

## Heat and momentum transport in a gaseous dilute solution

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(Received 3 February 1993)

A kinetic study of a gaseous dilute solution in a stationary nonequilibrium state is performed in the tracer limit. The state is characterized by the presence of velocity and temperature gradients (steady Couette flow) and uniform molar fraction. The results are derived from the Gross-Krook model [Phys. Rev. **102**, 593 (1956)] of the Boltzmann equation for a binary mixture. The ratio between the temperatures of the solute and the solvent, as well as the main transport coefficients, are obtained in terms of the shear rate and the mass and size ratios. Furthermore, the velocity distribution functions are explicitly derived.

PACS number(s): 51.10.+y, 05.20.Dd, 05.60.+w

### I. INTRODUCTION

The statistical-mechanical study of fluid mixtures far from equilibrium is a very interesting subject from a theoretical as well as a practical point of view. The general description of these systems is much more complicated than that of a single fluid. Not only is the number of transport coefficients much higher but also they are functions of parameters such as the molar fractions, the mass ratios, and the size ratios. Due to the complexity of the general problem, tractable specific situations must be considered.

Recently, generalized Green-Kubo formulas for self-diffusion [1] and mutual diffusion [2] tensors of a shearing fluid have been derived. In the case of dilute binary mixtures, where a Boltzmann description [3] is adequate, diffusion of tagged particles has also been analyzed in several nonequilibrium states [4–6]. Similar studies have been carried out to extend the previous problems to the case of unequal masses when the solute component is present in tracer concentration [7–10]. All these studies refer to situations in which the solvent is in a state arbitrarily far from equilibrium. On the other hand, the Fokker-Planck equation for a Brownian particle when the solvent is described by the first-order Chapman-Enskog approximation has been derived in Ref. [11].

In this paper, we consider a low-density binary mixture with a solute molar fraction much smaller than 1 (tracer limit). As a consequence, it is assumed that the state of the solvent is not disturbed by the presence of the solute particles. Further, the effect on the state of the solute of collisions among the solute particles themselves can be neglected. On the other hand, our description applies to arbitrary mass and size ratios. The mixture is in a steady planar Couette flow with a uniform molar fraction. Consequently, no mutual diffusion appears in the system. Because of the mathematical complexity embodied in the Boltzmann equation, no solution for the steady planar Couette flow is known, even in the case of a single gas. In order to avoid the above difficulties, we use the nonlinear

kinetic model for mixtures proposed by Gross and Krook (GK) [12], which is constructed in the same spirit as the well-known Bhatnagar-Gross-Krook (BGK) model for a single gas [13]. While keeping the main physical features of the Boltzmann equation, these models allow for the explicit derivation of the velocity distribution function. An exact solution of the BGK equation for the steady planar Couette flow has recently been found [14,15].

Here we are mainly interested in evaluating the coefficients describing the transport of momentum and energy associated with the solute particles. These coefficients are nonlinear functions of the mass and the size ratios and of the shear rate. In contrast to what happens in the case of tagged particles, the transport coefficients of the solute differ appreciably from those of the solvent. In particular, one can distinguish between two “temperatures” measuring the mean kinetic energy of each component.

The plan of the paper is as follows. Section II starts with a brief survey of the GK model. Then, the physical problem we are interested in is introduced. The section ends with a summary of the results derived from the BGK equation for a single gas in steady Couette flow. The temperature and the main transport properties of the solute are obtained as functions of the shear rate and the mass and size ratios in Sec. III. In addition, the velocity distribution function of the solute is studied. Finally, the conclusions are presented in Sec. IV.

### II. DESCRIPTION OF THE PROBLEM

Let us consider a dilute binary mixture, with  $f_i(\mathbf{r}, \mathbf{v}; t)$  being the one-particle velocity distribution function of species  $i$  ( $i = 1, 2$ ). They satisfy the set of two coupled Boltzmann equations [3]

$$\begin{aligned} \frac{\partial}{\partial t} f_1 + \mathbf{v} \cdot \nabla f_1 &= J_{11}[f_1, f_1] + J_{12}[f_1, f_2], \\ \frac{\partial}{\partial t} f_2 + \mathbf{v} \cdot \nabla f_2 &= J_{22}[f_2, f_2] + J_{21}[f_2, f_1]. \end{aligned} \quad (2.1)$$

The terms appearing on the right-hand side of Eq. (2.1) represent the self- and cross collisions, respectively. They conserve the number of particles of each species, the total momentum, and the total energy. The local number density and mean velocity of species  $i$  are defined, respectively, by

$$n_i = \int d\mathbf{v} f_i, \quad (2.2)$$

$$\mathbf{u}_i = \frac{1}{n_i} \int d\mathbf{v} \mathbf{v} f_i. \quad (2.3)$$

We also introduce a local temperature  $T_i$  for each species as

$$\frac{3}{2} n_i k_B T_i = \int d\mathbf{v} \frac{m_i}{2} (\mathbf{v} - \mathbf{u}_i)^2 f_i, \quad (2.4)$$

where  $k_B$  is the Boltzmann constant and  $m_i$  is the mass of a particle of species  $i$ .

Due to the complicated structure of the collision operators  $J_{ij}$ , it is a very hard problem to solve the coupled set of Boltzmann equations (2.1), especially in far from equilibrium situations. This fact has motivated the search for kinetic models in which the Boltzmann operators are replaced by simpler terms that preserve the main physical properties. Here we adopt the GK model [12], in which the terms  $J_{ij}[f_i, f_j]$  in Eq. (2.1) are replaced by simple relaxation terms of the form

$$\nu_{ij}(f_i - f_{ij}^R), \quad (2.5)$$

where  $\nu_{ij}$  is an effective collision frequency satisfying the general property  $n_i \nu_{ij} = n_j \nu_{ji}$ , and the reference distribution function  $f_{ij}^R$  is given by

$$f_{ij}^R = n_i \left( \frac{m_i}{2\pi k_B T_{ij}} \right)^{3/2} \exp \left[ -\frac{m_i}{2k_B T_{ij}} (\mathbf{v} - \mathbf{u}_{ij})^2 \right]. \quad (2.6)$$

In this equation,

$$\mathbf{u}_{ij} = (m_i \mathbf{u}_i + m_j \mathbf{u}_j) / (m_i + m_j), \quad (2.7)$$

$$T_{ij} = T_i + 2 \frac{m_i m_j}{(m_i + m_j)^2} \left[ (T_j - T_i) + \frac{m_j}{6k_B} (\mathbf{u}_i - \mathbf{u}_j)^2 \right]. \quad (2.8)$$

The above expressions are obtained by requiring that the momentum and energy moments of the collision term (2.5) be the same as those of the Boltzmann collision term  $J_{ij}[f_i, f_j]$  for Maxwell molecules [16]. In order to follow the original Boltzmann equation as much as possible, we assume that particles of species  $i$  and  $j$  interact through the Maxwell potential, i.e.  $V_{ij}(r) = \kappa_{ij} r^{-4}$ . Consequently, we identify the effective collision frequency  $\nu_{ij}$  by

$$\nu_{ij} = A n_j \left[ \kappa_{ij} \frac{m_i + m_j}{m_i m_j} \right]^{1/2}, \quad (2.9)$$

where  $A = 4\pi \times 0.422$ . It is worth remarking that the results derived in this paper could be extended to more general potentials.

Due to the highly nonlinear character of the reference function  $f_{ij}^R$  in the GK model, it has the following shortcoming. In the special case of mechanically equivalent particles ( $m_1 = m_2$ ,  $\kappa_{11} = \kappa_{22} = \kappa_{12}$ ), the total distribution function  $f = f_1 + f_2$  does not obey a closed equation. This problem is avoided by a recently proposed kinetic model [17], which is especially useful for systems of like particles. In fact, this model has been used to get the shear-rate-dependent self-diffusion coefficient in the steady Couette flow [6]. Nevertheless, in the tracer limit for arbitrary mass ratio, the above shortcoming of the GK model does not apply. In that situation, the GK model is preferable to the model proposed in Ref. [17].

We now describe the physical problem we are interested in. A gas (the solvent) is enclosed between two infinite parallel plates (normal to the  $y$  axis) in relative motion (along the  $x$  axis) and, in general, at different temperatures. The stationary state of the gas under the above conditions will be referred to as steady Couette flow. At a given time, a small concentration of particles of a different species (the solute) is introduced. The resulting solution is assumed to be so dilute that the state of the solvent is not disturbed by the presence of the solute, while the collisions among solute particles themselves can be neglected versus the solute-solvent collisions. After a certain transient stage, the solute is expected to reach a steady state. Our goal here is to analyze this steady state.

Under these conditions, the GK model reduces to

$$v_y \frac{\partial f_1}{\partial y} = -\nu_{12}(f_1 - f_{12}^R) \quad (2.10)$$

for the solute component and

$$v_y \frac{\partial f_2}{\partial y} = -\nu_{22}(f_2 - f_{22}^R) \quad (2.11)$$

for the solvent component. From Eqs. (2.10) and (2.11) one easily gets the following hydrodynamic balance equations:

$$\frac{\partial}{\partial y} P_{i,xy} = -\nu_{i2} \frac{m_i m_2}{m_i + m_2} n_i (u_{i,x} - u_{2,x}), \quad (2.12)$$

$$\begin{aligned} \frac{\partial}{\partial y} q_{i,y} + P_{i,xy} \frac{\partial}{\partial y} u_{i,x} \\ = -\nu_{i2} \frac{m_i m_2}{(m_i + m_2)^2} \\ \times n_i [3k_B(T_i - T_2) - m_2(\mathbf{u}_i - \mathbf{u}_2)^2]. \end{aligned} \quad (2.13)$$

Here we have introduced the partial pressure tensor  $P_i$  and heat flux  $\mathbf{q}_i$ , defined by

$$P_i = m_i \int d\mathbf{v} (\mathbf{v} - \mathbf{u}_i)(\mathbf{v} - \mathbf{u}_i) f_i \quad (2.14)$$

and

$$\mathbf{q}_i = \int d\mathbf{v} \frac{m_i}{2} (\mathbf{v} - \mathbf{u}_i)^2 (\mathbf{v} - \mathbf{u}_i) f_i, \quad (2.15)$$

respectively.

The main advantage of the tracer limit ( $n_1/n_2 \ll 1$ ) is that  $f_2$  obeys a closed equation (the BGK model). Then, the explicit knowledge of  $f_2$  allows one to solve the kinetic equation for  $f_1$ . In the case of the steady Couette flow, a normal solution to Eq. (2.11) has been found [14,15]. This solution is characterized by the following hydrodynamic profiles:

$$p_2 \equiv n_2 k_B T_2 = \text{const}, \quad (2.16)$$

$$\frac{1}{\nu_{22}(y)} \frac{\partial}{\partial y} u_{2,x} = a = \text{const}, \quad (2.17)$$

$$\left[ \frac{1}{\nu_{22}(y)} \frac{\partial}{\partial y} \right]^2 T_2 = -\frac{2m_2}{k_B} \gamma(a) = \text{const}. \quad (2.18)$$

The reduced shear rate  $a$  measures the ratio between the mean free path and the hydrodynamic length associated with the spatial variation of the local velocity  $\mathbf{u}_2$ . Equations (2.17) and (2.18) indicate that, under an adequate change of spatial variable, the velocity profile is linear and the temperature profile is parabolic. The self-consistency of the solution allows one to relate the dimensionless parameter  $\gamma$  to the shear rate  $a$ . Nevertheless, we consider for the moment  $\gamma$  as a free parameter. Taking into account the profiles (2.16)–(2.18), one gets the relevant fluxes. In particular [14],

$$P_{2,xy} = -\frac{p_2}{\nu_{22}} F^{(0)}(\gamma) \frac{\partial}{\partial y} u_{2,x}, \quad (2.19)$$

$$q_{2,y} = -\frac{5p_2 k_B}{2m_2 \nu_{22}} \left[ \frac{a^2}{5\gamma} F^{(0)}(\gamma) + G(a, \gamma) \right] \frac{\partial}{\partial y} T_2, \quad (2.20)$$

where

$$F^{(0)}(\gamma) \equiv \frac{2}{\gamma} \int_0^\infty dt t \exp(-t^2/2) K_0(2\gamma^{-1/4} t^{1/2}), \quad (2.21)$$

$K_0$  being the zeroth-order modified Bessel function, and

$$G(a, \gamma) \equiv \frac{2}{5} F^{(2)}(\gamma) + \frac{1}{5} \left( 3 - \frac{a^2}{\gamma} \right) F^{(1)}(\gamma). \quad (2.22)$$

Here  $F^{(r)}(\gamma) \equiv \left( \frac{d}{d\gamma} \right)^r F^{(0)}(\gamma)$ . The behaviors of  $F^{(0)}(\gamma)$  for small and large  $\gamma$  are [14], respectively,  $F^{(0)}(\gamma) \approx 1 - 18\gamma$  and  $F^{(0)}(\gamma) \approx \frac{1}{2}\gamma^{-1} \ln \gamma$ . Formally, Eqs. (2.19) and (2.20) can be interpreted as giving the fluxes of  $f_2$  in terms of the moments characterizing  $f_{22}^R$ , namely  $n_2$ ,  $\mathbf{u}_{22} = \mathbf{u}_2$ , and  $T_{22} = T_2$ . The proposed hydrodynamic fields (2.16)–(2.18) and the resulting fluxes (2.19) and (2.20) are consistent with the balance equations (2.12) and (2.13) for  $i = 2$  if and only if the following relationship between  $\gamma$  and  $a$  is verified:

$$G(a, \gamma) = 0. \quad (2.23)$$

For small shear rates, the solution of Eq. (2.23) is  $\gamma \approx \frac{1}{5}a^2 + \frac{72}{125}a^4$ . In the opposite limit, one has  $\gamma \approx \frac{1}{3}a^2$ .

One of the main advantages of using kinetic models is the possibility of obtaining explicit expressions for the distribution functions. This is in general not possible in the case of the Boltzmann equation, even when the corresponding moment hierarchy is solvable. In the steady Couette flow problem, the explicit solution to Eq. (2.11) is [15]

$$f_2(\mathbf{r}, \mathbf{v}) = n_2 (m_2/2\pi k_B T_2)^{3/2} \frac{2\alpha(1+\alpha)^{3/2}}{\epsilon |\xi_y|} \times \int_{t_0}^{t_1} dt [2t - (1-\alpha)t^2]^{-5/2} \times \exp \left\{ -\frac{2\alpha}{1+\alpha} \frac{1-t}{\epsilon \xi_y} - \frac{1+\alpha}{2t - (1-\alpha)t^2} \left[ \left( \xi_x + \frac{2a\alpha}{1+\alpha} \frac{1-t}{\epsilon} \right)^2 + \xi_y^2 + \xi_z^2 \right] \right\}, \quad (2.24)$$

where  $(t_0, t_1) = (0, 1)$  if  $\xi_y > 0$  and  $(t_0, t_1) = [1, 2/(1-\alpha)]$  if  $\xi_y < 0$ . In this equation,

$$\epsilon \equiv \frac{1}{\nu_{22}} \left( \frac{2k_B T_2}{m_2} \right)^{1/2} \frac{1}{T_2} \frac{\partial}{\partial y} T_2, \quad (2.25)$$

$$\alpha(\gamma, \epsilon) \equiv \frac{\epsilon}{(\epsilon^2 + 8\gamma)^{1/2}}, \quad (2.26)$$

$$\xi \equiv (m_2/2k_B T_2)^{1/2} (\mathbf{v} - \mathbf{u}_2). \quad (2.27)$$

The task now is to solve the kinetic equation for the solute, Eq. (2.10), once the solution of the kinetic equation for the solvent, Eq. (2.11), is known.

### III. TRANSPORT PROPERTIES OF THE SOLUTE

On physical grounds, one expects that the steady state of the solute is characterized by a constant molar fraction  $x_1 = n_1/n_2$ , the absence of mutual diffu-

sion, i.e.,  $\mathbf{u}_1 = \mathbf{u}_2$ , and a constant temperature ratio  $T_1/T_2 \equiv \chi$ . The parameter  $\chi$  must depend on the shear rate  $a$ , the mass ratio  $\mu \equiv m_2/m_1$ , and the force ratio  $\omega \equiv (\kappa_{12}/\kappa_{22})^{1/4}$ . The explicit calculation of  $\chi(a, \mu, \omega)$  is one of the main objectives of this paper. Obviously,  $\chi = 1$  if (i) the mixture is at equilibrium ( $a = 0$ ) or (ii) the particles are mechanically indistinguishable ( $\mu = \omega = 1$ ). Although we are considering Maxwell molecules, we can assign an effective diameter  $\sigma_{ij}$  to the interaction between particles of species  $i$  and  $j$ . Dimensional analysis allows one to interpret  $\omega$  as the size ratio  $\sigma_{12}/\sigma_{22}$ .

According to the above assumptions, and by taking into account Eqs. (2.16)–(2.18), one has

$$n_1 k_B T_{12} = \text{const}, \quad (3.1)$$

$$\frac{1}{\nu_{12}(y)} \frac{\partial}{\partial y} u_{12,x} = \tilde{a} = \text{const}, \quad (3.2)$$

$$\left[ \frac{1}{\nu_{12}(y)} \frac{\partial}{\partial y} \right]^2 T_{12} = -\frac{2m_1}{k_B} \tilde{\gamma} = \text{const}, \quad (3.3)$$

where Eqs. (2.7) and (2.8) imply that  $\mathbf{u}_{12} = \mathbf{u}_1 = \mathbf{u}_2$  and  $T_{12}/T_2 = \chi + 2M(1 - \chi)$  with  $M \equiv \mu/(1 + \mu)^2$ . Consequently,

$$\tilde{a} \equiv \frac{a}{\omega^2[(1 + \mu)/2]^{1/2}} \quad (3.4)$$

and

$$\tilde{\gamma} \equiv \frac{2\mu}{1 + \mu} \frac{\chi + 2M(1 - \chi)}{\omega^4} \gamma. \quad (3.5)$$

Equations (3.1)–(3.3) define the profiles of the fields characterizing the reference distribution  $f_{12}^R$ . From a

formal point of view, the kinetic equation (2.11) becomes Eq. (2.10) by making the changes  $f_2 \rightarrow f_1$ ,  $f_{22}^R \rightarrow f_{12}^R$ , and  $\nu_{22} \rightarrow \nu_{12}$ . Consequently, the fluxes of  $f_1$  can be obtained from comparison with those of  $f_2$ . In particular,

$$P_{1,xy} = -\frac{n_1 k_B T_{12}}{\nu_{12}} F^{(0)}(\tilde{\gamma}) \frac{\partial}{\partial y} u_{12,x}, \quad (3.6)$$

$$q_{1,y} = -\frac{5n_1 k_B^2 T_{12}}{2m_1 \nu_{12}} \left[ \frac{\tilde{a}^2}{5\tilde{\gamma}} F^{(0)}(\tilde{\gamma}) + G(\tilde{a}, \tilde{\gamma}) \right] \frac{\partial}{\partial y} T_{12}, \quad (3.7)$$

where use has been made of Eqs. (2.19) and (2.20). The balance equation (2.12) is automatically satisfied. However, in order to verify the consistency of the energy balance equation (2.13), the parameter  $\tilde{\gamma}$  must be given by the following implicit equation:

$$G(\tilde{a}, \tilde{\gamma}) = \frac{3}{5\tilde{\gamma}} \frac{M(1 - \chi)}{\chi + 2M(1 - \chi)}, \quad (3.8)$$

where  $G$  is defined in Eq. (2.22). To close Eq. (3.8), one must use the relations (3.4) and (3.5). The solution gives  $\chi$  as a function of  $a$ ,  $\mu$ , and  $\omega$ . In general, this solution must be obtained numerically. However,  $\chi$  can be explicitly derived in some limiting cases. In the limit of small shear rates, one gets

$$\chi \approx 1 + \frac{2}{3} \frac{1 - \mu^2}{\omega^4 \mu} a^2. \quad (3.9)$$

On the other hand, for large shear rates,

$$\chi \approx \frac{1}{\mu}. \quad (3.10)$$

If we choose  $\omega = 1$ , the behavior of  $\chi$  in the case of similar masses is

$$\chi \approx 1 + \frac{2}{3} \frac{a^2 [F^{(2)}(\gamma) - 2F^{(1)}(\gamma)] - \gamma [2F^{(3)}(\gamma) + 3F^{(2)}(\gamma)]}{1 - \frac{2}{3} \{a^2 [F^{(2)}(\gamma) - F^{(1)}(\gamma)] - \gamma [2F^{(3)}(\gamma) + 3F^{(2)}(\gamma)]\}} (\mu - 1). \quad (3.11)$$

The temperature ratio  $\chi$  is plotted in Fig. 1 as a function of  $a^2$  for two values of the mass ratio. Two choices of  $\omega$  have been considered:  $\omega = 1$  (solid lines) and  $\omega = \mu^{-1/8}$  (dashed lines). The latter has been suggested [18] to model the mass dependence of the cross section observed in disparate mass binary mixtures. We observe that  $\chi \equiv T_1/T_2$  monotonically varies from 1 to  $m_1/m_2$  as the shear rate increases. This means that very far from equilibrium the mean-square velocities of each species tend to be equal, but the mean kinetic energies are different, while the converse happens at equilibrium (equipartition theorem). The fact that  $T_1 \neq T_2$  for arbitrary shear rate indicates that the standard one-temperature Chapman-Enskog theory [3] is not appropriate, especially for disparate masses. In this case, the so-called two-fluid theory must be used [19]. The monotonic behavior of  $\chi$  in the steady Couette flow contrasts with the behavior observed in the uniform shear flow [9]. In the latter

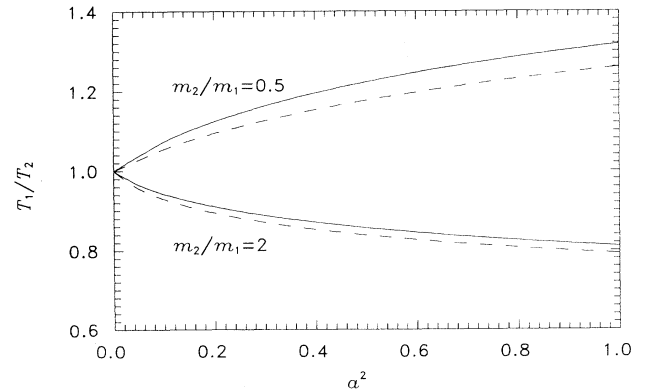


FIG. 1. Plot of the temperature ratio  $\chi \equiv T_1/T_2$  vs the reduced shear rate for two values of the mass ratio  $\mu \equiv m_2/m_1$  and two choices of the size ratio:  $\omega = 1$  (solid lines) and  $\omega = \mu^{-1/8}$  (dashed lines).

case, for each value of  $\mu$  there exists a particular value of  $a$  such that  $\chi = 1$ . For those combinations of  $\mu$  and  $a$  a one-temperature theory can be adequate, even in the case of disparate masses.

Once the function  $\chi$  is known, Eqs. (3.6) and (3.7) give the solute contribution to the momentum and heat transport across the system. It is convenient to define a dimensionless partial generalized shear viscosity  $\eta_1$  and a dimensionless partial generalized thermal conductivity  $\lambda_1$  through the relations

$$P_{1,xy} = -\frac{n_1 k_B T_2}{\nu_{12}} \eta_1 \frac{\partial}{\partial y} u_{2,x}, \quad (3.12)$$

$$q_{1,y} = -\frac{5n_1 k_B^2 T_2}{2m_1 \nu_{12}} \lambda_1 \frac{\partial}{\partial y} T_2. \quad (3.13)$$

The transport coefficients  $\eta_1$  and  $\lambda_1$  are normalized with respect to their Navier-Stokes values. In the case of particles mechanically identical, the transport coefficients of the solute coincide with those of the solvent [14]. The behaviors of  $\eta_1$  for small and large shear rates are, respectively,

$$\eta_1 \approx 1 - \frac{2}{15} \frac{5\mu^3 + 49\mu^2 + 5\mu - 5}{\omega^4 \mu(1 + \mu)} a^2, \quad (3.14)$$

$$\eta_1 \approx \frac{3}{4} \omega^4 \frac{1 + \mu \ln a^2}{\mu a^2}. \quad (3.15)$$

Analogously, the behaviors of  $\lambda_1$  for small and large shear rates are, respectively,

$$\lambda_1 \approx 1 - \frac{4}{75} \frac{25\mu^3 + 353\mu^2 - 110\mu - 25}{\omega^4 \mu(1 + \mu)} a^2, \quad (3.16)$$

$$\lambda_1 \approx \frac{9}{20} \omega^4 \frac{1 + \mu \ln a^2}{\mu^2 a^2}. \quad (3.17)$$

Equations (3.14) and (3.15) indicate that  $\eta_1$  monotonically decreases as the shear rate increases if  $\mu \gtrsim 0.27$ .

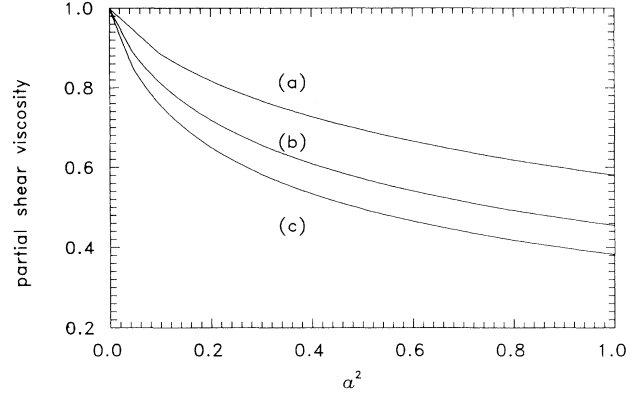


FIG. 2. Shear-rate dependence of the dimensionless partial shear viscosity  $\eta_1$  for  $\omega = 1$  and three values of the mass ratio: (a)  $\mu = 0.5$ , (b)  $\mu = 1$ , and (c)  $\mu = 2$ .

The same happens for  $\lambda_1$  if  $\mu \gtrsim 0.45$ . For smaller values of  $\mu$ , the partial transport coefficients increase for small shear rates but go to zero in the limit of large shear rates.

In Figs. 2 and 3 we plot the shear-rate dependence of  $\eta_1$  and  $\lambda_1$  for  $\omega = 1$  and some illustrative values of  $\mu$ . We observe that, at a given value of the shear rate, the solute contribution to the transport of momentum and energy increases with the solute mass relative to the solvent mass. Similar conclusions can be drawn by using other choices for  $\omega$ , such as  $\omega = \mu^{-1/8}$ .

Let us turn our attention now to the velocity distribution function  $f_1$ . By exploiting the formal analogy between Eqs. (2.10) and (2.11), we can easily obtain  $f_1$  from Eq. (2.24) by performing the following changes:  $n_2 \rightarrow n_1$ ,  $m_2 \rightarrow m_1$ ,  $T_2 \rightarrow T_{12}$ , and  $\nu_{22} \rightarrow \nu_{12}$ . Obviously, these changes must also be performed on  $\epsilon$ ,  $\alpha$ ,  $a$ , and  $\xi$ . The explicit expression for the solute distribution function is then given by

$$f_1(\mathbf{r}, \mathbf{v}) = n_1 (m_1 / 2\pi k_B T_2)^{3/2} \Phi(\xi), \quad (3.18)$$

where

$$\begin{aligned} \Phi(\xi) = & \omega^2 \left( \frac{1 + \mu}{2\mu} \right)^{1/2} [\chi + 2M(1 - \chi)]^{-3/2} \frac{2\alpha(1 + \alpha)^{3/2}}{\epsilon |\xi_y|} \\ & \times \int_{t_0}^{t_1} dt [2t - (1 - \alpha)t^2]^{-5/2} \\ & \times \exp \left\{ -\omega^2 \left( \frac{1 + \mu}{2\mu} \right)^{1/2} \frac{2\alpha}{1 + \alpha} \frac{1 - t}{\epsilon \xi_y} \right. \\ & \left. - [\chi + 2M(1 - \chi)]^{-1} \frac{1 + \alpha}{2t - (1 - \alpha)t^2} \left[ \left( \xi_x + \frac{2a\alpha}{1 + \alpha} \frac{1 - t}{\mu^{1/2} \epsilon} \right)^2 + \xi_y^2 + \xi_z^2 \right] \right\}. \quad (3.19) \end{aligned}$$

Here the integration limits are the same as in Eq. (2.24),  $\epsilon$  and  $\alpha$  are given by Eqs. (2.25) and (2.26), respectively, and now the reduced velocity  $\xi$  is defined as

$$\xi \equiv (m_1 / 2k_B T_2)^{1/2} (\mathbf{v} - \mathbf{u}_2). \quad (3.20)$$

In order to illustrate the shape of the solute distribution function, it is convenient to define the function

$$\varphi(\xi_y) \equiv \frac{\int_{-\infty}^{\infty} d\xi_x \int_{-\infty}^{\infty} d\xi_z \Phi(\xi)}{\int_{-\infty}^{\infty} d\xi_x \int_{-\infty}^{\infty} d\xi_z e^{-\xi^2}}. \quad (3.21)$$

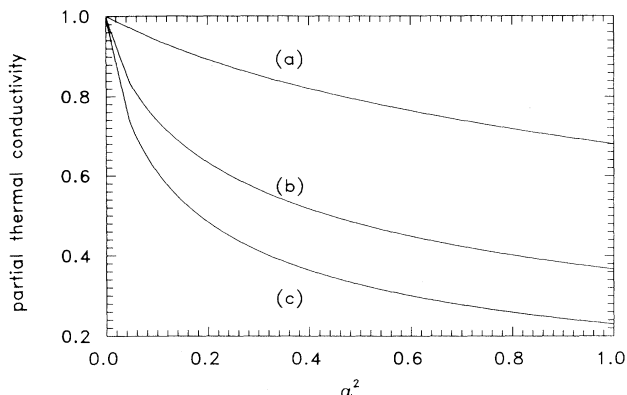


FIG. 3. Same as in Fig. 2, but for the dimensionless partial thermal conductivity  $\lambda_1$ .

This function is plotted in Fig. 4 for  $\omega = 1$ ,  $a = 1$ ,  $\epsilon = 1$ , and  $\mu = 0.5, 1$ , and  $2$ . We observe that, as  $\mu$  decreases, the fraction of solute particles with high energies increases. This is consistent with the fact that  $T_1/T_2$  also increases when  $\mu$  decreases, as seen in Fig. 1.

#### IV. CONCLUSIONS

In this paper, we have addressed the problem of a gaseous dilute solution far from equilibrium. The solution is assumed to be so dilute that the state of the solvent is not affected by the presence of the solute. Further, the mixture density is so low that a kinetic description is appropriate. Under these conditions, the solvent distribution function  $f_2$  obeys a closed Boltzmann equation, while the solute distribution function  $f_1$  obeys a Boltzmann-Lorentz equation. This situation is usually referred to as the tracer limit. The specific state that we have considered corresponds to the steady planar Couette flow, in which the system is enclosed between two parallel plates in relative motion. We have also assumed

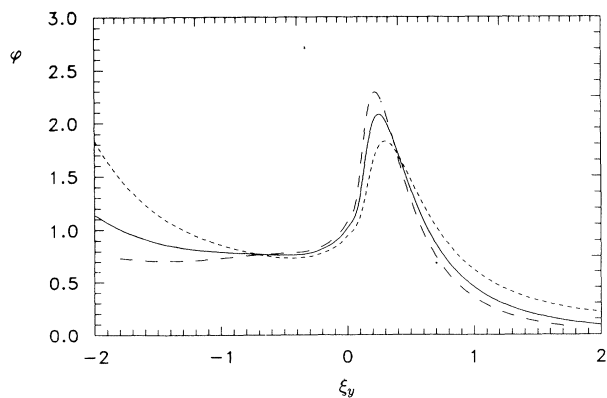


FIG. 4. Plot of the reduced distribution function  $\varphi(\xi_v)$  for  $a = 1$ ,  $\epsilon = 1$ ,  $\omega = 1$ , and three values of the mass ratio:  $\mu = 0.5$  (---),  $\mu = 1$  (—), and  $\mu = 2$  (- - -).

that the molar fraction is spatially uniform. This implies that no mutual diffusion appears in the system, so that we focus on the transport of momentum and energy.

The results have been derived from the nonlinear GK kinetic model for binary mixtures. In the tracer limit, the kinetic equation for the solvent reduces to the BGK equation, whose solution in the steady Couette flow is known [14,15]. Consequently, our task here has been to solve the kinetic equation for the solute. In order to do that, we have exploited a formal similarity between the equations for the solvent and the solute. In this problem, the crucial quantity is the ratio  $\chi \equiv T_1/T_2$  between the temperatures of the solute and the solvent. We have obtained an implicit equation, whose solution gives  $\chi$  as a nonlinear function of the shear rate  $a$ , the mass ratio  $\mu \equiv m_2/m_1$ , and the size ratio  $\omega$ . Of course,  $\chi = 1$  in the special case of mechanically equivalent particles [6]. In general, however,  $\chi$  varies monotonically from 1 (limit of vanishing shear rate) to  $1/\mu$  (limit of large shear rates). The fact that  $\chi \neq 1$  shows the failure of the equipartition theorem in nonequilibrium situations. More specifically, both the mean-square velocities and the mean kinetic energies are different for each species at finite shear rate. The mean-square velocities tend to equal as one departs from equilibrium, while the mean kinetic energies tend to equal as one approaches equilibrium. Since  $T_1 \neq T_2$  at nonzero shear rate, a two-fluid theory is much more appropriate than the standard one-temperature Chapman-Enskog theory.

From the knowledge of  $\chi$ , the main transport properties of the solute have been determined, namely the (partial) shear viscosity  $\eta_1$  and thermal conductivity  $\lambda_1$ , as functions of the shear rate and the mass and size ratios. For values of  $\mu$  smaller than about 0.27, the shear viscosity does not behave monotonically as a function of the shear rate. In the region of small shear rates it is an increasing function, while the opposite happens in the region of large shear rates. For  $\mu \gtrsim 0.27$ ,  $\eta_1$  monotonically decreases as the shear rate increases (shear thinning). Similar behavior is exhibited by the thermal conductivity depending on whether  $\mu$  is smaller or greater than about 0.45. On the other hand, both  $\eta_1$  and  $\lambda_1$  increase as  $\mu$  decreases at a given value of  $a$ .

In addition, an explicit expression for the velocity distribution function  $f_1$  has been derived. This function depends not only on the shear rate and the mass and size ratios, but also on the local thermal gradient  $\epsilon$ . Both  $a$  and  $\epsilon$  are the parameters measuring the departure away from equilibrium. Although the dependence of  $f_1$  on  $\epsilon$  is highly nonlinear, the momentum flux is independent of  $\epsilon$  and the heat flux is linear in  $\epsilon$ . Concerning the influence of  $\mu$  on  $f_1$ , we have observed a significant distortion with respect to  $f_2$ , especially in the high-velocity region.

From our point of view, the motivation for this work is twofold. First, the characterization of gaseous dilute solutions in stationary states far from equilibrium is an interesting problem itself. In this context, the solute and the solvent distribution functions have been recently compared in a homogeneous and isotropic problem [20]. Second, in order to study a tracer diffusion problem under steady Couette flow, the results derived in this paper

are needed as a starting point. More specifically, the idea consists of performing a perturbation expansion around the distribution  $f_1$  obtained here, by considering the gradient of molar fraction as the perturbation parameter [5,6,8,9]. In this way, one can get the diffusion tensor as a function of  $a$ ,  $\mu$ , and  $\omega$ . Work along these lines is in progress.

#### ACKNOWLEDGMENT

This research has been supported by the Dirección General de Investigación Científica y Técnica (DGICYT) of the Spanish Government through Grant No. PB91-0316.

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