-(t+u)} = \frac{4}{\sqrt{\pi}} \int_0^\infty dt e^{-t} \int_0^\infty du u^2 e^{-u^2} (1 + 2\gamma_{ij} u^2 t^2)^{-1}. \tag{C.9}$$

Substitution of Eq. (C.9) into Eq. (C.6) leads to Eq. (A.33) for the xy element of P_i . Then, the function $F_1(\gamma_{ij})$ is given by

$$F_1(\gamma_{ij}) = \frac{d}{d\gamma_{ij}} (\gamma_{ij} F_0(\gamma_{ij})) = \frac{4}{\sqrt{\pi}} \int_0^\infty dt e^{-t} \int_0^\infty du u^2 e^{-u^2} (1 + 2\gamma_{ij} u^2 t^2)^{-2} = \frac{1}{2} \gamma_{ij}^{-1} - \frac{1}{\sqrt{\pi}} \gamma_{ij}^{-1} \int_0^\infty dt e^{-t} \int_0^\infty du e^{-u^2} (1 + 2\gamma_{ij} u^2 t^2)^{-1}, \tag{C.10}$$

where the last equality has been obtained after integrating by parts in the t integral. From Eqs. (C.10) and (C.5), one gets the expression (A.32) for $P_{i,zz}$. The function $F_2(\gamma_{ij})$ is given by

$$F_2(\gamma_{ij}) = \frac{d}{d\gamma_{ij}} (\gamma_{ij} F_1(\gamma_{ij})) = \frac{2}{\sqrt{\pi}} \int_0^\infty dt t^2 e^{-t} \int_0^\infty du u^2 e^{-u^2} (1 + 2\gamma_{ij} u^2 t^2)^{-2}. \tag{C.11}$$

Substitution of Eqs. (C.10) and (C.11) into Eq. (C.4) yields Eq. (A.31) when one takes into account the following integration by parts in the u integral:

$$\int_0^\infty du \frac{u^2 e^{-u^2}}{1 + 2\gamma_{ij} u^2 t^2} = \frac{1}{2} \int_0^\infty du e^{-u^2} \frac{1 - 2\gamma_{ij} u^2 t^2}{(1 + 2\gamma_{ij} u^2 t^2)^2}. \tag{C.12}$$

The expression (A.30) for $P_{i,xx}$ can be easily obtained from Eqs. (C.3) and (C.10).

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