

Uniform shear flow in a binary mixture with general repulsive interactions

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A kinetic model for a binary mixture under uniform shear flow is exactly solved. The model incorporates a temperature dependence of the collision frequencies that allows the consideration of general repulsive interactions. The rheological properties of the mixture are obtained as functions of the shear rate, the parameters of the mixture (particle masses, concentrations, and force constants), and a parameter characterizing the interaction considered. In addition, the velocity distribution functions are explicitly obtained. While the transport coefficients are hardly sensitive to the interaction potential, the distribution functions are clearly influenced by the interaction parameter. In the tracer limit, a transition to an alternative state recently found in the context of Boltzmann equation is exactly identified in the case of Maxwell molecules. For non-Maxwell molecules, preliminary results suggest that this transition is also present although the phenomenon is less significant. A comparison with previous results derived from the a Boltzmann equation for Maxwell molecules is also carried out. © 1996 American Institute of Physics. [S1070-6631(96)01010-0]

I. INTRODUCTION

The analysis of transport phenomena occurring in a binary mixture far away from equilibrium is certainly a very hard task since the transport coefficients are not only functions of the nonequilibrium parameters (hydrodynamic gradients, external forces, . . .), but also of parameters such as masses, concentrations, and sizes. This complexity leads us to consider tractable situations for which a complete description can be given. Perhaps, one of the most extensively studied cases corresponds to the so-called uniform shear flow (USF). In this state, the only nonzero gradient (which is a constant) is $\partial u_x / \partial y = a$, where \mathbf{u} is the flow velocity. The constant shear rate a measures the distance of the system from equilibrium. The USF problem is a useful prototype for evaluating transport properties under extreme conditions (far away from equilibrium). In “computer experiments” this state is generated by applying Lees-Edwards periodic boundary conditions.¹ This type of boundary conditions do work on the system so that the temperature increases with time. In order to achieve a stationary situation, an artificial (microscopic) force is usually introduced. Although the USF may be experimentally unrealizable for large shear rates, the results derived in this (idealized) problem are of great value in order to gain insight into the understanding of more realistic flows.

In the USF state the most important transport properties are related to the pressure tensor \mathbf{P} , whose elements define the nonlinear shear viscosity η and viscometric functions $\Psi_{1,2}$. Recently, we have obtained these quantities for a binary mixture of Maxwell molecules (r^{-5} repulsive intermolecular force) from an *exact* solution of the coupled set of Boltzmann equations.² The transport coefficients η and $\Psi_{1,2}$ are given as nonlinear functions of the shear rate and the parameters of the mixture (mass ratio, concentration ratio, and force constant ratios). This work extends the well-known Ikenberry-Truesdell solution³ for a *single* component gas of Maxwell molecules.

Nevertheless, the above solution has two important limi-

tations. First, it cannot be regarded as general since the model of Maxwell molecules is not a realistic example of intermolecular interactions. As a consequence, the predictions made in Ref. 2 cannot *in principle* be extrapolated to other interaction potentials. Second, and due to the mathematical difficulties embodied in the Boltzmann collision operators, no explicit expressions for the velocity distribution functions are known, even for Maxwell molecules. A possible alternative to overcome analytically both limitations is to use a kinetic model. The idea is to replace the Boltzmann collision integrals (which contain a detailed description of the two-body interactions) by simple collision terms which retain the main physical properties of the true collision operators. The usefulness of such an approach has been widely demonstrated in the past with the Bhatnagar-Gross-Krook (BGK) equation⁴ in the case of a monocomponent gas under USF.⁵

The aim of this paper is to reexamine the USF problem for a dilute binary mixture. The starting point is a generalization of the well-known Gross-Krook (GK) kinetic model⁶ for a binary mixture where the effective collision frequencies depend on the “temperature” of each species. This allows for the consideration of general repulsive intermolecular forces. Our motivation is twofold. On the one hand, we find explicit expressions for the velocity moments and the velocity distribution functions in terms of the shear rate, the ratios of mass, concentration, and force constants and a parameter characterizing the intermolecular interaction considered. The latter allows us to assess the influence of the interaction potential on the main transport properties. In this sense, in this paper we extend previous works about the USF problem in the tracer limit.^{7,8} On the other hand, and as a test of validation of the kinetic model, we compare the shear-rate dependence of the temperature ratio, the shear viscosity, and viscometric functions with the one given from the exact Boltzmann equation for Maxwell molecules. Such a comparison shows that the rheological properties of the mixture derived from the GK and Boltzmann equations do not coincide although they exhibit a qualitative agreement for not too

large shear rates and/or not too large a disparity of the parameters of the mixture.

As a final point, it is interesting to investigate what happens in the tracer limit, i.e. when the molar fraction of one of the species tends to zero. In this limit, a transition to an alternative state has been *exactly* identified from the Boltzmann solution.⁹ In this new state, the tracer species contribute significantly to the total properties of the mixture. In the same way as in the Boltzmann equation, an exact analysis of the tracer limit for Maxwell molecules shows that such a transition is also present in the GK solution. For non-Maxwell molecules, numerical results suggest that this phenomenon also appears although it is much less important as the interaction becomes harder.

The plan of the paper is as follows. In Sec. II we describe the problem we are interested in and introduce the kinetic model. Section III is concerned with the calculation of the steady transport properties and the corresponding comparison with the Boltzmann results. The velocity distribution functions are explicitly obtained in Sec. IV, while the tracer limit is studied in Sec. V. Finally, some concluding remarks close the paper in Sec. VI.

II. DESCRIPTION OF THE PROBLEM

Let us consider a dilute binary mixture. In terms of the velocity distribution function $f_s(\mathbf{r}, \mathbf{v}; t)$ of species s ($s \equiv 1, 2$), the number density and mean velocity of species s are defined, respectively, as

$$n_s = \int d\mathbf{v} f_s, \quad (1)$$

$$\mathbf{u}_s = \frac{1}{n_s} \int d\mathbf{v} \mathbf{v} f_s. \quad (2)$$

These quantities define the total number density $n = n_1 + n_2$ and the flow velocity $\mathbf{u} = (\rho_1 \mathbf{u}_1 + \rho_2 \mathbf{u}_2) / \rho$, where $\rho_s = m_s n_s$ is the mass density of species s , m_s is the mass of a particle of species s , and $\rho = \rho_1 + \rho_2$ is the total mass density. It is usual to define a local “temperature” for each species through

$$\frac{3}{2} n_s k_B T_s = \frac{m_s}{2} \int d\mathbf{v} (\mathbf{v} - \mathbf{u}_s)^2 f_s, \quad (3)$$

which is related to the mean kinetic energy of each species. Here, k_B is the Boltzmann constant. From these partial temperatures, the temperature of the mixture T (which is the relevant one at a hydrodynamic level) is

$$n k_B T = \sum_{s=1}^2 \left(n_s k_B T_s + \frac{1}{3} \rho_s (\mathbf{u}_s - \mathbf{u})^2 \right). \quad (4)$$

The uniform shear flow (USF) state is characterized by a linear profile of the x component of the flow velocities along the y axis, constant densities n_s , and uniform temperatures T_s :

$$u_{s,i} = u_i = a_{ij} r_j, a_{ij} = a \delta_{ix} \delta_{jy}, \quad (5)$$

$$n_s = \text{const}, \quad (6)$$

$$\nabla T_s = 0, \quad (7)$$

a being the constant shear rate. Since no mutual diffusion appears in the system, the only nonequilibrium parameter (which may be arbitrarily large) is the shear rate. As a consequence, the relevant transport phenomenon is the momentum transport which is measured by the pressure tensor

$$\mathbf{P} = \sum_{s=1}^2 m_s \int d\mathbf{v} \mathbf{V} \mathbf{V} f_s, \quad (8)$$

where $\mathbf{V} = \mathbf{v} - \mathbf{u}$ is the peculiar velocity. The elements of the pressure define the main transport coefficients of the problem, namely, the shear viscosity,

$$\eta(a) = -\frac{P_{xy}}{a}, \quad (9)$$

and the viscometric functions,

$$\Psi_1(a) = \frac{P_{yy} - P_{xx}}{a^2}, \quad (10)$$

$$\Psi_2(a) = \frac{P_{zz} - P_{yy}}{a^2}. \quad (11)$$

The USF is not stationary since the temperature increases in time due to viscous heating. Thus, Eqs. (9)–(11) must be understood in the long-time limit where the influence of the initial conditions has disappeared.

The USF state becomes spatially homogeneous when the velocities of the particles are referred to the Lagrangian frame moving with the flow velocity \mathbf{u} . In this new frame, the distribution function adopts the form $f_s(\mathbf{r}, \mathbf{v}; t) \equiv f_s(\mathbf{V}; t)$. For this reason, the USF state have been extensively studied in the past years, especially in the case of a single gas. Recently, *exact* expressions for the rheological properties of a binary mixture of Maxwell molecules (particles interacting via a repulsive r^{-5} force) under USF have been obtained.² To the best of our knowledge, this is the first exact solution of the Boltzmann equation for a binary mixture in an inhomogeneous state far from equilibrium. Beyond the Maxwell interaction, it is a very difficult problem to get explicit information about the shear-rate dependence of the transport coefficients from the Boltzmann equation. Since we are interested in offering a theory with a wider applicability than just for Maxwell molecules, here we will consider a kinetic model suitable for arbitrary repulsive forces. Specifically, for molecules interacting through a repulsive force $\mathbf{F}_{rs} = \hat{\mathbf{r}} \kappa_{rs} / r^\gamma$ ($\gamma = 5, \dots, \infty$), the Boltzmann collision integrals $J_{rs}[f_r, f_s]$ are replaced by relaxation terms of the form

$$-v_{rs}(f_r - f_{rs}), \quad (12)$$

where

$$f_{rs} = n_r \left(\frac{m_r}{2\pi k_B T_{rs}} \right)^{3/2} \exp \left[-\frac{m_r}{2k_B T_{rs}} (\mathbf{v} - \mathbf{u}_{rs})^2 \right], \quad (13)$$

$$\mathbf{u}_{rs} = \frac{m_r \mathbf{u}_r + m_s \mathbf{u}_s}{m_r + m_s}, \quad (14)$$

$$T_{rs} = T_r + 2 \frac{m_r m_s}{(m_r + m_s)^2} \left[(T_s - T_r) + \frac{m_s}{6k_B} (\mathbf{u}_r - \mathbf{u}_s)^2 \right], \quad (15)$$

and ν_{rs} is a velocity independent collision frequency given by

$$\nu_{rs} = A(\beta) n_s \left(\kappa_{rs} \frac{m_r + m_s}{m_r m_s} \right)^{(1-\beta)/2} \left(\frac{2k_B T_r}{m_r} + \frac{2k_B T_s}{m_s} \right)^{\beta/2}. \quad (16)$$

Here, $\beta \equiv (\gamma - 5)/(\gamma - 1)$ and $A(\beta)$ is a constant for a given interparticle potential.¹⁰ The quantities \mathbf{u}_{rs} , T_{rs} , and ν_{rs} are determined by imposing that the total momentum and energy are conserved and that the first five collisional moments as computed with Eq. (13) be the same as those computed with the exact $J_{rs}[f_r, f_s]$. In order to evaluate the last requirement for non-Maxwell molecules, one needs to introduce approximate forms for the above collisional moments.¹¹ The kinetic model defined by Eqs. (12)–(16) can be seen as a generalization of the Gross-Krook (GK) model⁶ (which was originally introduced for Maxwell molecules, i.e. $\beta = 0$) to general repulsive interactions. All the details of the interaction potential are taken into account through ν_{rs} , which depend on temperatures T_r and T_s . This model has been recently used to study tracer diffusion in uniform shear flow.⁸

Under the conditions of the USF state, the velocity distribution function f_1 verifies the kinetic equation

$$\frac{\partial f_1}{\partial t} - \frac{\partial}{\partial V_i} a_{ij} V_j f_1 = -\nu_{11}(f_1 - f_{11}) - \nu_{12}(f_1 - f_{12}), \quad (17)$$

and a similar equation holds for f_2 . It is interesting to note that Eq. (17) admits a scaling property in the special case of Maxwell molecules. Let us introduce the scaled quantities

$$\bar{\mathbf{V}} = e^{-\alpha t} \mathbf{V}, \quad (18)$$

$$\bar{f}_s(\bar{\mathbf{V}}, t) = e^{3\alpha t} f_s(\mathbf{V}, t), \quad (19)$$

where α is an arbitrary constant. For Maxwell molecules ($\beta = 0$), $\bar{\nu}_{rs} = \nu_{rs}$ so that Eq. (17) reduces to

$$\frac{\partial \bar{f}_1}{\partial t} - \frac{\partial}{\partial \bar{V}_i} (a_{ij} \bar{V}_j + \alpha \bar{V}_i) \bar{f}_1 = -\bar{\nu}_{11}(\bar{f}_1 - \bar{f}_{11}) - \bar{\nu}_{12}(\bar{f}_1 - \bar{f}_{12}). \quad (20)$$

This equation can be seen as the one corresponding to the USF in the presence of a nonconservative external force $\mathbf{F}_1 = -m_1 \alpha \mathbf{V}$. Consequently, there is an exact equivalence between the description with and without the drag forces \mathbf{F}_s (with arbitrary α). From a computational point of view, it is desirable to measure the transport coefficients in a steady state. For this reason, it is usual in molecular dynamics simulations¹ to choose α as a function of the shear rate by the condition that the temperature reaches a constant value in the long time limit. In this sense, \mathbf{F}_s plays the role of a thermostat force. Here, we also adopt this point of view and will incorporate thermostat forces to achieve a steady state. Nevertheless, it must be remarked that for non-Maxwell molecules this type of force does not play a neutral role in the transport properties of the system.¹²

Now, we will start from Eq. (20) with $\partial \bar{f}_1 / \partial t = 0$ and will determine α by consistency. Further, for simplicity, we will drop the bars in Eq. (20).

III. TRANSPORT PROPERTIES

Let us assume that, after a transient period, the system has reached a steady state. In this situation, our goal is to evaluate the main transport properties of the mixture. To this end, it is useful to define the reduced velocity moments $M_{k,\ell,m}^{(s)}$ corresponding to species s as

$$M_{k,\ell,m}^{(s)} = \frac{1}{n_s} \left(\frac{2k_B T}{m_s} \right)^{-(1/2)(k+\ell+m)} \int d\mathbf{V} V_x^k V_y^\ell V_z^m f_s(\mathbf{V}). \quad (21)$$

In the following we will focus on the properties of species 1. Multiplying both sides of Eq. (20) (with $\partial f_1 / \partial t = 0$) by $V_x^k V_y^\ell V_z^m$ and integrating over the velocity space, one gets

$$akM_{k-1,\ell+1,m}^{(1)} + [\nu_1 + \alpha(k+\ell+m)]M_{k,\ell,m}^{(1)} = N_{k,\ell,m}^{(1)}, \quad (22)$$

where $\nu_1 = \nu_{11} + \nu_{12}$, and

$$N_{k,\ell,m}^{(1)} = \pi^{-3/2} C_k C_\ell C_m [\nu_{11} \chi_1^{(k+\ell+m)/2} + \nu_{12} \chi_{12}^{(k+\ell+m)/2}], \quad (23)$$

where $C_k = \Gamma((k+1)/2)$ if k is even, being zero otherwise. Here, we have introduced the temperature ratios $\chi_1 = T_1/T$ and $\chi_{12} = T_{12}/T$.

In order to study the nonlinear transport properties of the system, it is convenient to introduce dimensionless quantities. In general, the collision frequencies ν_{rs} depend on the shear rate through their dependence on the temperatures T_r and T_s . In the absence of shear field, $T_r = T_s = T$ and one recovers the expressions of the equilibrium collision frequencies,

$$\nu_{rs}^{(0)} = A(\beta) n_s \kappa_{rs}^{(1-\beta)/2} \left(\frac{m_r + m_s}{m_r m_s} \right)^{1/2} (2k_B T)^{\beta/2}. \quad (24)$$

Since our description applies for arbitrary mass, concentration, and size ratios, we choose for simplicity an effective collision frequency $\zeta = (n/n_2) \nu_{12}^{(0)}$ and take ζ^{-1} as the time unit. Thus, we will use the dimensionless quantities $a^* = a/\zeta$, $\alpha^* = \alpha/\zeta$, and

$$\nu_{11}^* = \frac{\nu_{11}}{\zeta} = \frac{\delta}{1+\delta} w_{11}^{(1-\beta)/2} \left(\frac{2}{1+\mu} \right)^{1/2} \chi_1^{\beta/2}, \quad (25)$$

$$\nu_{12}^* = \frac{\nu_{12}}{\zeta} = \frac{1}{1+\delta} \left(\frac{\chi_1}{1+\mu} + \frac{\mu}{1+\mu} \chi_{12} \right)^{\beta/2}, \quad (26)$$

where $\mu \equiv m_1/m_2$ is the mass ratio, $\delta \equiv n_1/n_2$ is the concentration ratio, and $w_{11} \equiv \kappa_{11}/\kappa_{12}$. For the sake of brevity, henceforth we will omit the asterisks.

In terms of the above reduced quantities, the solution to Eq. (22) can be written as⁸

$$M_{k,\ell,m}^{(1)} = \sum_{q=0}^k \frac{k!}{(k-q)!} (-a)^q [\nu_1 + (k+\ell+m)\alpha]^{-(1+q)} N_{k-q,\ell+q,m}^{(1)}, \quad (27)$$

where $N^{(1)}$ is assumed to be identically zero when any of its indices is negative. Equation (27) is still a formal expression as we do not know the shear-rate dependence of the thermo-

stat parameter α and the temperature ratios χ_1 and χ_2 . These quantities must be consistently determined from the requirements

$$\frac{3}{2}\chi_1 = M_{200}^{(1)} + M_{020}^{(1)} + M_{002}^{(1)}, \quad (28)$$

$$\frac{3}{2}\chi_2 = M_{200}^{(2)} + M_{020}^{(2)} + M_{002}^{(2)}, \quad (29)$$

$$\chi_2 = 1 + \delta(1 - \chi_1), \quad (30)$$

which follow from Eqs. (3) and (4). In Eq. (29), the moments $M_{k,l,m}^{(2)}$ of the distribution f_2 can be easily obtained from Eq. (27) by the adequate changes: $\mu \leftrightarrow \mu^{-1}$, $\delta \leftrightarrow \delta^{-1}$, $w_{11} \leftrightarrow w_{22}$. Except in the particular case of Maxwell molecules ($\beta=0$), the collision frequencies are nonlinear functions of the partial temperatures, so that it is not possible to get a closed equation for α or χ_1 . Thus, one must solve numerically the following coupled set of nonlinear algebraic equations:

$$(A_1 - 3)(A_2 - 3) - B_1 B_2 = 0, \quad (31)$$

$$\frac{\chi_1}{1 + \delta(1 - \chi_1)} = \frac{3 - A_2}{B_2}, \quad (32)$$

where

$$A_1 = \frac{\nu_{11} + \nu_{12}(1 - 2M)}{\nu_1 + 2\alpha} \left[3 + \frac{2a^2}{(\nu_1 + 2\alpha)^2} \right], \quad (33)$$

$$B_1 = \frac{2M\nu_{12}}{\nu_1 + 2\alpha} \left[3 + \frac{2a^2}{(\nu_1 + 2\alpha)^2} \right], \quad (34)$$

and the remaining coefficients are obtained by the adequate changes.

Nevertheless, there are some limit cases for which Eqs. (31) and (32) can be solved analytically. For instance, in the case of mechanically equivalent particles ($\mu=1, \kappa_{11}=\kappa_{22}=\kappa_{12}$), one gets that $\chi_1=\chi_2$ and α verifies the cubic equation

$$3\alpha(1 + 2\alpha)^2 = a^2, \quad (35)$$

whose real (physical) root is $\alpha(a) = \frac{1}{2}F(a)$ with

$$F(a) = \frac{4}{3} \sinh^2 \left[\frac{1}{6} \cosh^{-1}(1 + 9a^2) \right]. \quad (36)$$

In this case, all the results are independent of the potential model considered. In addition, the elements of the pressure tensor coincide with the ones obtained from the Boltzmann equation for Maxwell molecules when one adjusts conveniently the collision frequency.⁵ This fact shows the relevance of the kinetic model for evaluating transport properties. On the other hand, in the case of dissimilar particles and for small shear rates, $\alpha \approx \alpha_0 a^2$ and $\chi_1 \approx 1 + \chi_{10} a^2$ where

$$\alpha_0 = \frac{1}{3(\delta+1)} \left(\frac{\delta}{\nu_1^{(0)}} + \frac{1}{\nu_2^{(0)}} \right), \quad (37)$$

$$\chi_{10} = \frac{1}{3M(\delta+1)} \left(\frac{1}{\nu_2^{(0)}} - \frac{1}{\nu_1^{(0)}} \right), \quad (38)$$

being $M = \mu/(1 + \mu)^2$. Notice that all the dependence on β appears implicitly through $\nu_r^{(0)}$. For large shear rates, the behaviors for Maxwell molecules are

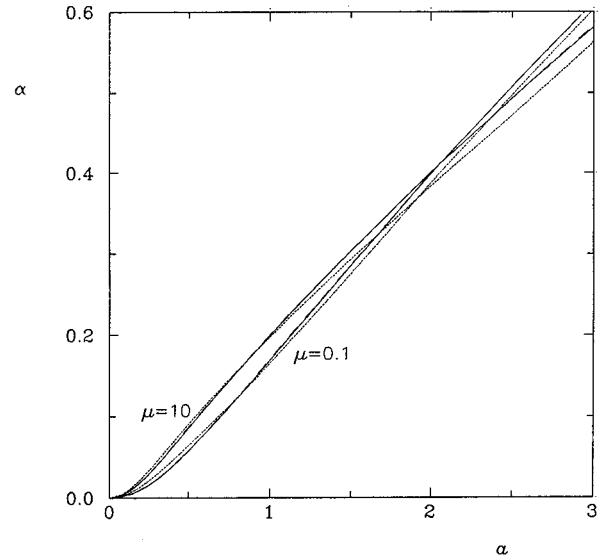


FIG. 1. Shear-rate dependence of the thermostat parameter α for $w_{11}=w_{22}=1$, $\delta=5$, and two values of the mass ratio μ . The solid and dashed lines refer to the GK results for Maxwell molecules and hard spheres, respectively, while the dotted line corresponds to the Boltzmann results for Maxwell molecules.

$$\alpha \approx \frac{\nu_1^{(0)}}{12} a^{2/3}, \quad (39)$$

$$\chi_1 \approx \frac{2M\delta + (\nu_1^{(0)} - \nu_2^{(0)})(\delta+1)}{\delta(2M + \nu_1^{(0)} - \nu_2^{(0)})}. \quad (40)$$

Since in the special case of Maxwell molecules ν_{rs} is independent of the temperature ratio, Eq. (31) reduces to a sixth-degree equation in α . The solution of this equation gives α as a function of a , μ , δ , w_{11} , and w_{12} . Obviously, this solution must also be obtained numerically. In Fig. 1, we plot the largest root $\alpha(a)$ (which is the physical solution) as a function of the shear rate given from the GK model and from the Boltzmann equation for $\delta=5$ and two values of μ . To make such a comparison, we have taken for the constant A appearing in Eq. (24) the value that gives the same results between the GK and Boltzmann equations in the case of identical particles. We observe a good agreement between both descriptions. In terms of α , the explicit expression for χ_1 is

$$\chi_1 = \left[1 + \frac{3\alpha(\nu_1 + 2\alpha)^2 - a^2\nu_1}{M\nu_{12}(\delta+1)[3(\nu_1 + 2\alpha)^2 + 2a^2]} \right]^{-1}. \quad (41)$$

For non-Maxwell molecules ($\beta \neq 0$), α and χ_1 are coupled through ν_{rs} and they do not obey closed equations. In order to analyze the effect of the intermolecular interaction on these quantities, we have considered the extreme case of hard spheres ($\beta=1$). According to Fig. 1, the curves corresponding to Maxwell molecules and hard spheres for $\alpha(a)$ are practically indistinguishable. This means that most of the influence of the potential has been scaled out by the choice of the reduced quantities. The temperature ratio $\chi_1 = T_1/T$ is plotted as a function of the shear rate in Fig. 2 for the same cases as those considered in Fig. 1. We observe that the qualitative trends predicted by the Boltzmann equa-

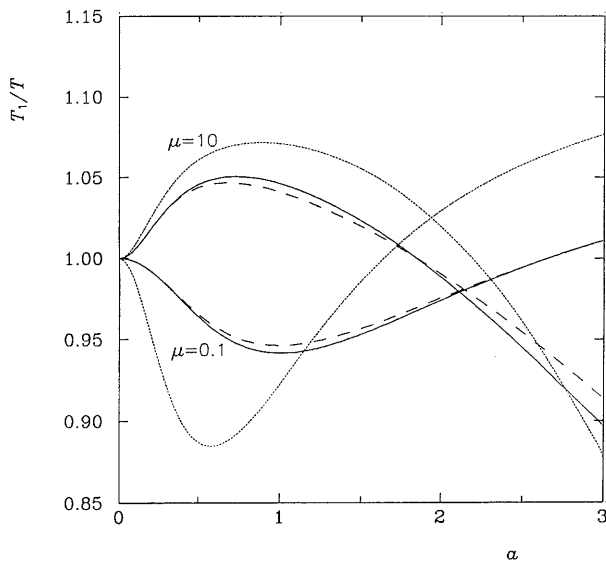


FIG. 2. Shear-rate dependence of the temperature ratio T_1/T for $w_{11}=w_{22}=1$, $\delta=5$, and two values of the mass ratio μ . The symbols are the same as those used in the previous figure.

tion are retained by the GK model since T_1/T does not present a monotonic behavior. In particular, $T_1=T_2=T$ at a certain value of the shear rate which depends on the parameters of the mixture. At a quantitative level, the discrepancies between the exact results and those from the model are more significant when the mass of the excess component is smaller than that of the defect component. With respect to the influence of the interaction potential, we see again that T_1/T is insensitive to the interaction potential in the region of small shear rates. As a increases, the influence of the potential becomes apparent for both values of the mass ratio.

Once α and χ_1 are determined, all the velocity moments of f_1 are explicitly known. The most important quantity of the USF problem is the nonlinear shear viscosity η defined in Eq. (9). Its expression can be obtained from Eq. (27) and its counterpart for $M^{(2)}$. It is given by

$$\eta(a) = \frac{1}{1+\delta} \left[\delta \frac{\nu_{11}\chi_1 + \nu_{12}\chi_{12}}{(\nu_1 + 2\alpha)^2} + \frac{\nu_{22}\chi_2 + \nu_{21}\chi_{21}}{(\nu_2 + 2\alpha)^2} \right] \frac{p}{\zeta}, \quad (42)$$

$p = nk_B T$ being the hydrostatic pressure. This equation provides the expression of the shear viscosity of a binary mixture with general repulsive interactions and subjected to an arbitrarily large shear rate. It is a highly nonlinear function of a and the parameters of the mixture. For vanishing shear rate, one gets the Navier-Stokes shear viscosity coefficient η_0 :

$$\eta_0 = \frac{1}{1+\delta} \left(\frac{\delta}{\nu_1^{(0)}} + \frac{1}{\nu_2^{(0)}} \right) \frac{p}{\zeta}. \quad (43)$$

Except in the case of mechanically equivalent particles, this expression differs from the one derived from the Boltzmann equation for Maxwell molecules.² Before considering nonlinear effects in the momentum transport, it is illustrative to compare the results obtained from the GK and Boltzmann equations for η_0 . In Fig. 3 we plot the ratio $\eta_0^{\text{GK}}/\eta_0^{\text{B}}$ as a function of the mass ratio for several values of the concen-

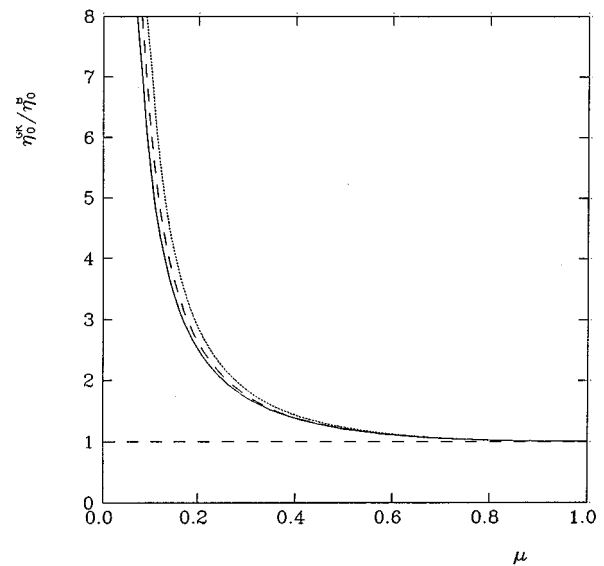


FIG. 3. Plot of the ratio between the Navier-Stokes shear viscosities of the GK and Boltzmann equations, $\eta_0^{\text{GK}}/\eta_0^{\text{B}}$ as a function of the mass ratio for $w_{11}=w_{22}$ and $\delta=2$ (solid line), $\delta=0.5$ (dashed line), and $\delta=0.2$ (dotted line).

tration ratio in the special case of Maxwell molecules. Here, η_0^{GK} and η_0^{B} denote the Navier-Stokes shear viscosities of the GK and Boltzmann equations, respectively. For simplicity, we have set $w_{11}=w_{22}=1$. We observe that the discrepancies between both equations increase significantly as the disparity of the masses increases. In fact, these discrepancies tend to disappear as the mass ratio approaches unity (system of like particles). Beyond the linear regime, the interesting problem is to analyze the shear-rate dependence of the nonlinear shear viscosity η relative to its Navier-Stokes value η_0 . Figure 4 shows η/η_0 for $\delta=5$ and two values of μ for the cases of

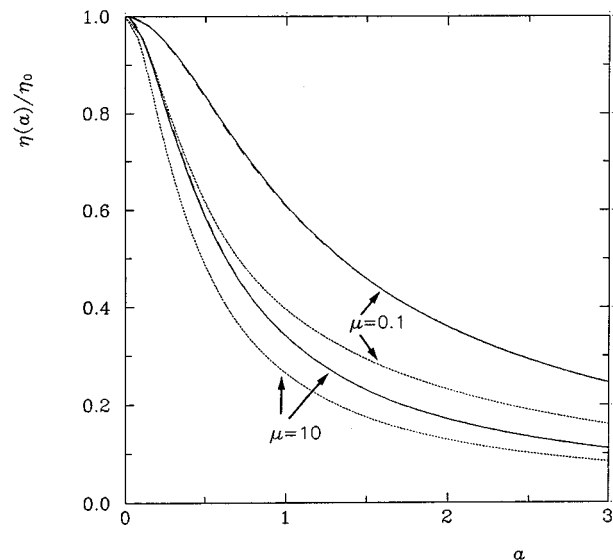


FIG. 4. Shear-rate dependence of the reduced shear viscosity for $w_{11}=w_{22}=1$, $\delta=5$, and two values of the mass ratio μ . The solid and dashed lines refer to the GK results for Maxwell molecules and hard spheres, respectively, while the dotted line corresponds to the Boltzmann results for Maxwell molecules.

Maxwell molecules and hard spheres. In the same way as the Boltzmann results for Maxwell molecules, the GK solution predicts that $\eta(a)$ decreases as a increases (shear thinning) whatever the interaction potential considered. The inhibition of momentum transport is more noticeable when the defect particles are lighter than the excess particles. The comparison with the exact results shows again a better agreement when the mass of the excess component is larger than that of the defect component. We also observe that, according to the GK model, the general shape of the relative viscosity is rather insensitive to the details of the interaction potential. This ‘‘universal’’ character has been recently also observed in the case of a single component gas under shear flow.¹³ The extrapolation of this character to binary mixtures, as the GK model suggests, remains at this stage to be confirmed.

From a rheological point of view, the normal stresses are also important. They are measured by the viscometric functions Ψ_1 and Ψ_2 , defined in Eqs. (10) and (11), respectively. From the expressions of the velocity moments, one gets that $P_{yy} = P_{zz}$. Consequently, the second viscometric function is zero whatever the values of a , μ , δ , w_{11} , w_{22} , and β . This result is exact for Maxwell molecules,² although for $\beta \neq 0$ one expects that $\Psi_2 \neq 0$ as happens in the single component gas.¹⁴ This drawback of the model may be related to the fact that the generalized GK model gives what Chapman and Cowling¹⁰ call the first approximation of the transport coefficients. The first viscometric function is given by

$$\Psi_1(a) = -2 \left[\frac{\delta}{\delta+1} (\nu_1 + 2a)^{-3} (\nu_{11}\chi_1 + \nu_{12}\chi_{12}) + \frac{1}{1+\delta} (\nu_2 + 2a)^{-3} (\nu_{22}\chi_2 + \nu_{21}\chi_{21}) \right] \frac{p}{a^2 \xi^2}. \quad (44)$$

In the limit $a \rightarrow 0$, one gets

$$\Psi_1(0) = -\frac{2}{1+\delta} \left(\frac{\delta}{\nu_1^{(0)2}} + \frac{1}{\nu_2^{(0)2}} \right) \frac{p}{\xi^2}, \quad (45)$$

which is a Burnett coefficient. This coefficient does not coincide with the one obtained from the Boltzmann equation.² In Fig. 5 we show the dependence of $\Psi_1(a)/\Psi_1(0)$ with the shear rate for the same cases as those considered in Fig. 4. We see that $\Psi_1(a)$ is a decreasing function and its dependence on the parameters of the mixture is similar to that of the shear viscosity. We note again a weak influence of the interaction potential on $\Psi_1(a)$.

IV. VELOCITY DISTRIBUTION FUNCTIONS

The general description of transport processes in the mixture requires the knowledge of the velocity distribution functions f_s . Even in the case of Maxwell molecules, an explicit solution to the Boltzmann equation in the USF state is not known and the information about f_s is obtained only indirectly through the knowledge of the first hydrodynamic moments. This is one of the main reasons to use a kinetic model since its simplicity allows one to get the distribution functions. In the case of a single component gas under USF, the velocity distribution function obtained from the BGK

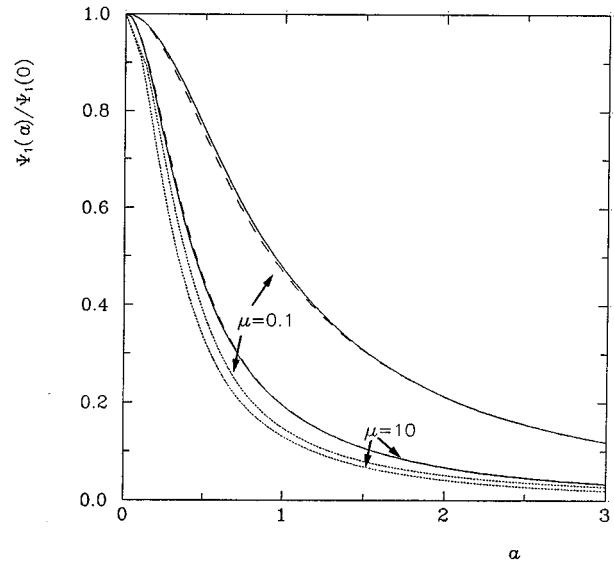


FIG. 5. The same as in Fig. 4, but for the first viscometric function.

equation presents a good qualitative agreement with Monte Carlo simulations^{13,14} except in the high-velocity region. This fact shows the reliability of kinetic models for describing the ‘‘real’’ distribution at least in the region of thermal velocities.

In the steady state, a formal solution to Eq. (20) compatible with the moments (27) can be written as

$$f_1(\mathbf{V}) = \left[\nu_1 - 3\alpha - a_{ij} V_j \frac{\partial}{\partial V_i} - \alpha \mathbf{V} \cdot \frac{\partial}{\partial \mathbf{V}} \right]^{-1} \Phi_1(\mathbf{V}) \\ = \int_0^\infty d\tau e^{-(\nu_1 - 3\alpha)\tau} \exp \left[a\tau V_y \frac{\partial}{\partial V_x} + \alpha\tau \mathbf{V} \cdot \frac{\partial}{\partial \mathbf{V}} \right] \Phi_1(\mathbf{V}), \quad (46)$$

where $\Phi_1 = \nu_{11} f_{11} + \nu_{12} f_{12}$. The explicit expression of $f_1(\mathbf{V})$ can be derived when one takes into account the action of the exponential operator:

$$\exp \left[a\tau V_y \frac{\partial}{\partial V_x} + \alpha\tau \mathbf{V} \cdot \frac{\partial}{\partial \mathbf{V}} \right] \Phi_1(V_x, V_y, V_z) \\ = \Phi_1(e^{\alpha\tau}(V_x + a\tau V_y), e^{\alpha\tau}V_y, e^{\alpha\tau}V_z). \quad (47)$$

To get $f_1(\mathbf{V})$ in a compact form, it is convenient to introduce the dimensionless quantities (25) and (26) and also define the reduced velocity $\xi = (2k_B T/m_1)^{-1/2} \mathbf{V}$. In terms of these quantities and using the identity (47), $f_1(\xi)$ can be written as

$$f_1(\mathbf{V}) = n_1 \left(\frac{m_1}{2k_B T} \right)^{3/2} g_1(\xi), \quad (48)$$

where the reduced distribution $g_1(\xi)$ is

$$g_1(\boldsymbol{\xi}) = \pi^{-3/2} \int_0^\infty d\tau e^{-(\nu_1 - 3\alpha)\tau} \tau [\nu_{11} \chi_1^{-3/2} \times \exp(-\chi_1^{-1} e^{2\alpha\tau} \boldsymbol{\xi} \cdot \boldsymbol{\Gamma}_\tau \cdot \boldsymbol{\xi}) + \nu_{12} \chi_{12}^{-3/2} \times \exp(-\chi_{12}^{-1} e^{2\alpha\tau} \boldsymbol{\xi} \cdot \boldsymbol{\Gamma}_\tau \cdot \boldsymbol{\xi})], \quad (49)$$

and $\boldsymbol{\Gamma}_\tau$ is the matrix,

$$\boldsymbol{\Gamma}_\tau = \begin{pmatrix} 1 & a\tau & 0 \\ a\tau & 1+a^2\tau^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (50)$$

The distribution g_1 happens to be a highly nonlinear function of the shear rate and the parameters of the mixture. The dependence of g_1 on a appears explicitly and also through the functions $\alpha(a)$, $\chi_1(a)$, $\nu_{11}(a)$, and $\nu_{12}(a)$. By making use of Eqs. (37) and (38), the first few terms of the Chapman-Enskog expansion¹⁰ of the distribution function can easily be obtained. Up to Burnett hydrodynamic order, one has

$$g_1(\boldsymbol{\xi}) = g_1^{(0)}(\boldsymbol{\xi}) + a g_1^{(1)}(\boldsymbol{\xi}) + a^2 g_1^{(2)}(\boldsymbol{\xi}) + \vartheta(a^3), \quad (51)$$

where

$$g_1^{(0)}(\boldsymbol{\xi}) = \pi^{-3/2} e^{-\xi^2}, \quad (52)$$

$$g_1^{(1)}(\boldsymbol{\xi}) = -2 \frac{\xi_x \xi_y}{\nu_1^{(0)}} g_1^{(0)}(\boldsymbol{\xi}), \quad (53)$$

$$g_1^{(2)}(\boldsymbol{\xi}) = \left\{ \frac{\alpha_0}{\nu_1^{(0)}} (3 - 2\xi^2) - \frac{5}{2\nu_1^{(0)}} \left[\nu_{11}^{(0)} + \frac{1 - 2\mu\delta + \mu^2}{(1 + \mu)^2} \nu_{12}^{(0)} \right] \chi_{10} - \frac{2}{\nu_1^{(0)2}} \xi_y^2 (1 - 2\xi_x^2) \right\} g_1^{(0)}(\boldsymbol{\xi}). \quad (54)$$

Notice that, up to the Burnett approximation, the interaction parameter only appears implicitly through the quantities $\nu_{rs}^{(0)}$ and χ_{10} . This means that the influence of the potential law on the distribution function can only be significant at large shear rates. According to Eq. (49), note that g_1 diverges to infinity at $\boldsymbol{\xi} = \mathbf{0}$ when $\nu_1 \leq 3\alpha$. This singularity was already found in the monocomponent gas case.¹⁵ The origin of this divergence at vanishing velocity is related to the viscous heating effect inherent to the USF. For the sake of clarity, let us consider the Maxwell interaction for which ν_1 is independent of the shear rate. Two exponential terms compete in Eq. (49): on the one hand, $\exp(-\nu_1\tau)$ gives the fraction of particles of species 1 that have not collided after τ effective collision times; on the other hand, $\exp(3\alpha\tau)$ is a consequence of the presence of the thermostat (viscous heating). For small shear rates [$\alpha(a) < \nu_1/3$], the viscous heating is not sufficiently large to exceed the effect of collisions and g_1 is finite at $\boldsymbol{\xi} = \mathbf{0}$. However, if $\alpha(a) \geq \nu_1/3$ the opposite occurs and there exists a ‘‘condensation’’ of particles of species 1 around $\boldsymbol{\xi} = \mathbf{0}$.

Since $g_1(\boldsymbol{\xi})$ depends on the three components of $\boldsymbol{\xi}$, it is useful to define some marginal distribution functions:

$$g_{1,x}(\xi_x; a) \equiv \int_0^\infty d\xi_y \int_{-\infty}^\infty d\xi_z g_1(\boldsymbol{\xi}), \quad (55)$$

$$g_{1,y}(\xi_y; a) \equiv \int_0^\infty d\xi_x \int_{-\infty}^\infty d\xi_z g_1(\boldsymbol{\xi}). \quad (56)$$

From Eq. (49) it is a simple matter of algebra to get these functions. They are given by

$$g_{1,x}(\xi_x; a) = \frac{1}{2\sqrt{\pi}} \int_0^\infty d\tau \frac{e^{-(\nu_1 - a)\tau}}{(1 + a^2\tau^2)^{1/2}} \left\{ \nu_{11} \chi_1^{-1/2} \times \exp\left[-\frac{e^{2\alpha\tau}}{\chi_1} \frac{\xi_x^2}{1 + a^2\tau^2}\right] \times \operatorname{erfc}\left[\frac{e^{\alpha\tau}}{\chi_1^{1/2}} \frac{a\tau}{(1 + a^2\tau^2)^{1/2}} \xi_x\right] + \nu_{12} \chi_{12}^{-1/2} \exp\left[-\frac{e^{2\alpha\tau}}{\chi_{12}} \frac{\xi_x^2}{1 + a^2\tau^2}\right] \times \operatorname{erfc}\left[\frac{e^{\alpha\tau}}{\chi_{12}^{-1/2}} \frac{a\tau}{(1 + a^2\tau^2)^{1/2}} \xi_x\right] \right\}, \quad (57)$$

$$g_{1,y}(\xi_y; a) = \frac{1}{2\sqrt{\pi}} \int_0^\infty d\tau e^{-(\nu_1 - a)\tau} \left\{ \nu_{11} \chi_1^{-1/2} \times \exp(-\chi_1^{-1} e^{2\alpha\tau} \xi_y^2) \operatorname{erfc}[\chi_1^{-1/2} a \tau \xi_y e^{\alpha\tau}] + \nu_{12} \chi_{12}^{-1/2} \exp(-\chi_{12}^{-1} e^{2\alpha\tau} \xi_y^2) \times \operatorname{erfc}[\chi_{12}^{-1/2} a \tau \xi_y e^{\alpha\tau}] \right\}, \quad (58)$$

where $\operatorname{erfc}(x)$ is the complementary error function.¹⁶ For the sake of illustration, we plot the ratios $\varphi_x(\xi_x) \equiv g_{1,x}(\xi_x; a)/g_{1,x}(\xi_x; 0)$ and $\varphi_y(\xi_y) \equiv g_{1,y}(\xi_y; a)/g_{1,y}(\xi_y; 0)$ for $w_{11} = 1$, $\delta = 5$, $\mu = 0.1, 1$ and 10 in the cases of Maxwell molecules and hard spheres. In Figs. 6 and 7 we show the shape of these ratios for $a = 1$. For this not too large a shear rate, the distributions for Maxwell molecules and hard spheres agree rather well. In general, the distortion from local equilibrium ($\varphi_{x,y} = 1$) is significant for all the mass ratios considered. The dependence of φ_x with μ depends if the x component of the thermal velocity is positive or negative, namely, it increases (decreases) with μ if $\xi_x < 0$ ($\xi_x > 0$). According to the predictions for φ_y , we observe that while the high-velocity population of the solvent increases as its mass is lighter than that of the solute, the opposite happens in the region of very small velocities. In order to analyze the influence of the repulsion law on the distribution function in far from equilibrium states, we have considered $a = 8$ in Figs. 8 and 9 for the same cases as in the two previous figures. Since $a = 8$ is larger than the threshold values of these systems, the functions diverge in the vicinity of $\xi_x = 0$ and $\xi_y = 0$. The qualitative differences between Maxwell molecules and hard spheres are now quite evident, especially in the region of high velocities. In this region, the population increases as the potential becomes harder. These discrepancies are more significant when the mass of the defect particles is smaller than that of the excess component. Nevertheless, despite these

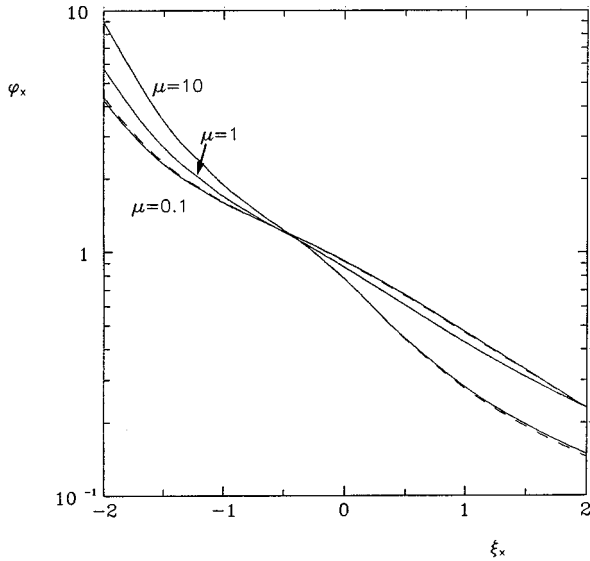


FIG. 6. Reduced distribution function $\varphi_x(\xi_x)$ versus ξ_x for $a=1$, $w_{11}=w_{22}=1$, $\delta=5$, and three values of the mass ratio μ . The solid lines refer to Maxwell molecules while the dashed lines refer to hard spheres.

discrepancies among the velocity distribution functions for thermal velocities, the rheological properties are practically independent of the potential considered.

V. TRACER LIMIT

The results presented in previous sections apply for arbitrary values of masses, concentrations, and force constants. An interesting physical limit corresponds to the so-called tracer limit, namely, $n_1 \ll n_2$. In this situation, one usually assumes that the excess component is not disturbed by the presence of the tracer particles and, in addition, one neglects the effect on the state of the tracer component of collisions among tracer particles themselves. As a consequence, one expects that the tracer particles do not contribute signifi-

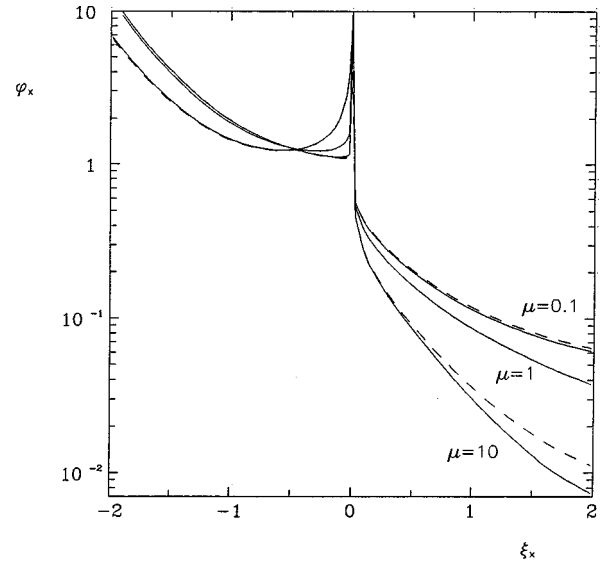


FIG. 8. The same as Fig. 6, but for $a=8$.

cantly to the total properties of the mixture. Nevertheless, and quite surprisingly, recent results derived from the Boltzmann equation for Maxwell molecules⁹ show a transition to a new state in which the relative contribution of the tracer species to the properties of the mixture does not tend to zero as $\delta \rightarrow 0$ when the mixture is sufficiently far from equilibrium. Now we are going to analyze the tracer limit in the context of the GK equation.

For the sake of simplicity, let us consider first the special case of Maxwell molecules, for which the thermostat parameter α verifies the closed equation (31). Taking carefully the limit $\delta \rightarrow 0$, Eq. (31) factorizes into two cubic equations:

$$3\alpha(v_{22} + 2\alpha)^2 = v_{22}a^2, \quad (59)$$

$$3(\alpha + M)(1 + 2\alpha)^2 = (1 - 2M)a^2. \quad (60)$$

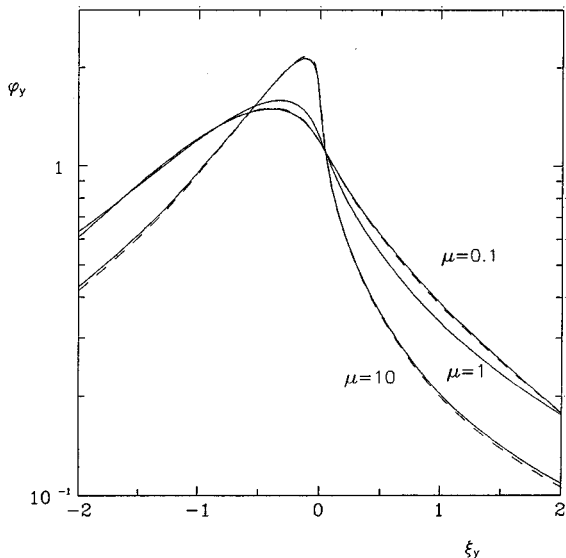


FIG. 7. The same as Fig. 6, but for $\varphi_y(\xi_y)$ as a function of ξ_y .

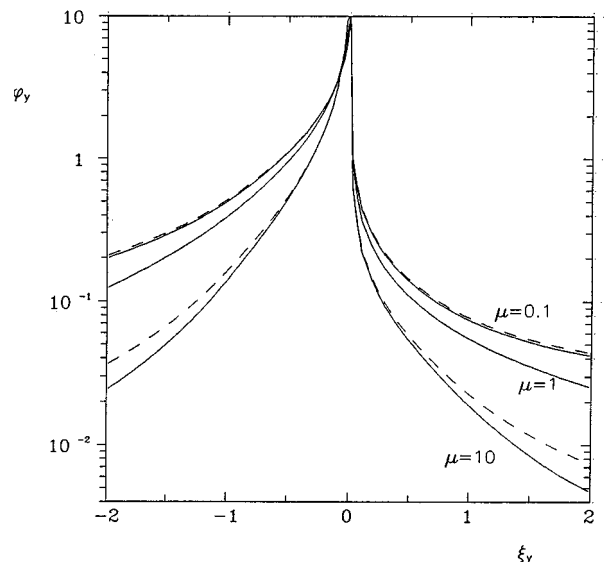


FIG. 9. The same as Fig. 7, but for $a=8$.

Equation (59) is associated with the time evolution of the excess component, while Eq. (60) gives the transient behavior of the tracer species. The real roots (which give the dominant behavior in the long-time limit) of both equations are, respectively,

$$\alpha = \frac{\nu_{22}}{2} F\left(\frac{a}{\nu_{22}}\right), \quad (61)$$

$$\alpha' = \left(\frac{1}{2} - M\right) F\left(\frac{a}{1-2M}\right) - M, \quad (62)$$

where $F(x)$ is defined in Eq. (36). According to the analysis carried out in Ref. 9, the adequate thermostat to achieve steady values for T_1 and T_2 is $\alpha_{\max} = \max(\alpha, \alpha')$. As long as $\delta \neq 0$, the difference between the two largest roots of the

sixth-degree equation (31) does not vanish for any value of the shear rate and the parameters of the mixture. In the same way as in the Boltzmann description, for a given choice of the force constants, it turns out that $\alpha_{\max} = \alpha$ if μ is larger than a certain threshold value μ_0 , which is the solution of $2M + \nu_{22} = 1$. On the other hand, if $\mu < \mu_0$, then $\alpha_{\max} = \alpha'$ for shear rates larger than a critical value $a_c(\mu)$. The main physical consequence of the existence of $a_c(\mu)$ is that the tracer species have a finite contribution to the total properties of the mixture when $a > a_c(\mu)$ and $\mu < \mu_0$. For instance, let us consider the ratio p_1/p , where $p_1 = n_1 k_B T_1$. This ratio represents the relative contribution of the tracer particles to the total energy of the system. From Eq. (41), one gets that in the tracer limit $p_1/p \approx 0$ if $a < a_c(\mu)$ and

$$\frac{p_1}{p} = \frac{4\alpha'^3(\lambda + 2M - 1) + 12\alpha'^2 M \lambda + \alpha' \lambda [1 - \lambda + 2M(2 + \lambda)] + M \lambda}{[4\alpha'^2 + 8\alpha' M + 2M(1 + \lambda) - \lambda](M + \alpha')(\lambda - 1)}, \quad (63)$$

if $a > a_c(\mu)$. Here, $\lambda \equiv [2\mu w_{22}/(1 + \mu)]^{1/2}$. Although the molar fraction of the tracer particles is negligible, their contribution to the total energy may be relevant for sufficiently large shear rates. Obviously, identical conclusions can be obtained for other transport properties of the mixture. Possible physical implications of the singularity have been discussed in Ref. 9.

A natural question is whether the above phenomenon can be extended to other interaction potentials. Since for non-Maxwell molecules no explicit closed equation for α can be obtained, it is a complex problem to analyze with detail the tracer limit. One possibility is to numerically solve the coupled equations for α and χ_1 for very small values of the concentration ratio. For illustrative purposes, Fig. 10 shows $p_1/p - n_1/n$ versus a for $\mu = 0.1$ and $\delta = 10^{-4}$ in the case $w_{11} = w_{22} = 1$. We have considered $r^{-\gamma}$ repulsive forces, with $\gamma = 5, 7, 9, 13$, and ∞ . We have also included the exact tracer limit ($\delta = 0$) for Maxwell molecules ($\gamma = 5$), which is indistinguishable from the one corresponds to $\delta = 10^{-4}$. For this interaction potential, $a_c(0.1) \approx 3.906$. According to Fig. 10, it is evident that p_1/p is only negligible for $a \leq a_c$. This indicates the different qualitative behavior of the system depending on whether a is larger or not than a certain critical value a_c , which might be a weak function of the interaction parameter. The curves also show that the contribution of the tracer species to the total energy of the mixture decreases as γ increases. In fact, $p_1/p \approx 0$ in the limit of hard spheres ($\gamma \rightarrow \infty$) for the range of shear rates considered. Nevertheless, these conclusions must be taken with caution since they require an accurate analysis of the tracer limit for general repulsive potentials. We plan to address this study in the near future.

VI. CONCLUDING REMARKS

In this paper we have considered a binary mixture with repulsive intermolecular interactions under uniform shear

flow. The macroscopic state is characterized by uniform density and temperature and a linear profile of the x component of the flow velocity along the y direction. In principle, this state is not stationary since the temperature increases in time due to viscous heating. To prevent this effect, and in the same way as in computer simulations, a drag external force is introduced. The only nonequilibrium parameter is the constant shear rate a , which measures the deviation from equilibrium. The main transport property is in this case the momentum transport, which is related to the pressure tensor. On the other hand, the transport coefficients also depend on the parameters of the mixture, namely the mass, concentration,

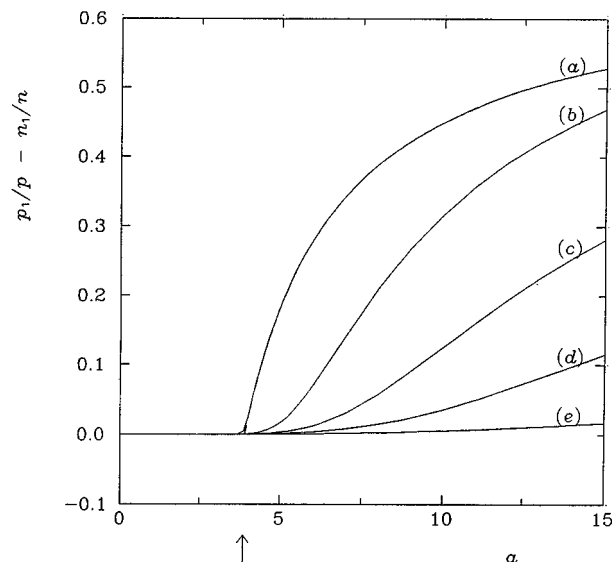


FIG. 10. Shear-rate dependence of $p_1/p - n_1/n$ for $w_{22} = 1$, $\mu = 0.1$, and $\delta = 10^{-4}$ for several $r^{-\gamma}$ repulsive forces: (a) $\gamma = 5$, (b) $\gamma = 7$, (c) $\gamma = 9$, (d) $\gamma = 13$, and (e) $\gamma = \infty$. We have also included the case $\delta = 0$ for Maxwell molecules (dashed line). The arrow indicates the location of the critical value a_c for Maxwell molecules.

and size of each species. In this situation, only the special case of Maxwell molecules allows one to obtain explicit results for the rheological properties within the framework of the Boltzmann equation.² In order to analyze the problem for more realistic intermolecular potentials, one needs to resort to a kinetic model. In the model considered here all the details of the interaction potential are introduced through effective collision frequencies ν_{rs} , which depend on the temperatures of each species. Furthermore, and due to the simplicity of the model, explicit expressions for the velocity distribution functions can be derived.

All the velocity moments are obtained as nonlinear functions of the shear rate, the ratios of mass, concentration, and force constants and a parameter characterizing the interaction potential. The expressions of such moments are given in terms of the thermostat parameter α and the temperature ratios χ_s , which are in general coupled. The rheological properties (namely the non-Newtonian shear viscosity η and the viscometric function Ψ_1) decrease as the shear rate increases, whatever the parameters of the mixture and the interaction potential considered are. Another interesting property is the temperature ratio, which is a measure of the distribution of the kinetic energy between both species. This ratio does not present a monotonic behavior with the shear rate, since it has a maximum or minimum depending on the parameters of the mixture. Concerning the influence of the interaction potential considered, 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 power law. This influence is more significant in the case of the temperature ratio. A comparison with related results derived from the Boltzmann equation for Maxwell molecules² indicate a reasonably good agreement for not too large shear rates, especially for systems of like particles.

Another interesting aspect addressed in this paper is the analysis of the dependence of the velocity distribution functions on the parameters of the problem as well as on the interaction potential. With respect to the first point, we observe that these distributions are strongly distorted from their equilibrium values. This fact could be in principle anticipated on the basis of the highly nonlinear dependence of the transport coefficients on the shear rate and the parameters of the mixture. On the other hand, other nonlinear effects that are not present in the velocity moments, such as the divergence of the distribution function at zero velocity, emerge for large shear rates. With respect to the effect of the repulsive intermolecular law, and in contrast to the weak influence of the interaction model on the transport properties, we conclude that the shape of the distribution function is affected by the hardness of the interaction very far from equilibrium. This influence becomes more noticeable in the domain of high speeds, especially when the excess component is heavier than that of the defect component.

In the tracer limit, it is worthwhile to remark that the GK model also predicts a transition to a new state. This transition had been previously identified from the Boltzmann solution in the case of Maxwell molecules.^{2,9} The numerical calculations reported in this paper suggest that this phenomenon

also appears for non-Maxwell molecules, although it is less strong as the potential becomes harder. As a matter of fact, it might disappear in the limit of hard spheres. We plan to present a more detailed analysis of the tracer limit in the context of the GK model in order to support the above expectations.

The analysis carried out refers to a binary mixture in the low-density regime. The extrapolation of the conclusions drawn out here to dense fluids must be taken with caution since the dominant mechanism of collisional transfer is absent in the dilute gas regime. Nevertheless, qualitative features in appropriate scaled variables may still be useful for interpretation of simulation results in fluids.⁵ In the particular case of the uniform shear flow, one could obtain a qualitative agreement with the shear thinning observed in simulations at liquid densities whether one scales the shear viscosity to a convenient dimensionless form.

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