

Nonlinear Couette flow in a dilute gas: Comparison between theory and molecular-dynamics simulation

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(Received 20 February 1998)

Nonlinear transport properties of a d -dimensional dilute gas subjected to a planar Couette flow are determined. The results are obtained from a kinetic model that accounts for the correct value of the Prandtl number. The solution is characterized by constant pressure and linear velocity and parabolic temperature profiles with respect to a scaled variable. The main transport coefficients are explicitly obtained as nonlinear functions of the reduced shear rate. A comparison with recent molecular-dynamics simulations of a bidimensional gas of hard disks [D. Risso and P. Cordero, Phys. Rev. E **56**, 489 (1997)] is carried out. Such a comparison shows that our results are in better agreement with the computer simulations than those previously derived from other approximations, especially in the case of the thermal conductivity tensor. [S1063-651X(98)03308-X]

PACS number(s): 05.20.Dd, 47.50.+d, 51.10.+y, 05.60.+w

I. INTRODUCTION

The Boltzmann equation provides an adequate framework to analyze transport phenomena occurring in dilute gases. The standard method of solving it is the Chapman-Enskog series expansion in gradients of the hydrodynamic fields. Nevertheless, this approach is not very useful when one deals with far from equilibrium situations for which, due to the complexity of the Boltzmann collision term, it is a formidable task to find exact solutions [1]. This problem has stimulated in the past the search for alternative approximate schemes to overcome the above difficulties. In the context of analytical methods, the use of kinetic models [2] as well as Grad's moment expansion method [3] can be considered *a priori* as reliable procedures to study such nonlinear transport problems. However, it is not evident which approximate scheme should be used in each case. As a complementary tool to analytical methods, one can get *semiexperimental* results from microscopic computational techniques using molecular-dynamics and/or Monte Carlo simulations.

One of the most interesting problems for which the exact solution of the Boltzmann equation is not known is the steady planar Couette flow. It corresponds to a gas between two parallel plates in relative motion and kept, in general, at different temperatures. These boundary conditions lead to combined heat and momentum transport so that the relevant fluxes are the pressure tensor \mathbf{P} and the heat flux vector \mathbf{q} . From the knowledge of the above fluxes, one can identify the main transport coefficients of the problem, namely, the shear viscosity coefficient η and the nonzero elements of the thermal conductivity tensor $\boldsymbol{\kappa}$. In the context of the Boltzmann equation and for a three-dimensional (3D) gas of Maxwell molecules, Tij and Santos [4] have obtained the above coef-

ficients by using a perturbation expansion in powers of the shear rate up to the super-Burnett approximation. Moreover, very recently Risso and Cordero [5] have explicitly evaluated η and $\boldsymbol{\kappa}$ in the case of a 2D gas of hard disks by applying Grad's method to the Boltzmann equation. Beyond the Navier-Stokes regime, they found that these coefficients turn out to be highly nonlinear functions of the (dimensionless) shear rate. In addition, and in order to validate their analytical predictions, they have also performed molecular-dynamics simulations. The comparison shows good agreement for the nonlinear shear viscosity in the range of shear rates considered while the discrepancies become important in the case of the thermal conductivity tensor, especially when the shear rate is large. Given this fact, a natural question is whether the above analytical predictions could be improved if one uses a suitable kinetic model.

The aim of this paper is to analyze the transport properties of the Couette flow state by starting from the so-called ellipsoidal statistical (ES) kinetic model [6]. In this model, the Boltzmann collision term is replaced by a simpler one $J[f, f] \rightarrow \nu(f_0 - f)$, where f_0 is an anisotropic Gaussian that involves the pressure tensor and the Prandtl number Pr . This quantity can be considered as an extra parameter (apart from the collision frequency ν) to be adjusted to give the same Navier-Stokes transport coefficients as those obtained from the Boltzmann equation. That happens if $Pr = \frac{2}{3}$ in the 3D case or $Pr = \frac{1}{2}$ in the 2D case [6]. Besides, if $Pr = 1$, one recovers the well-known Bhatnagar-Gross-Krook (BGK) model [7], so that the latter can be considered as a particular case of the ES model. The goal is to solve the ES model for a d -dimensional system subjected to the planar Couette flow. This study extends previous results obtained in the Couette flow for the 3D case by using the ES model [8]. Now, our main motivation is to compare the results derived from the ES and BGK models and from Grad's solution with those obtained in the Boltzmann equation from a perturbation expansion (3D case) [4] and from molecular-dynamics simulations for hard disks [5]. This comparison allows one to infer

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the degree of reliability of the *nonlinear* transport coefficients obtained from the different approximations.

The plan of the paper is as follows. In Sec. II we solve the ES model in the steady planar Couette flow. We provide explicit expressions of the relevant transport coefficients of the problem in terms of the shear rate, the thermal gradient, the dimensionality of the system, and the Prandtl number Pr . In Sec. III we compare the Boltzmann and molecular-dynamics results with the predictions made from the different approximations (kinetic models and Grad's method). In general, the comparison shows a superiority of the kinetic models over Grad's approximation, especially in the case of the ES model at the level of the thermal conductivity tensor. A few concluding remarks close the paper in Sec. IV.

II. SOLUTION OF THE ELLIPSOIDAL STATISTICAL MODEL IN THE COUETTE FLOW

A kinetic model is constructed by replacing the complicated Boltzmann collision operator $J[f, f]$ by a simpler collision term that retains the qualitative and average properties of the true $J[f, f]$. In the case of the ES kinetic model [6] one replaces $J[f, f]$ by $J^{\text{ES}} \equiv -\nu(f - f_0)$, where ν is an effective collision frequency that can depend on the density and temperature and

$$f_0(\mathbf{v}) = n \pi^{-d/2} (\det \Lambda)^{1/2} \exp(-\Lambda_{ij} V_i V_j), \quad (1)$$

where $d=2,3$ refers to the dimensionality of the system, $\Lambda = [A\mathbf{1} - (B/\rho)\mathbf{P}]^{-1}$, $\mathbf{1}$ is the unit tensor, $\rho = mn$, $A = (2k_B T/m)\text{Pr}^{-1}$, and $B = 2(\text{Pr}^{-1} - 1)$. Here m is the mass of a particle, k_B is the Boltzmann constant,

$$n = \int d\mathbf{v} f(\mathbf{v}) \quad (2)$$

is the local number density, $\mathbf{V} = \mathbf{v} - \mathbf{u}$,

$$\mathbf{u} = \frac{1}{n} \int d\mathbf{v} \mathbf{v} f(\mathbf{v}) \quad (3)$$

is the local flow velocity,

$$T = \frac{m}{dnk_B} \int d\mathbf{v} V^2 f(\mathbf{v}) \quad (4)$$

is the local temperature, and

$$\mathbf{P} = m \int d\mathbf{v} \mathbf{V} \mathbf{V} f \quad (5)$$

is the pressure tensor. The quantity Pr is an extra parameter that plays the role of the Prandtl number. It is easy to see that if $\text{Pr} = 1$, f_0 reduces to the local Maxwellian and one recovers the well-known BGK equation [7]. In contrast to the BGK approximation, the ES collision term involves not only the first five conserved hydrodynamic fields but also the dissipative momentum flux. The other relevant dissipative flux is the heat flux \mathbf{q} defined as

$$\mathbf{q} = \frac{m}{2} \int d\mathbf{v} \mathbf{V}^2 \mathbf{V} f. \quad (6)$$

The ES model can be seen as an extension of the simple BGK model to account for the correct Prandtl number. This can be particularly important in situations where combined heat and momentum transport occur, as it is the case of steady Couette flow. In the ES model, it is straightforward to evaluate the Navier-Stokes transport coefficients, namely, the shear viscosity coefficient η_0 and the thermal conductivity coefficient κ_0 . The result is [9]

$$\eta_0 = \frac{nk_B T}{\nu \text{Pr}^{-1}}, \quad (7)$$

$$\kappa_0 = \frac{d+2}{2} \frac{nk_B^2 T}{m\nu}. \quad (8)$$

If we identify ν with a given eigenvalue of the linearized Boltzmann collision operator and take $\text{Pr} = 1 - 1/d$, then expressions (7) and (8) coincide with those derived from the Boltzmann equation in the first Sonine approximation [6].

We describe now the nonlinear problem we are interested in. Let us consider a dilute gas enclosed between two parallel plates in relative motion and kept at different temperatures (planar Couette flow). Let the x axis be parallel to the motion and the y axis be normal to the plates. We want to compute the transport properties in a steady state under *arbitrary* velocity and temperature gradients along the y direction. Under the geometry of the Couette flow, the ES equation reads

$$v_y \frac{\partial}{\partial y} f = -\nu(f - f_0). \quad (9)$$

In the same way as in previous descriptions [8,10,11], our interest lies in obtaining the hydrodynamic profiles in the bulk region far away from the boundaries. Therefore, instead of introducing appropriate boundary conditions to Eq. (9), we first assume a given form of the profiles and then verify their consistency. We expect to describe the state of the gas in the bulk by looking for a consistent solution regardless the actual characterization of the boundaries. Following the work of Risso and Cordero [5], we choose $\zeta = \nu \text{Pr}^{-1} = nk_B T / \eta_0$ as a convenient collision frequency to reduce all the quantities of the problem with respect to it. Thus let us assume that Eq. (9) admits a consistent solution characterized by the hydrodynamic profiles

$$p = nk_B T = \text{const}, \quad (10)$$

$$\frac{\partial}{\partial s} u_x = a = \text{const}, \quad (11)$$

$$\frac{\partial^2}{\partial s^2} T = -\frac{2m}{k_B} \gamma(a) = \text{const}, \quad (12)$$

where $ds = \zeta(y) dy$ is a scaled space variable. In terms of s , our results are independent of the interaction potential considered. Obviously, when one returns to the actual space coordinate y , the profiles depend on the interaction law through the dependence of the collision frequency ν on the temperature. Thus, for instance, for repulsive potentials of the form $r^{-\ell}$, $\nu \propto n T^\mu$, with $\mu = \frac{1}{2} - (d-1)/\ell$. The dimensionless function $\gamma(a)$ (which measures the curvature of the tempera-

ture profile) is a nonlinear function of the reduced shear rate a to be determined by consistency.

As stated in the Introduction, the fluxes P_{xy} , q_y , and q_x define the most relevant nonlinear transport coefficients of the problem, namely, the generalized shear viscosity $\eta(a)$,

$$P_{xy} = -\eta(a) \frac{\partial}{\partial y} u_x, \tag{13}$$

the generalized thermal conductivity coefficient $\kappa_{yy}(a)$,

$$q_y = -\kappa_{yy}(a) \frac{\partial}{\partial y} T, \tag{14}$$

and a transport coefficient $\kappa_{xy}(a)$, which measures the heat flux along the x direction induced by the shear flow

$$q_x = -\kappa_{xy}(a) \frac{\partial}{\partial y} T. \tag{15}$$

The evaluation of these three generalized coefficients is the main objective of this paper [12].

In order to determine $\gamma(a)$ and the corresponding fluxes it is sufficient to use the following formal solution to Eq. (9):

$$f = \left(1 + \text{Pr}^{-1} v_y \frac{\partial}{\partial s} \right)^{-1} f_0 = \sum_{k=0}^{\infty} \text{Pr}^{-k} (-v_y)^k \frac{\partial^k}{\partial s^k} f_0. \tag{16}$$

This solution is consistent with the profiles (10)–(12) if and only if

$$\int d\mathbf{v} \{1, \mathbf{V}, V^2\} f = \left\{ n, \mathbf{0}, d \frac{n k_B T}{m} \right\}. \tag{17}$$

The fulfillment of these conditions requires the evaluation of the nonzero elements of the pressure tensor. Since the mathematical procedures to verify Eq. (17) and to get the transport coefficients (13)–(15) are identical to those employed in Ref. [8] for the 3D case, here we only quote the final results and refer the interested reader to the corresponding Appendixes of Ref. [8] for further details.

It is convenient to introduce an auxiliary parameter β , related to the shear rate a through the implicit equation

$$a^2 = \frac{[\text{Pr}(\text{Pr} + \overline{\text{Pr}}C_1)]^2 [2F_2 + dF_1(\text{Pr} + \overline{\text{Pr}}C_1)]}{\text{Pr}(F_0^2 \overline{\text{Pr}} + F_1 \text{Pr}) + \overline{\text{Pr}}C_1(F_0^2 \overline{\text{Pr}} + 2F_1 \text{Pr}) + C_1^2 F_1 \overline{\text{Pr}}^2 - 2\beta F_0^2 F_2 \overline{\text{Pr}}^2} \beta, \tag{18}$$

where $\overline{\text{Pr}} = \text{Pr} - 1$,

$$C_1(\beta) = 2\beta(F_1 + 2F_2) - 1, \tag{19}$$

and $F_r(\beta) = [(d/d\beta)\beta]^r F_0(\beta)$, where

$$F_0(\beta) = \frac{2}{\beta} \int_0^\infty dt t e^{-t^2/2} K_0(2\beta^{-1/4} t^{1/2}), \tag{20}$$

K_0 being the zeroth-order modified Bessel function. The function $\gamma(a)$ that measures the temperature curvature [cf. Eq. (12)] is given by

$$\gamma = [1 + \overline{\text{Pr}}(1 + C_1)] \text{Pr}^2 \beta. \tag{21}$$

The nonlinear transport coefficients can be written as

$$\eta(a) = \eta_0 F_\eta(a), \tag{22}$$

$$\kappa_{yy}(a) = \kappa_0 F_\kappa(a), \tag{23}$$

$$\kappa_{xy}(a) = -\kappa_0 \Phi(a), \tag{24}$$

where η_0 and κ_0 are given by Eqs. (7) and (8), respectively, and

$$F_\eta = \frac{\text{Pr}^2 F_0}{(\text{Pr} + \overline{\text{Pr}}C_1)^2}, \tag{25}$$

$$F_\kappa = \frac{\text{Pr}}{2+d} \frac{a^2}{\gamma} F_\eta, \tag{26}$$

$$\begin{aligned} \Phi = & \frac{\text{Pr}^{-3}}{2+d} C_4 \{ 4a^3 C_4 (F_2 + 5F_3 + 8F_4 + 4F_5) \\ & + 6 \text{Pr} a^2 C_4 C_6 (F_2 + 4F_3 + 4F_4) + \text{Pr}^2 a \\ & \times [6C_3 F_2 + C_4 (F_2 + 2F_3) (2 + 3C_6^2) + 2(d-2)C_5 F_2] \\ & + \text{Pr}^3 C_6 [3C_3 F_1 + C_4 (F_1 + 2F_2) (1 + C_6^2) \\ & + (d-2)C_5 F_1] \}. \end{aligned} \tag{27}$$

In the above equations

$$C_2(\beta) = 2\beta F_1 - 1, \tag{28}$$

$$\begin{aligned} C_3(\beta) = & \frac{1}{(\text{Pr} + \overline{\text{Pr}}C_1)^3 (\text{Pr} + \overline{\text{Pr}}C_2)} \\ & \times \{ (\overline{\text{Pr}}C_1 + \text{Pr})^2 [C_1 \overline{\text{Pr}} (dC_2 \overline{\text{Pr}} + d \overline{\text{Pr}} + 2) \\ & + \overline{\text{Pr}}C_2 (d \text{Pr} - 1) + \text{Pr} (d \overline{\text{Pr}} + 1)] \\ & - a^2 F_0^2 \text{Pr}^{-2} \overline{\text{Pr}}^2 (\text{Pr} + \overline{\text{Pr}}C_2) \}, \end{aligned} \tag{29}$$

$$C_4(\beta) = \frac{1}{\text{Pr} + C_1 \overline{\text{Pr}}}, \tag{30}$$

$$C_5(\beta) = \frac{1}{\text{Pr} + C_2 \overline{\text{Pr}}}, \tag{31}$$

$$C_6(\beta) = \frac{F_0 \text{Pr}^{-1} \overline{\text{Pr}}}{\text{Pr} + C_1 \text{Pr}} a. \quad (32) \quad + 4 + 2d] a^2 + O(a^4) \Big\}, \quad (34)$$

Equations (22)–(27), (21), and (18) provide expressions for the transport coefficients and the hydrodynamic profiles as implicit functions of the shear rate a . Although this quantity is the natural physical independent parameter, from a practical point of view it is convenient to take β as the independent variable since all the unknowns are explicitly expressed in terms of it.

When $a=0$, one has $F_\eta = F_\kappa = 1$ and $\Phi = 0$, so that the Navier-Stokes transport coefficients (7) and (8) are reobtained. Before analyzing the shear-rate dependence of the transport coefficients, it is worthwhile to consider the limit of small shear rates, in which case one gets

$$\beta = \frac{\text{Pr}^{-2}}{2+d} a^2 \left\{ 1 - \frac{2 \text{Pr}^{-1}}{(2+d)^2} [\text{Pr}^2(7+8d) - \text{Pr}(52+11d) + 8+4d] a^2 + O(a^4) \right\}, \quad (33)$$

$$\gamma = \frac{\text{Pr}}{2+d} a^2 \left\{ 1 - \frac{4 \text{Pr}^{-2}}{(2+d)^2} [\text{Pr}^2(1+2d) - \text{Pr}(23+4d) \right.$$

$$F_\eta = 1 - \frac{6 \text{Pr}^{-1}(1+2 \text{Pr})}{2+d} a^2 + O(a^4), \quad (35)$$

$$F_\kappa = 1 - \text{Pr}^{-2} \frac{\text{Pr}^2(20+4d) + \text{Pr}(104+22d) - 16-8d}{(2+d)^2} a^2 + O(a^4), \quad (36)$$

$$\Phi = \text{Pr}^{-1} \frac{(4+d)(\text{Pr}+1)}{2+d} a + O(a^3). \quad (37)$$

Apart from obtaining the nonlinear transport coefficients, the use of a kinetic model allows one to explicitly get the velocity distribution function $f(\mathbf{r}, \mathbf{v})$. This quantity, which cannot be determined from the Boltzmann equation, provides all the information on the planar Couette flow problem. Following similar mathematical steps as the ones used in Ref. [8], the distribution function can be written as $f(\mathbf{r}, \mathbf{v}) = n(m/2\pi k_B T)^{d/2} \Psi(\boldsymbol{\xi})$, where

$$\begin{aligned} \Psi(\boldsymbol{\xi}) = & \frac{2\delta(1+\delta)^{d/2}}{\text{Pr}^{-1}\epsilon|\xi_y|} (C_3 C_4)^{-1/2} C_5^{1-d/2} \int_{t_0}^{t_1} dt [2t - (1-\delta)t^2]^{-(1+d/2)} \exp\left(-\frac{2\delta}{1+\delta} \frac{1-t}{\text{Pr}^{-1}\epsilon\xi_y}\right) \\ & \times \exp\left[-\frac{1+\delta}{2t-(1-\delta)t^2} \left[c_3^{-1} \left(\xi_x + \frac{2a\delta}{1+\delta} \frac{1-t}{\epsilon} \right)^2 + (C_4^{-1} + C_6^2 C_3^{-1}) \xi_y^2 + (d-2) C_5^{-1} \xi_z^2 \right. \right. \\ & \left. \left. + 2C_6 C_3^{-1} \xi_y \left(\xi_x + \frac{2a\delta}{1+\delta} \frac{1-t}{\epsilon} \right) \right] \right]. \end{aligned} \quad (38)$$

Here $(t_0, t_1) \equiv (0, 1)$ if $\xi_y > 0$ and $(t_0, t_1) \equiv [1, 2/(1-\delta)]$ if $\xi_y < 0$. Furthermore, $\boldsymbol{\xi} = (m/2k_B T)^{1/2} \mathbf{V}$,

$$\delta = \frac{\epsilon}{(\epsilon^2 + 8\gamma)^{1/2}}, \quad (39)$$

and

$$\epsilon = \left(\frac{2k_B}{mT} \right)^{1/2} \frac{1}{\zeta} \frac{\partial T}{\partial y} \quad (40)$$

is a reduced local thermal gradient. The nonlinear dependence of $\Psi(\boldsymbol{\xi})$ on the dimensionless gradients a and ϵ is very apparent.

III. COMPARISON WITH EXACT BOLTZMANN RESULTS AND MOLECULAR-DYNAMICS SIMULATIONS

As said before, very recently Risso and Cordero [5] have performed computer molecular-dynamics experiments to study the shear-rate dependence of F_η , F_κ , and Φ for a hard disk gas ($d=2$). Furthermore, they compared their simula-

tion data with theoretical results derived from Grad's method of the Boltzmann equation. While they found good agreement for the shear viscosity, the same did not happen in the case of the thermal conductivity tensor. On the other hand, in the 3D case, Tij and Santos [4] have obtained corrections to the Navier-Stokes equations in the limit of small shear rates from an exact analysis of the Boltzmann equation for Maxwell molecules. Since the calculations presented in the preceding section are not restricted to a given value of the dimensionality d , now we can compare all the above analytical and computational predictions with those obtained from the BGK ($\text{Pr}=1$) and ES ($\text{Pr}=1-1/d$) models. This comparison will be useful to assess the reliability of the approximate methods or kinetic models.

Let us start with a three-dimensional system. In this case, for small shear rates and taking into account only terms up to the third (super-Burnett) order in a , the transport coefficients can be written as $F_\eta(a) = 1 + F_\eta^{(2)} a^2 + \dots$, $F_\kappa(a) = 1 + F_\kappa^{(2)} a^2 + \dots$, and $\Phi(a) = \Phi^{(1)} a + \dots$, where the numerical values of the coefficients $F_\eta^{(2)}$, $F_\kappa^{(2)}$, and $\Phi^{(1)}$ depend on the approximation used [13]. In Table I we show the differ-

TABLE I. Coefficients $F_\eta^{(2)}$, $F_\kappa^{(2)}$, and $\Phi^{(1)}$ for a three-dimensional gas as obtained from the Boltzmann equation for Maxwell molecules (B), from Grad's method (G), from the Bhatnagar-Gross-Krook (BGK) model, and from the ellipsoidal statistical (ES) model.

Coefficient	B	G	BGK	ES
$F_\eta^{(2)}$	$-\frac{149}{45}$	$-\frac{13}{5}$	$-\frac{18}{5}$	$-\frac{21}{5}$
$F_\kappa^{(2)}$	-7.259	$\frac{21}{50}$	$-\frac{162}{25}$	$-\frac{389}{50}$
$\Phi^{(1)}$	$\frac{7}{2}$	$\frac{7}{2}$	$\frac{14}{5}$	$\frac{7}{2}$

ent values of these coefficients according to the Boltzmann equation [4], Grad's method [5], and the BGK and ES models. According to the values reported in Table I, we see that in the case of the shear viscosity, all the approximations predict the correct sign of $F_\eta^{(2)}$. Further, the relative errors are around 21% for Grad's method, 26% for the ES model, and 9% in the BGK model. Concerning the thermal conductivity coefficient, in contrast to what happens in the kinetic models, Grad's approximation does not give the correct sign of $F_\kappa^{(2)}$. At a quantitative level, the BGK model estimates $F_\kappa^{(2)}$ with a deviation of around 11%, while in the ES model this coefficient is estimated with a deviation of around 7%. With respect to $\Phi^{(1)}$, both the Grad and ES approximations give the exact Boltzmann value, while the relative error in the BGK model is around 20%.

Unfortunately, beyond the small shear rate limit, no exact results are known, so that the only way to validate the different approximations is to use computer simulation data. To the best of our knowledge, the simulation of Risso and Cordero for a two-dimensional dilute gas [5] is the only computer experiment in which the planar Couette flow problem has been studied. Although the Boltzmann equation is only valid in the zero-density limit, it is evident that in a molecular-dynamics experiment one needs to fix a nonzero (but very small) average density. As a consequence, the collisional contributions to the transport coefficients are not *strictly* zero. This implies that the Boltzmann equation cannot exactly reproduce the simulation data, although the discrepancies between both can be neglected as the density becomes very small. In particular, in the simulation of Risso and Cordero, the fraction of area covered by the disks was 1%, so that, for instance, the nonideal corrections to the equation of state are less than 2%. In Figs. 1–3 we show the shear-rate dependence of the dimensionless functions F_η , F_κ , and Φ , respectively, as obtained from simulations (circles), the ES model (solid line), Grad's method (dotted line), and the BGK model (dashed line). In the case of the nonlinear shear viscosity (Fig. 1) we see that the qualitative trends predicted by the simulation results are retained by all the approximations, namely, the viscosity decreases as the shear rate increases (shear thinning effect). At a quantitative level, the kinetic models and Grad's method present good agreement with simulation data, especially in the case of the BGK model. For instance, at $a \approx 0.2$ (which is the largest value considered in the simulation), the discrepancies of the ES model and Grad's method with the simulation result are less than 3% and less than 2% for the BGK model. For larger shear rates, we would need more simulation data to state

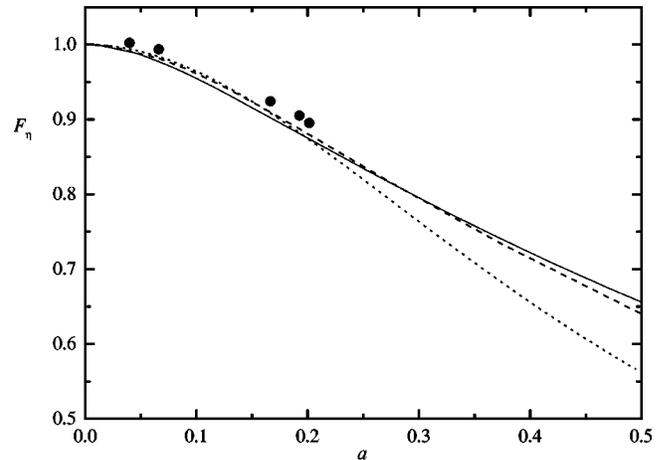


FIG. 1. Plot of the reduced nonlinear shear viscosity $F_\eta(a) = \eta(a)/\eta_0$ versus the reduced shear rate a for a hard disk gas as obtained from molecular-dynamics simulation (circles), the ES model (solid line), Grad's method (dotted line), and the BGK model (dashed line).

which approximation is superior. In the case of the heat transport, it is evident from Fig. 2 that Grad's solution does not estimate qualitatively well the shear-rate dependence of F_κ . This failure could be anticipated from the comparison with the perturbation solution in the 3D case. On the other hand, for the function $F_\kappa(a)$, the agreement between the ES and BGK models and simulation data is excellent, especially for the ES model where the discrepancies between theory and simulation are smaller than 1%. In the case of the BGK model, the discrepancies are smaller than 3%. In the case of Φ , Fig. 3 shows clearly the superiority of the ES model over the remaining approximations, the discrepancies for this coefficient being smaller than 6%. Although Grad's solution gives the exact asymptotic value $\Phi^{(1)}$, its predictions worsen significantly as the shear rate increases. On the other hand, in contrast to what happens for η and F_κ , the BGK model does not provide a good estimate of Φ within the range of shear

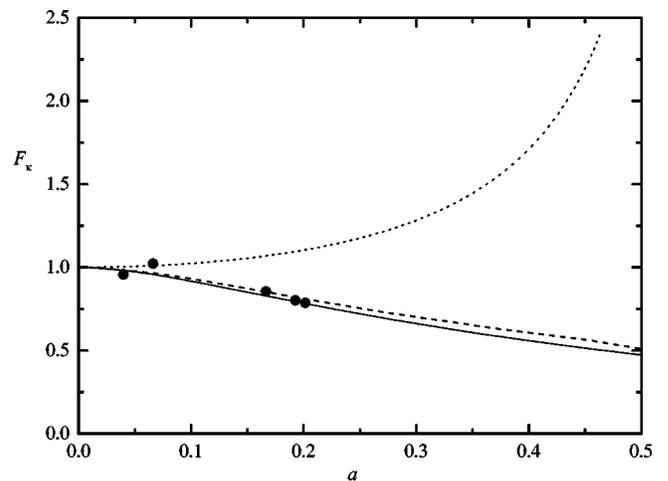


FIG. 2. Plot of the reduced nonlinear thermal conductivity $F_\kappa(a) = \kappa_{yy}(a)/\kappa_0$ versus the reduced shear rate a for a hard disk gas as obtained from molecular-dynamics simulation (circles), the ES model (solid line), Grad's method (dotted line), and the BGK model (dashed line).

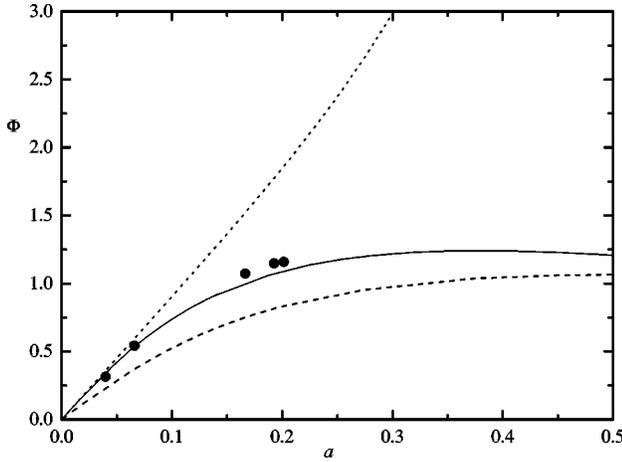


FIG. 3. Plot of the reduced nonlinear cross coefficient $\Phi(a) = -\kappa_{xy}(a)/\kappa_0$ versus the reduced shear rate a for a hard disk gas as obtained from molecular-dynamics simulation (circles), the ES model (solid line), Grad's method (dotted line), and the BGK model (dashed line).

rates considered in the simulations. Thus, at $a \approx 0.2$, the relative error is around 40%. The fact that the BGK model leads to significant quantitative discrepancies for the coefficient Φ can justify the use of more sophisticated kinetic models (such as the ES approximation) in the Couette problem, at the expense, however, of the simplicity of the model.

Finally, in spite of the lack of simulation data, it is also interesting to compare the distribution functions as given by the several theories. For the sake of illustration, for a two-dimensional gas, let us consider the marginal distribution

$$R_y(\xi_y) \equiv \frac{\int_{-\infty}^{+\infty} d\xi_x f(\xi)}{\int_{-\infty}^{+\infty} d\xi_x f^{\text{LE}}(\xi)}, \quad (41)$$

where

$$f^{\text{LE}} = n \left(\frac{m}{2\pi k_B T} \right)^{d/2} e^{-m v^2 / 2k_B T} \quad (42)$$

is the local equilibrium distribution function. The distribution $R_y(\xi_y)$ measures the distortion of f with respect to the local equilibrium. Notice that in the case of Grad's theory, $R_y(\xi_y) = 1$ and consequently the behavior of Grad's distribution $f(\xi)$ is very close to a Gaussian form. This is not what happens in the BGK and ES models, for which Fig. 4 shows a high distortion of both distributions from local equilibrium. Although the shapes of the BGK and ES distributions are in general similar, we observe significant quantitative differences between both distributions, especially for large and negative ξ_y . This could explain the discrepancies observed at the level of Φ .

IV. CONCLUDING REMARKS

In this paper we have considered the state of a d -dimensional dilute gas subject to steady planar Couette flow. The physical situation corresponds to a gas enclosed

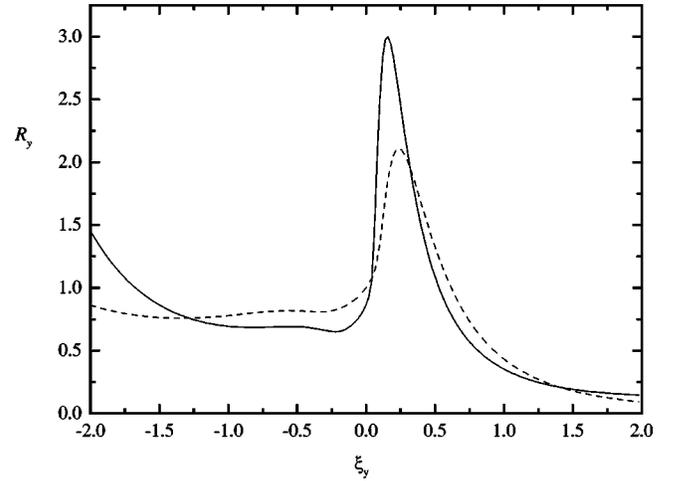


FIG. 4. Plot of the marginal distribution $R_y(\xi_y)$ versus ξ_y for $a=1$ and $\epsilon=1$. The solid line refers to the ES model, while the dashed line corresponds to the BGK model.

between two infinite parallel plates and maintained at different temperatures. As a consequence, combined heat and momentum transport are induced in the system. Our interest has been to get the transport properties for arbitrary values of both velocity and temperature gradients. Since in this problem the Prandtl number Pr plays a relevant role, we have used a kinetic model (ES kinetic model) that leads to the correct value of Pr . When $\text{Pr}=1$, the ES model reduces to the well-known BGK model. The solution is characterized by $p = \text{const}$, $\partial u_x / \partial s = a = \text{const}$, and $\partial^2 T / \partial s^2 = -(2m/k_B) \gamma(a) = \text{const}$, where s is a scaled space variable [Eqs. (10)–(12)]. We have found that the pressure tensor, and hence the nonlinear shear viscosity $\eta(a) = \eta_0 F_\eta(a)$, is independent of the thermal gradient, while the heat flux verifies a generalized Fourier law (proportional to the thermal gradient) with a shear-rate-dependent thermal conductivity tensor κ . The two nonzero elements of κ are $\kappa_{xy} = \kappa_0 \Phi(a)$ (which vanishes in the limit of zero shear rate) and $\kappa_{yy} = \kappa_0 F_\kappa(a)$ (which can be interpreted as a generalization of the thermal conductivity coefficient). Our calculations show that F_η , Φ , and F_κ are highly nonlinear functions of the shear rate.

The present work has been mainly motivated by a recent paper of Risso and Cordero [5], who use computer molecular-dynamics experiments to study the shear-rate dependence of η , κ_{xy} , and κ_{yy} for a hard disk gas. In addition, Risso and Cordero also derived expressions of such nonlinear coefficients by using Grad's method of the Boltzmann equation. In the case of the shear viscosity, the comparison of the theoretical predictions given by the ES and BGK models and Grad's method with the simulation results shows good agreement. In the range of shear rates analyzed, the discrepancies observed are smaller than 3% in the case of the ES and Grad approximations, while for the BGK model the discrepancies are smaller than 2%. Nevertheless, in the case of the coefficients $\kappa_{yy}(a)$ and $\kappa_{xy}(a)$, the discrepancies between simulation and Grad's theory become important. This is in contrast to what happens in the ES model, where the agreement is excellent, especially in the case of κ_{yy} with a relative error less than 1%. Although the BGK prediction for κ_{yy} is very close to that of the ES model, it does not give a

good estimate of Φ since the discrepancies are around 40%. All these results clearly show that, at least in the range of shear rates considered in the simulation, the ES model provides a shear-rate dependence of the transport coefficients in the Couette flow problem that is consistent with the observations made in the bulk region by Risso and Cordero [5]. Since the Couette flow is essentially two-dimensional, one expects that the above conclusions can be extended to the 3D case. The comparison with the perturbation solution of Tij and Santos [4] supports the above expectation. It must be noticed that, while the choice of unit of time is irrelevant in the case of the ES model, this is not the case for the BGK model. In this equation, its collision frequency ν can be adjusted to reproduce either the exact Navier-Stokes shear viscosity η_0 ($\nu = p/\eta_0$) or the exact Navier-Stokes thermal conductivity κ_0 ($\nu = [(d+2)/2]pk_B/m\kappa_0$). While in the former case the BGK equation presents good agreement with simulation results (except in the case of Φ), we have verified that the latter choice leads to discrepancies with computer experiments much more important than those obtained here.

On the other hand, apart from density effects, it is possible that the differences observed between theory and simulation could be also in part due to boundary effects that have not been completely eliminated in the bulk region. In the simulation of Risso and Cordero [5], the gas can be seen as enclosed between two baths at local equilibrium at the same temperature and different velocities. A possible way to inhibit the boundary effects could be to assume that both baths

are out of equilibrium in a state close to the one of the actual gas. The use of this type of condition has been shown to be more appropriate to analyze bulk transport properties [14] in the planar Fourier problem (both walls at rest). As a final point, we want to remark that in spite of the simplicity of the kinetic models, the results presented here can be taken as a good example to assess their reliability in evaluating nonlinear transport properties. In this context, it would be very interesting to investigate whether the good agreement observed here between theory and simulation could be extended when one considers shear rates larger than the ones considered by Risso and Cordero. As an alternative to overcome the difficulties associated with molecular-dynamics simulations for achieving very large shear rates in the low-density regime, one could perhaps use the direct simulation Monte Carlo method [15], which has been shown to be very fruitful in the past few years.

ACKNOWLEDGMENTS

We are grateful to Dr. Patricio Cordero for providing us with the correct expressions of the 3D case prior to publication. We also thank Dr. Andrés Santos for a critical reading of the manuscript. Partial support from the DGICYT (Spain) through Grant No. PB97-1501 and from the Junta de Extremadura (Fondo Social Europeo) through Grant No. PRI97C1041 is acknowledged.

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