ELSEVIER

Physica A 243 (1997) 113–128

PHYSICA A

Kinetic model for uniform shear flow

V. Garzó

Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain

Received 10 December 1996

Abstract

The so-called ellipsoidal statistical (ES) kinetic model is used to study the uniform shear flow problem in a dilute gas. This model is an extension of the well-known BGK kinetic to account for the correct Prandtl number. The velocity moments and the velocity distribution function are obtained in terms of the shear rate and a parameter Pr which plays the role of the Prandtl number. It is shown that, independently of the numerical value of Pr, the expressions of the second-degree velocity moments (which are related to the pressure tensor) coincide with the ones derived from the Boltzmann equation for Maxwell molecules. A comparison with previous results obtained from the Boltzmann equation for the fourth-degree velocity moments and for the velocity distribution function is carried out. Surprisingly enough, the comparison shows a superiority of the BGK model ($\mathrm{Pr}=1$) over the ES model ($\mathrm{Pr}=\frac{2}{3}$) in this problem. If one chooses values of Pr larger than one, the ES predictions are improved significantly.

PACS: 47.50.+d; 47.50.-n; 51.10.+y; 05.20.Dd

Keywords: Dilute gas; Kinetic model; Prandtl number; Uniform shear flow

1. Introduction

A well-known problem in dealing with the Boltzmann equation is the intricacy of its collision term. This is specially manifest when one attempts to analyze situations far away from equilibrium. One possibility to overcome such problem is to use kinetic models, namely, equations where the Boltzmann collision term is replaced by a simple relaxation term. The physical idea behind such an approximation is to assume that the net effect of collisions is to make the distribution function to tend toward a certain reference function with a characteristic relaxation time ν^{-1}. The most widely known collision model of the Boltzmann equation is the Bhatnagar–Gross–Krook (BGK) kinetic equation [1], where the reference distribution is the local equilibrium distribution function. Although this model has been shown to be very fruitful in the past years, it

PII S0378-4371(97)00262-8

presents an important defficiency since it does not lead to the correct Prandtl number. For this reason other kinetic models have been proposed. Nevertheless, either they are constructed specially for linearized problems [2,3] or suffer from a drawback [2,4], namely, their distribution functions may turn out to be negative.

One model in which neither of these limitations appears is the ellipsoidal statistical (ES) model [5,6]. In this model, the local Maxwellian (which is an isotropic Gaussian) of the BGK collision term is replaced by an anisotropic three-dimensional Gaussian which involves the Prandtl number Pr. This quantity can be seen as an extra parameter (apart from ν) that can be chosen in principle arbitrarily. If $\mathrm{Pr}=1$, we recover the BGK model, so that the latter can be considered as a particular case of the ES model. When one chooses $\mathrm{Pr}=\frac{2}{3}$, one obtains the same expressions for the shear viscosity and thermal conductivity coefficients as the ones given from the Boltzmann equation for a Maxwell gas [6]. This fact encourages the use of the ES approximation to analyze general transport phenomena. However, beyond the linear domain and to the best of our knowledge, the problem of validation of the ES model through a comparison with an exact solution of the Boltzmann equation has not been treated so far. This circumstance is clearly related to the difficulty of finding exact solutions of the Boltzmann equation. In this paper, we solve the ES model in the so-called uniform shear flow (USF) problem and perform a comparison with the exact expressions derived from the Boltzmann equation. The natural expectation is that the ES equation improves the results previously obtained from the BGK equation.

The USF problem is one of the few non-homogeneous situations for which a solution of the Boltzmann equation can be given in terms of the velocity moments. In this state, the only non-zero hydrodynamic gradient is $\partial u_x/\partial y=a$, where $\mathbf{u}$ is the flow velocity and a is the constant shear rate. In the especial case of Maxwell molecules (particles interacting via an r^{-4} potential), Ikenberry and Truesdell [7] showed that the infinite hierarchy of velocity moments could be recursively solved and, in particular, they obtained the elements of the pressure tensor (which are related to the second-degree velocity moments) as non-linear functions of the shear rate. The expression of the pressure tensor exactly coincides with the one given from the BGK model [8,9]. More recently, the fourth-degree velocity moments have also been evaluated [10]. Since the exact velocity distribution function is not known, the comparison with the fourth-degree moments allows one to infer the degree of reliability of the distribution functions obtained from the ES and the BGK equations.

The plan of the paper is as follows. In Section 2 we give a brief description of the ES model. In Section 3, we solve the ES model in the USF state. We provide explicit expressions of the velocity moments as well as the velocity distribution function in terms of the shear rate and the Prandtl number Pr. In Section 4, we compare the results obtained from the ES ($\mathrm{Pr}=\frac{2}{3}$) and the BGK ($\mathrm{Pr}=1$) approximations with those obtained from the Boltzmann equation. In this comparison we also include recent simulation results [11] obtained for the velocity distribution function. A few concluding remarks close the paper in Section 5.

2. The ellipsoidal statistical (ES) model for dilute gases

A kinetic model is constructed by replacing the complicated Boltzmann collision operator $J[f,f]$ by a simpler collision term which retains only the qualitative and average properties of the true $J[f,f]$. The usual choice is a relaxation term of the form

$$J[f,f] = -\nu(f - f_0), \tag{1}$$

where $f(\mathbf{r},\mathbf{v};t)$ is the velocity distribution function and $f_0(\mathbf{r},\mathbf{v};t)$ is a certain distribution function determined by requering that Eq. (1) preserves the local conservation laws of mass, momentum and energy. Its explicit form may be chosen in different ways. All the details of the interaction potential are taken into account through a velocity independent collision frequency $\nu(\mathbf{r};t)$, which can depend on the density and temperature. Thus, for $r^{-\ell}$ potentials, $\nu \propto nT^{-\mu}$ with $\mu = \frac{1}{2} - 2/\ell$. The simplest collision model is the BGK equation [1] where $f_0(\mathbf{r},\mathbf{v};t)$ is the local equilibrium distribution function $f^{\mathrm{LE}}(\mathbf{r},\mathbf{v};t)$, i.e.

$$f_0^{\mathrm{BGK}} \equiv f^{\mathrm{LE}} = n\left(\frac{m}{2\pi k_B T}\right)^{3/2} \exp\left(-\frac{m}{2k_B T}V^2\right). \tag{2}$$

Here, m is the mass of a particle, k_B is the Boltzmann constant,

$$n = \int d\mathbf{v} f(\mathbf{v}) \tag{3}$$

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

$$\mathbf{u} = \frac{1}{n}\int d\mathbf{v}\mathbf{v} f(\mathbf{v}) \tag{4}$$

is the local flow velocity, and

$$T = \frac{m}{3nk_B}\int d\mathbf{v} V^2 f(\mathbf{v}) \tag{5}$$

is the local temperature. In spite of its simplicity, the BGK model has been shown to be very fruitful in the past years. However, it presents an important defficiency since it leads to a Prandtl number of 1 instead of the correct value of $\frac{2}{3}$ [2]. To improve such prediction, other more sophisticated selections for f_0 have been proposed [2–4]. A disadvantage of grand part of them is that the corresponding distribution function may turn out to be negative for large velocities.

A non-linear model that does not present neither of the above drawbacks is the so-called ellipsoidal statistical (ES) model [5,6]. In the ES model, one takes for f_0 the distribution

$$f_0(\mathbf{v}) = n\pi^{-3/2}(\det \mathbf{\Lambda})^{1/2} \exp(-\Lambda_{ij} V_i V_j), \tag{6}$$

where $\Lambda = [AI - (B/\rho)P]^{-1}$, $\rho = mn$, $A = (2k_BT/m)\mathrm{Pr}^{-1}$, $B = 2(\mathrm{Pr}^{-1} - 1)$, and

$$P = \int d\mathbf{v}\, \mathbf{V}\mathbf{V} f \tag{7}$$

is the pressure tensor. The quantity Pr is an extra parameter which plays the role of the Prandtl number. It is easy to see that if $\mathrm{Pr} = 1$, f_0 reduces to the local Maxwellian f^{LE} and one recovers the BGK equation. In contrast to the BGK approximation, its collision term involves not only the first five conserved hydrodynamic fields but the dissipative momentum flux.

As a final point in this section, it is interesting to give the expressions of the Navier–Stokes transport coefficients obtained from the ES model. After a simple calculation, the shear viscosity η_0 and thermal conductivity κ_0 coefficients are given by [6]

$$\eta_0 = \frac{nk_BT}{\nu \mathrm{Pr}^{-1}}, \tag{8}$$

$$\kappa_0 = \frac{5}{2}\frac{nk_B^2T}{m\nu}. \tag{9}$$

If we identify ν with a given eigenvalue of the linearized Boltzmann collision operator and take $\mathrm{Pr} = \frac{2}{3}$, then the expressions (8) and (9) coincide with those derived from the Boltzmann equation [2].

3. Solution of the ES model in the uniform shear flow

As said in the Introduction, the only non-zero hydrodynamic gradient in the uniform shear flow (USF) state corresponds to $\partial u_x/\partial y = a$, where a is the constant shear rate. This quantity measures the departure of the system from equilibrium. The USF is not stationary since the temperature increases in time due to viscous heating. In order to prevent this effect, a drag force of the form $-m\alpha\mathbf{V}$ is usually introduced [12], where α is a function of the shear rate to be determined by consistency. It is important to remark that *only* in the especial case of Maxwell molecules ($\mu = 0$), there is an exact equivalence between the results with and without a thermostat [13]. Furthermore, the velocity distribution function becomes spatially homogeneous when one refers the velocities of the particles to the flow velocity $\mathbf{u}$, namely, $f(\mathbf{r}, \mathbf{v}) = f(\mathbf{V})$.

The USF state must not be confused with the so-called steady planar Couette flow. In the latter, apart from the linear profile of the velocity, the temperature varies spatially so that combined heat and momentum transport appears in the system. Both kinds of shear flow are generated in computer simulations by means of different boundary conditions [14] and the corresponding rheological properties are different beyond the Navier–Stokes approximation [15]. As a matter of fact, and in contrast to what happens in the USF problem [7], no exact solution of the Boltzmann equation is known for the planar Couette problem.

Under the conditions established in the USF state, the stationary ES equation can be written as [10]

$$-\frac{\partial}{\partial V_i}(a_{ij}V_j + \alpha V_i)f = -\nu(f - f_0), \tag{10}$$

where $a_{ij} = a\delta_{ix}\delta_{jy}$, and $f_0(\mathbf{V})$ is given by Eq. (6) with

$$\mathbf{\Lambda} = \frac{\rho}{\Delta}\begin{pmatrix} A\rho - BP_{yy} & BP_{xy} & 0 \\ BP_{xy} & A\rho - BP_{xx} & 0 \\ 0 & 0 & \dfrac{\Delta}{A\rho - BP_{zz}} \end{pmatrix}. \tag{11}$$

Here, $\Delta = A^2\rho^2 - AB\rho(P_{xx} + P_{yy}) + B^2(P_{xx}P_{yy} - P_{xy}^2)$. The structure of $\mathbf{\Lambda}$ reflects the geometry of the USF. The fact that the temperature is controlled by the thermostat force implies that the collsion frequency is constant, and consequently all the results apply for any potential. On the other hand, the reference function f_0 is given in terms of the pressure tensor whose shear rate dependence is not known. In order to get this quantity, let us define now the reduced velocity moments

$$M_{k_1,k_2,k_3} = \frac{1}{n}\left(\frac{m}{2k_BT}\right)^{(k_1+k_2+k_3)/2}\int d\mathbf{v}\, V_x^{k_1}V_y^{k_2}V_z^{k_3} f\,. \tag{12}$$

Taking velocity moments in Eq. (10), the following moment hierarchy is obtained:

$$ak_1M_{k_1-1,k_2+1,k_3} + [\nu + \alpha(k_1 + k_2 + k_3)]M_{k_1,k_2,k_3} = \nu N_{k_1,k_2,k_3}\,, \tag{13}$$

where N_{k_1,k_2,k_3} is (see the appendix)

$$N_{k_1,k_2,k_3} = \pi^{-3/2}\sum_{\ell=0}^{k_1}\frac{k_1!}{\ell!(k_1-\ell)!}b_x^{-\frac{1}{2}(k_1-\ell)}b_y^{-\frac{1}{2}(k_2+\ell)}b_z^{-k_3/2}(-c)^{\ell}C_{k_1-\ell}C_{k_2+\ell}C_{k_3} \tag{14}$$

with $C_k = \Gamma((k+1)/2)$ if $k =$ even, being zero otherwise. Furthermore, we have introduced the functions $b_x = (2k_BT/m)\Lambda_{xx}$, $b_y = (2k_BT/m)[\Lambda_{yy} - (\Lambda_{xy}^2/\Lambda_{xx})]$, $b_z = (2k_BT/m)\Lambda_{zz}$, and $c = \Lambda_{xy}/\Lambda_{xx}$.

Let us introduce $\tau = \nu\mathrm{Pr}^{-1}$ as a convenient unit of time. Henceforth, all the quantities will be reduced with respect to τ. Thus, the solution to Eq. (13) can be recast into the form

$$M_{k_1,k_2,k_3} = \sum_{q=0}^{k_1}\mathrm{Pr}^{-q}(-a)^q\frac{k_1!}{(k_1-q)!}[1 + \mathrm{Pr}^{-1}\alpha(k_1 + k_2 + k_3)]^{-(q+1)}N_{k_1-q,k_2+q,k_3}\,. \tag{15}$$

Notice that in Eq. (15), N is zero if any of its indices is negative. To close the expression (15), it still remains to determine the second-degree moments (pressure tensor) and α as functions of a and Pr. They can be obtained self-consistently from the definition (7). After a simple algebra, one gets

$$M_{200} = \frac{1}{2}\frac{1}{1+2\alpha}\left[1+\frac{2a^2}{(1+2\alpha)^2}\right], \tag{16}$$

$$M_{020} = M_{002} = \frac{1}{2}\frac{1}{1+2\alpha}, \tag{17}$$

$$M_{110} = -\frac{1}{2}\frac{a}{(1+2\alpha)^2}. \tag{18}$$

The requirement $M_{200}+M_{020}+M_{002}=\frac{3}{2}$ yields a cubic equation for α, whose real (physical) solution is

$$\alpha(a) = \tfrac{2}{3}\sinh^2\left[\tfrac{1}{6}\cosh^{-1}(1+9a^2)\right]. \tag{19}$$

The expressions (16)–(19) coincide with those obtained from the Boltzmann equation for Maxwell molecules [7] and from the BGK equation [10]. This fact shows the relevance of the BGK and ES models for computing the rheological properties of the system. The knowledge of the second-degree moments allows one to get the parameters b_i and c. They are given by

$$b_x = \frac{\mathrm{Pr}(\mathrm{Pr}+2\alpha)(1+2\alpha)}{3\alpha(\mathrm{Pr}-1)(4\alpha+\mathrm{Pr}+1)+(2\alpha+\mathrm{Pr})^2}, \tag{20}$$

$$b_y = b_z = \mathrm{Pr}\frac{1+2\alpha}{\mathrm{Pr}+2\alpha}, \tag{21}$$

$$c = \frac{\mathrm{Pr}-1}{(1+2\alpha)(\mathrm{Pr}+2\alpha)}a. \tag{22}$$

Now, all the velocity moments of f can be obtained from Eq. (15). They are given as non-linear functions of the shear rate a and the Prandtl number Pr.

The use of the simplified collision term (1) allows one to explicitly get the velocity distribution function $f(\mathbf{V})$, which cannot be determined from the Boltzmann equation even in the case of Maxwell molecules. This fact is one of the main reasons for using kinetic models. A formal solution to Eq. (10) compatible with the moments (15) is given by

$$\begin{aligned} f(\mathbf{V}) &= \left[1-3\mathrm{Pr}^{-1}\alpha-\mathrm{Pr}^{-1}aV_y\frac{\partial}{\partial V_x}-\mathrm{Pr}^{-1}\alpha\mathbf{V}\cdot\frac{\partial}{\partial\mathbf{V}}\right]^{-1}f_0(\mathbf{V}) \\ &= \int_0^\infty e^{-(1-3\mathrm{Pr}^{-1}\alpha)s}\exp\left(\mathrm{Pr}^{-1}asV_y\frac{\partial}{\partial V_x}+\mathrm{Pr}^{-1}\alpha s\mathbf{V}\cdot\frac{\partial}{\partial\mathbf{V}}\right)f_0(\mathbf{V}). \end{aligned} \tag{23}$$

The action of the operator is

$$\begin{aligned} &\exp\left(msV_y\frac{\partial}{\partial V_x}+ns\mathbf{V}\cdot\frac{\partial}{\partial\mathbf{V}}\right)f_0(V_x,V_y,V_z) \\ &\quad = f_0(e^{ns}(V_x+msV_y), e^{ns}V_y, e^{ns}V_z). \end{aligned} \tag{24}$$

In terms of the reduced velocity $\boldsymbol{\xi}=(m/2k_BT)^{1/2}\mathbf{V}$, and taking into account the identity (24), the distribution function can be written as $f(\mathbf{V})=n(2k_BT/m)^{-3/2}g(\boldsymbol{\xi})$, where

$$g(\boldsymbol{\xi})=\pi^{-3/2}(b_xb_yb_z)^{1/2}\int_0^\infty ds\exp[-(1-3\mathrm{Pr}^{-1}\alpha)s]$$
$$\times\exp(-e^{2\mathrm{Pr}^{-1}\alpha s}\boldsymbol{\xi}\cdot\boldsymbol{\Omega}(s)\cdot\boldsymbol{\xi}). \tag{25}$$

Here, $\boldsymbol{\Omega}(s)$ is a matrix whose non-zero elements are $\Omega_{xx}=b_x$, $\Omega_{xy}=b_x(c+\mathrm{Pr}^{-1}as)$, $\Omega_{yy}=b_y+b_x(c^2+2\mathrm{Pr}^{-1}acs+\mathrm{Pr}^{-2}a^2s^2)$, and $\Omega_{zz}=b_y$. The dependence of g on a appears explicitly and also through $\alpha(a)$ and the parameters $b_i(a)$ and $c(a)$. For small shear rates,

$$g(\boldsymbol{\xi};a)=g^{(0)}(\boldsymbol{\xi})+a\,g^{(1)}(\boldsymbol{\xi})+a^2g^{(2)}(\boldsymbol{\xi})+a^3g^{(3)}(\boldsymbol{\xi})+\mathcal{O}(a^4), \tag{26}$$

where

$$g^{(0)}(\boldsymbol{\xi})=\pi^{-3/2}\exp(-\xi^2), \tag{27}$$

$$g^{(1)}(\boldsymbol{\xi})=-2\xi_x\xi_y\,g^{(0)}(\boldsymbol{\xi}), \tag{28}$$

$$g^{(2)}(\boldsymbol{\xi})\doteq\frac{1}{\mathrm{Pr}^2}[\tfrac{1}{6}(4\mathrm{Pr}+5\mathrm{Pr}^2-3)-\tfrac{2}{3}\mathrm{Pr}^2\xi^2-(1+\mathrm{Pr}^2)\xi_y^2(1-2\xi_x^2)$$
$$-(1-\mathrm{Pr}^2)\xi_x^2]g^{(0)}(\boldsymbol{\xi}), \tag{29}$$

$$g^{(3)}(\boldsymbol{\xi})=\frac{1}{3\mathrm{Pr}^3}\xi_x\xi_y[6(\mathrm{Pr}^3-3\mathrm{Pr}^2+9\mathrm{Pr}-1)\xi_y^2+4\mathrm{Pr}^2(1+\mathrm{Pr})\xi^2$$
$$+6\mathrm{Pr}(1-\mathrm{Pr}^2)\xi_x^2-4(\mathrm{Pr}^3-3\mathrm{Pr}^2+9\mathrm{Pr}-1)\xi_x^2\xi_y^2$$
$$+\mathrm{Pr}(\mathrm{Pr}^2-14\mathrm{Pr}-7)]g^{(0)}(\boldsymbol{\xi}). \tag{30}$$

At the level of Navier-Stokes, the ES and BGK distributions coincide with the one given from the Boltzmann equation for Maxwell molecules. Beyond the linear regime, an explicit dependence on the parameter Pr appears.

Once the velocity distribution function is known, it is instructive to obtain the non-equilibrium entropy S in terms of a and Pr. Let us define the reduced excess entropy per particle as [16]

$$\mathcal{S}(a)\equiv(S-S_{\mathrm{eq}})/Nk_B=-\int d\boldsymbol{\xi}\,g(\boldsymbol{\xi};a)\log\frac{g(\boldsymbol{\xi};a)}{g^{(0)}(\boldsymbol{\xi})}, \tag{31}$$

where S_{eq} is the entropy per particle of an ideal gas at equilibrium. Although $g(\boldsymbol{\xi};a)$ is given by Eq. (25) for arbitrary values of the shear rate, it is a very complex problem to get the full nonlinear dependence of $\mathcal{S}(a)$. Here, we evaluate the first few terms of the expansion of the reduced entropy in powers of the shear rate. After some algebra, one gets

$$\mathcal{S}(a)=\mathcal{S}^{(2)}a^2+\mathcal{S}^{(4)}a^4+\mathcal{O}(a^6), \tag{32}$$

where

$$\mathscr{S}^{(2)} = -\tfrac{1}{2}\,, \tag{33}$$

$$\mathscr{S}^{(4)} = \frac{73\mathrm{Pr}^4 - 50\mathrm{Pr}^3 - 56\mathrm{Pr}^2 + 78\mathrm{Pr} - 36}{36\mathrm{Pr}^4}\,. \tag{34}$$

Upon deriving the above expressions use has been made of the property

$$\int d\xi\, g^{(k)}(\xi) = 0 \tag{35}$$

for $k \geqslant 1$, which follows from the normalization of g.

4. Comparison with the Boltzmann results

The calculations presented in the above section apply for arbitrary values of the Prandtl number Pr. This quantity can be seen as an additional parameter to adjust the transport coefficients of the ES model to those given by the Boltzmann equation. Nevertheless, in the case of the USF problem, the ES equation gives the exact *nonlinear* transport coefficients independently of the numerical value of Pr. This implies that no restriction about the value of Pr exists, except that $\mathrm{Pr} \geqslant \frac{2}{3}$ to assure the positive definitness of $\boldsymbol{\Lambda}$ [6]. Here, we will only consider the most interesting physical cases of $\mathrm{Pr} = \frac{2}{3}$ (correct Prandtl number) and $\mathrm{Pr} = 1$ (BGK model).

The knowledge of the explicit shear rate dependence of the fourth-degree moments derived from the Boltzmann equation [10] allows one to perform a detailed comparison with the corresponding moments given by the ES model. This comparison extends the one previously made between the Boltzmann and BGK equations [17]. Due to the symmetry of the problem, there are in principle 9 independent fourth-degree moments. Here, we take the following set $\{M_{400}, M_{040}, M_{004}, M_{022}, M_{202}, M_{220}, M_{112}, M_{130}, M_{310}\}$. The expressions of these moments are given in the appendix. The first five moments of the set are even functions of the shear rate, while the remaining three moments are odd functions. The analysis of the small shear rate limit shows that the BGK ($\mathrm{Pr} = 1$) and ES ($\mathrm{Pr} = \frac{2}{3}$) approximations are exact up to first order in a, while the predictions of the BGK model for the Burnett and super-Burnett transport coefficients are closer to the exact ones [10] than those obtained from the ES model. This is indicative of what happens for finite shear rates. For the sake of illustration, in Figs. 1–4 we show the shear rate dependence of the reduced moments $\mathscr{M}_{400} = M_{400}/(\frac{3}{4})$, $\mathscr{M}_{040} = M_{040}/(\frac{3}{4})$, $\mathscr{M}_{220} = M_{220}/(\frac{1}{4})$, and $\mathscr{M}_{112} = -M_{112}/(a/4)$, respectively, according to the ES results, the BGK results and the Boltzmann results. We see that in general, the qualitative trends predicted by the Boltzmann equation are retained by both the BGK and ES models, at least for the range of shear rates considered in the figures. Nevertheless, at a quantitative level, the results from the BGK model are in better agreement with the exact results than those given from the ES model, except for $\mathscr{M}_{040}$. For instance, at $a \simeq 0.5$ (where the shear viscosity is about 1.25 times smaller than its zero shear rate value), the

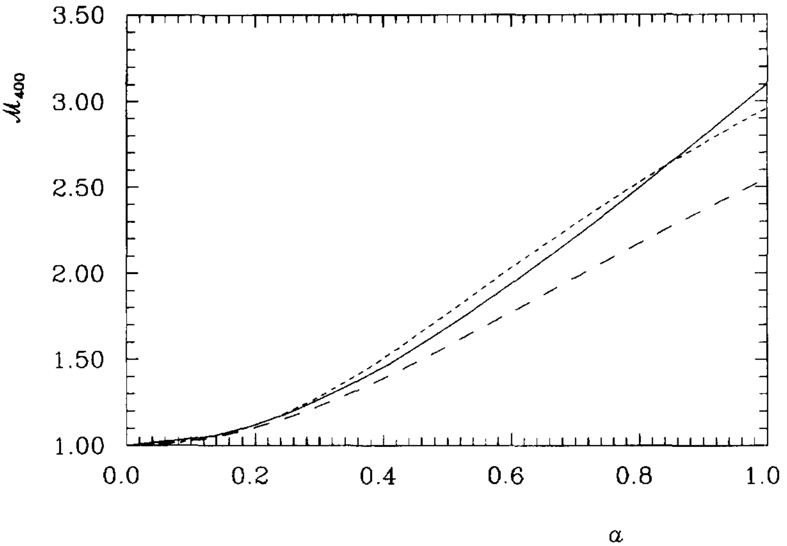

Fig. 1. Shear rate dependence of M_{400}, relative to its equilibrium value, according to the Boltzmann equation (——), the ES model (— — —) and the BGK model (- - -).

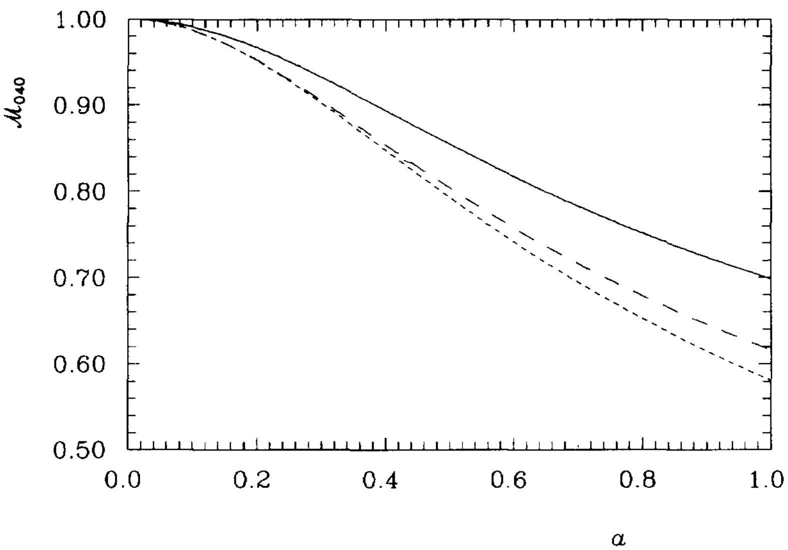

Fig. 2. Shear rate dependence of M_{040}, relative to its equilibrium value, according to the Boltzmann equation (——), the ES model (— — —) and the BGK model (- - -).

comparison with the Boltzmann prediction for M_{400}, M_{040}, M_{220}, and M_{112} indicates that the relative error for the BGK model is around 4.7%, 7%, 0.6% and 14%, respectively, while for the ES model is around 31%, 5.8%, 6.4% and 23%, respectively. Obviously, these discrepancies increase as the shear rate increases. We have also compared the

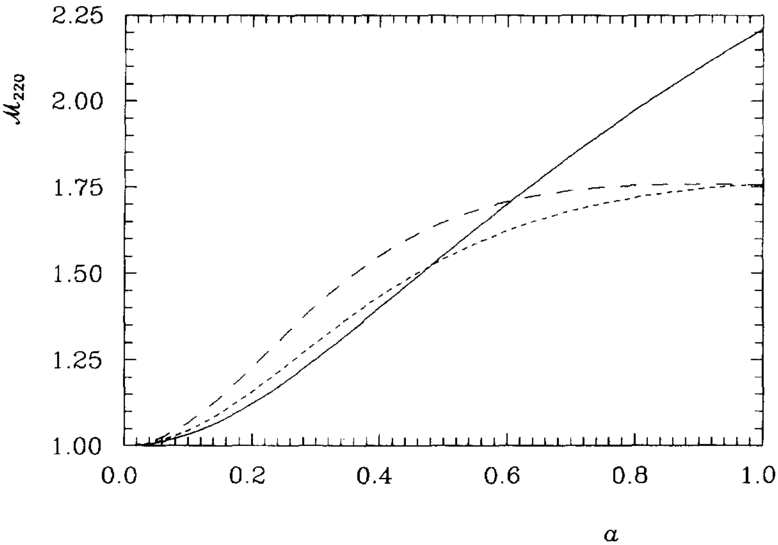

Fig. 3. Shear rate dependence of M_{220}, relative to its equilibrium value, according to the Boltzmann equation (——), the ES model (— — —) and the BGK model (- - -).

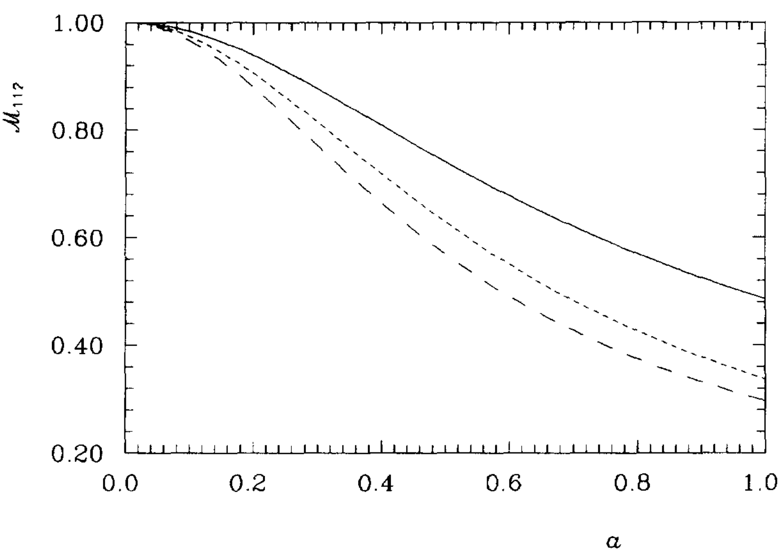

Fig. 4. Shear rate dependence of M_{112}, relative to its Navier–Stokes value, according to the Boltzmann equation (——), the ES model (— — —) and the BGK model (- - -).

remaining independent fourth-degree moments and similar conclusions can be obtained, especially for moments in which the component V_x is the most relevant one. Another possibility in the above comparison is to choose for the parameter Pr the value that gives the same results for the fourth-degree moments between the ES and Boltzmann

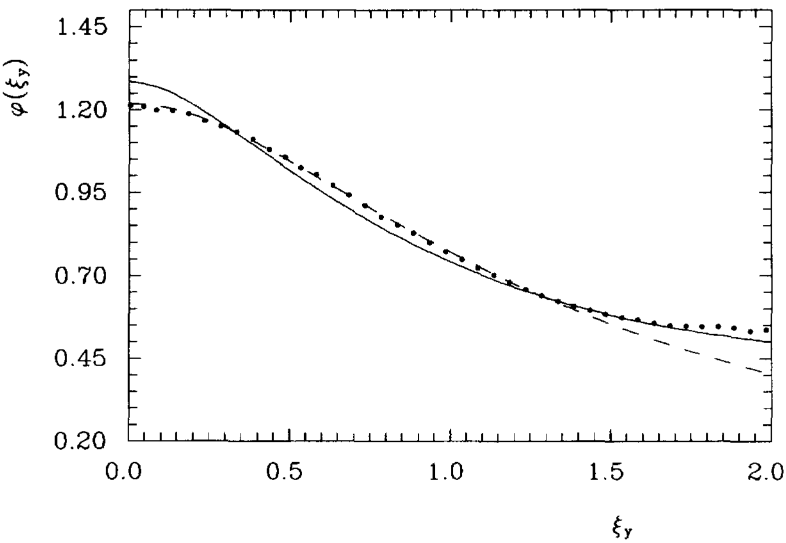

Fig. 5. Plot of the marginal distribution $\varphi(\xi_y)$ for $a=1$, as obtained from the ES model (solid line), the BGK model (dashed line) and from simulation results for Maxwell molecules (dotted line).

equations at the level of the Burnett order and/or at the level of the super-Burnett order. In this way, one could obtain a good agreement between both descriptions for not too large shear rates. Nevertheless, the price to be paid is that the corresponding values for Pr are larger than 1 (in fact, in some cases the values are around 1.7), and consequently one gets an incorrect Prandtl number.

The above conclusions can be also extended to the coefficients $\mathscr{S}^{(2)}$ and $\mathscr{S}^{(4)}$, which have been recently evaluated in the Boltzmann equation [16]. In this case, $\mathscr{S}^{(2)}=-\frac{1}{2}$ and $\mathscr{S}^{(4)}\simeq 0.58417$. The coefficient $\mathscr{S}^{(2)}$ is the same as the one given from the ES and BGK approximations. This a consequence of the fact that the ES and BGK equations coincide with the Boltzmann equation to Navier–Stokes order. In the case of the coefficient $\mathscr{S}^{(4)}$, the ES equation $(\mathrm{Pr}=\frac{2}{3})$ gives the value $-47/36$ and the BGK equation $(\mathrm{Pr}=1)$ gives $\frac{1}{4}$. The BGK equation estimates $\mathscr{S}^{(4)}$ with a deviation of about 50% while the ES equation does not give the same sign as the exact one. If one takes $\mathrm{Pr}\simeq 1.218$, Eq. (34) leads to the same value as the Boltzmann equation.

Since the velocity distribution function depends on the three components of the velocity, in Fig. 3 we plot the marginal distribution

$$\varphi(\xi_y)=\sqrt{\pi}e^{\xi_y^2}\int_{-\infty}^{\infty} d\xi_x \int_{-\infty}^{\infty} d\xi_z\, g(\boldsymbol{\xi}) \tag{36}$$

for $a=1$ and for the ES model $(\mathrm{Pr}=\frac{2}{3})$ and the BGK model $(\mathrm{Pr}=1)$. We have also included the velocity distribution function obtained from Monte Carlo simulations for

Maxwell molecules [11]. Since the shear rate is large, the distortion from equilibrium is quite evident in both distributions. Their shape is rather similar, at least in the range of velocities considered. This is consistent with the fact that both distributions lead to the same transport coefficients. On the other hand, it is clear that the comparison with the simulation results shows again the superiority of the BGK distribution over the ES distribution, especially in the region of thermal velocities ($\xi_y \sim 1$). Further, since the fourth-degree moments obtained from both models are generally smaller than the exact ones, the high-velocity population is possibly underestimated by both approximations. This expectation has been recently confirmed by computer simulations [11].

5. Concluding remarks

One of the main advantages of the knowledge of exact solutions is the possibility of testing approximation methods. In the case of a dilute gas, the BGK model is usually used as an approximation of the Boltzmann equation. However, the fact that the BGK equation leads to an incorrect Prandtl number has estimulated the search for other kinetic equations. Although the majority of these models [2,4] give correctly the Navier–Stokes transport coefficients, their velocity distribution functions may turn out to be negative. This problem is especially important in far from equilibrium situations. A good candidate to overcome such difficulties is the ellipsoidal statistical (ES) model [5,6]. This model introduces a further adjustable parameter Pr, which can be adapted to a given Prandtl number. If $\mathrm{Pr} = \frac{2}{3}$, the ES model yields the same Navier–Stokes transport coefficients as the Boltzmann equation.

The motivation of this paper has been to validate the ES model through a comparison with an exact solution of the Boltzmann equation in the uniform shear flow (USF) state. In the USF state, the only nonequilibrium control parameter is the constant shear rate a. We have obtained the velocity moments and the velocity distribution function of the ES model for arbitrary values of both the shear rate a and the Prandtl number Pr. When $\mathrm{Pr} = 1$ we recover previous results derived in the context of the BGK model [9]. We have shown that, by a convenient scaling, the rheological properties (which are related to the second-degree velocity moments) are identical to those given from the BGK and Boltzmann equations [7], independently of the value of the Prandtl number Pr. Beyond the second-degree moments, the results obtained from the ES model ($\mathrm{Pr} = \frac{2}{3}$) and from the BGK model ($\mathrm{Pr} = 1$) are different. In the case of the fourth-degree moments, a comparison with the exact results of the Boltzmann equation indicates that, in general, the BGK predictions are closer to the exact ones than those obtained from the ES model. This conclusion can also be extended to the velocity distribution function where a comparison with simulation results has been carried out.

It is known that some of the shortcomings of the BGK model can be avoided by suitable modifications, at the expense however, of the simplicity of the model. The extension of the BGK model represented by the ES model might be expected to lead to a better agreement with the Boltzmann results, especially in far from equilibrium situations. Nevertheless, this is not the case for the USF problem. Perhaps, this conclusion is related to the fact that in the USF state, where *only* momentum transport appears, the Prandtl number does not play an important role. On the other hand, one could consider Pr as an additional parameter which value is chosen by requiring that the ES model gives the nonlinear shear viscosity and the viscometric functions of the Boltzmann equation in the USF state. As shown, these quantities are identical to those given in the Boltzmann equation for *any* value of Pr so that Pr can be taken a priori arbitrarily. If one chooses values of Pr larger than one, the results derived from the ES equation are in better agreement with the Boltzmann results as those derived from the BGK model. Finally, we want to remark that the conclusions reported here should not be extrapolated to other non-linear problems, especially those where the Prandtl number plays a *relevant* role (such as combined heat and momentum transport). In this sense, recent results [18] obtained in the planar Couette flow state shows a superiority of the ES model over other approximations when one chooses $\mathrm{Pr} = \frac{2}{3}$.

Acknowledgements

I am grateful to Dr. Andrés Santos for a critical reading of the manuscript and to Dr. José María Montanero for providing simulation results. Partial support from the DGICYT (Spain) through Grant No. PB94-1021 and from the Junta de Extremadura (Fondo Social Europeo) through Grant No. EIA94-39 is acknowledged.

Appendix A. Some mathematical results

Let us evaluate the expression of N_{k_1,k_2,k_3} appearing in Eq. (13). In order to compute this term, it is convenient to rewrite the exponential $\exp(-\Lambda_{ij}V_iV_j)$ in the form

$$\exp(-\Lambda_{ij}V_iV_j) = \exp\left(cV_y\frac{\partial}{\partial V_x}\right)\exp\left(-\frac{m}{2k_BT}b_iV_i^2\right), \tag{A.1}$$

where $b_x = (2k_BT/m)\Lambda_{xx}$, $b_y = (2k_BT/m)[\Lambda_{yy} - (\Lambda_{xy}^2/\Lambda_{xx})]$, $b_z = (2k_BT/m)\Lambda_{zz}$, and $c = \Lambda_{xy}/\Lambda_{xx}$. Here, use has been made of the identity

$$\exp\left(cV_y\frac{\partial}{\partial V_x}\right)\Phi(V_x, V_y, V_z) = \Phi(V_x + cV_y, V_y, V_z)\,. \tag{A.2}$$

It is easy to show that $\det\mathbf{\Lambda} = (m/2k_BT)^3 b_x b_y b_z$ and in the following, we will make use of the general property

$$\int d\mathbf{V} G(\mathbf{V}) e^{cV_y\partial/\partial V_x} F(\mathbf{V}) = \int d\mathbf{V} F(\mathbf{V}) e^{-cV_y\partial/\partial V_x} G(\mathbf{V})\,. \tag{A.3}$$

Now, we are in conditions to evaluate N_{k_1,k_2,k_3}. It is given by

$$\begin{aligned}
N_{k_1,k_2,k_3} &= \frac{1}{n}\left(\frac{m}{2k_BT}\right)^{(k_1+k_2+k_3)/2} \int d\mathbf{V}\; V_x^{k_1} V_y^{k_2} V_z^{k_3} f_0(\mathbf{V}) \\
&= \left(\frac{m}{2k_BT}\right)^{(k_1+k_2+k_3)/2} \pi^{-3/2} (\det\mathbf{\Lambda})^{1/2} \\
&\quad \times \int d\mathbf{V}\; V_x^{k_1} V_y^{k_2} V_z^{k_3} e^{cV_y\partial/\partial V_x} \exp\left(-\frac{m}{2k_BT} b_i V_i^2\right) \\
&= \left(\frac{m}{2k_BT}\right)^{(k_1+k_2+k_3)/2} \pi^{-3/2} (\det\mathbf{\Lambda})^{1/2} \\
&\quad \times \int d\mathbf{V}\; (V_x - cV_y)^{k_1} V_y^{k_2} V_z^{k_3} \exp\left(-\frac{m}{2k_BT} b_i V_i^2\right) \\
&= \pi^{-3/2} b_y^{-k_2/2} b_z^{-k_3/2} \int d\boldsymbol{\xi}\; (b_x^{-1/2}\xi_x - c b_y^{-1/2}\xi_y)^{k_1} \xi_y^{k_2} \xi_z^{k_3} e^{-\xi^2} \\
&= \pi^{-3/2} b_z^{-k_3/2} \sum_{\ell=0}^{k_1} \frac{k_1!}{\ell!(k_1-\ell)!} b_x^{-\frac{1}{2}(k_1-\ell)} b_y^{-\frac{1}{2}(k_2+\ell)} (-c)^\ell \\
&\quad \times \int d\boldsymbol{\xi}\; \xi_x^{k_1-\ell} \xi_y^{k_2+\ell} \xi_z^{k_3} e^{-\xi^2}\,.
\end{aligned} \tag{A.4}$$

By performing the integral one gets Eq. (14).

The explicit expressions of the fourth-degree moments are

$$M_{040} = M_{004} = 3M_{022} = \frac{3}{4\mathrm{Pr}} \frac{(\mathrm{Pr}+2\alpha)^2}{(1+2\alpha)^2(\mathrm{Pr}+4\alpha)}\,, \tag{A.5}$$

$$M_{112} = \frac{1}{3} M_{130} = -\frac{1}{4\mathrm{Pr}} \frac{a}{(1+2\alpha)^3} \frac{(\mathrm{Pr}+2\alpha)[4\alpha^2 + 2\alpha(3\mathrm{Pr}-1)\alpha + \mathrm{Pr}^2]}{(\mathrm{Pr}+4\alpha)^2}\,. \tag{A.6}$$

The remaining moments can be written in the form

$$M_{202} = \frac{(\mathrm{Pr}+2\alpha)}{4\mathrm{Pr}(\mathrm{Pr}+4\alpha)^3(1+2\alpha)^2} \Delta_{202}\,, \tag{A.7}$$

$$M_{220} = \frac{\Delta_{220}}{4\mathrm{Pr}(\mathrm{Pr}+4\alpha)^3(1+2\alpha)^2}\,, \tag{A.8}$$

$$M_{310} = -\frac{3a\Delta_{310}}{4\text{Pr}(\text{Pr}+4\alpha)^4(1+2\alpha)^3}, \tag{A.9}$$

$$M_{400} = \frac{3\Delta_{400}}{4\text{Pr}(\text{Pr}+4\alpha)^5(1+2\alpha)^2}, \tag{A.10}$$

where

$$\Delta_{202} = 48\alpha^4 + 8(21\text{Pr}-8)\alpha^3 + 4(15\text{Pr}^2+5\text{Pr}-3)\alpha^2 + 2\text{Pr}^2(3\text{Pr}+5)\alpha + \text{Pr}^3, \tag{A.11}$$

$$\Delta_{220} = 288\alpha^5 + 128(6\text{Pr}-1)\alpha^4 + 24(24\text{Pr}^2-3\text{Pr}+1)\alpha^3 + 4\text{Pr}(36\text{Pr}^2+10\text{Pr}+3)\alpha^2 + 6\text{Pr}^2(2\text{Pr}^2+2\text{Pr}+1)\alpha + \text{Pr}^4, \tag{A.12}$$

$$\Delta_{310} = 576\alpha^6 + 32(48\text{Pr}+1)\alpha^5 + 16(96\text{Pr}^2-\text{Pr}+11)\alpha^4 + 8(72\text{Pr}^3+30\text{Pr}^2+10\text{Pr}+3)\alpha^3 + 4\text{Pr}(24\text{Pr}^3+24\text{Pr}^2+13\text{Pr}+3)\alpha^2 + 2\text{Pr}^2(3\text{Pr}^3+8\text{Pr}^2+2\text{Pr}+3)\alpha + \text{Pr}^5, \tag{A.13}$$

$$\Delta_{400} = 13824\alpha^8 + 1536(24\text{Pr}+5)\alpha^7 + 128(360\text{Pr}^2+45\text{Pr}+68)\alpha^6 + 64(360\text{Pr}^3+234\text{Pr}^2+59\text{Pr}+42)\alpha^5 + 32(180\text{Pr}^4+240\text{Pr}^3+121\text{Pr}^2+39\text{Pr}+9)\alpha^4 + 16\text{Pr}(45\text{Pr}^4+120\text{Pr}^3+62\text{Pr}^2+48\text{Pr}+9)\alpha^3 + 4\text{Pr}^2(9\text{Pr}^4+60\text{Pr}^3+44\text{Pr}^2+12\text{Pr}+18)\alpha^2 + 4\text{Pr}^5(3\text{Pr}+5)\alpha + \text{Pr}^6. \tag{A.14}$$

Up to the super-Burnett order (a^3), they behave as

$$M_{040} = M_{004} = 3M_{022} = \frac{3}{4} - a^2 + \cdots, \tag{A.15}$$

$$M_{112} = \frac{1}{3}M_{130} = -\frac{1}{4}a + \frac{1}{3}\frac{3\text{Pr}^2+1}{2\text{Pr}^2}a^3 + \cdots, \tag{A.16}$$

$$M_{202} = \frac{1}{4} + \frac{a^2}{6} + \cdots, \tag{A.17}$$

$$M_{220} = \frac{1}{4} + \frac{1}{3}\frac{4\text{Pr}^2+3}{2\text{Pr}^2}a^2 + \cdots, \tag{A.18}$$

$$M_{310} = -\frac{3}{4}a - \frac{1}{2}\frac{2\mathrm{Pr}+3}{2\mathrm{Pr}^3}a^3 + \cdots , \tag{A.19}$$

$$M_{400} = \frac{3}{4} + 2a^2 + \cdots . \tag{A.20}$$

References

[1] P.L. Bhatnagar, E.P. Gross, M. Krook, Phys. Rev. 94 (1954) 511.
[2] C. Cercignani, Mathematical Methods in Kinetic Theory, Plenum, New York, 1990.
[3] F. Bouchut, B. Perthame, J. Stat. Phys. 71 (1993) 191.
[4] G. Liu, Phys. Fluids A 2 (1990) 277.
[5] C. Cercignani, G. Tironi, in: C.L. Brundin (Ed.), Rarefied Gas Dynamics, Academic Press, New York, 1967, vol. I, p. 441.
[6] L.H. Holway, Phys. Fluids 9 (1966) 1658.
[7] C. Truesdell, R. Muncaster, Fundamentals of Maxwells Kinetic Theory of a Simple Monoatomic Gas, Academic Press, New York, 1980.
[8] R. Zwanzig, J. Chem. Phys. 71 (1979) 4416.
[9] A. Santos, J.J. Brey, Physica A 174 (1991) 355.
[10] A. Santos, V. Garzó, Physica A 213 (1995) 409.
[11] J.M. Montanero, A. Santos, V. Garzó, Phys. Fluids 8 (1996) 1981.
[12] D.J. Evans, G.P. Morriss, Statistical Mechanics of Nonequilibrium Liquids, Academic Press, London, 1990.
[13] J.W. Dufty, A. Santos, J.J. Brey, R.F. Rodríguez, Phys. Rev. A 33 (1986) 459.
[14] S.Y. Liem, D. Brown, J.H.R. Clarke, Phys. Rev. A 45 (1992) 3706.
[15] A. Santos, V. Garzó, J.J. Brey, Phys. Rev. A 46 (1992) 8018.
[16] J.M. Montanero, A. Santos, Physica A 225 (1996) 7.
[17] V. Garzó, A. Santos, Physica A 213 (1995) 426.
[18] V. Garzó, M. Lopez de Haro, Phys. Fluids 9 (1997) 776.