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Kinetic model for transport around uniform shear flow

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Expressions for the heat and momentum transport around the state of uniform shear flow are given for a dilute gas. The results are obtained from a kinetic model recently proposed: the Liu model. This model improves some insufficiencies of the well-known Bhatnagar, Gross and Krook (BGK) equation. It is shown that the coexistence between both velocity and temperature gradients is only possible for interaction models with uniform collision frequency. In this case, the heat flux verifies a generalized Fourier's law where the thermal conductivity tensor depends on the shear rate. When considering systems where the collision frequency is not uniform, a perturbation method around the shear flow state is proposed. The irreversible fluxes are evaluated explicitly up to first order in the expansion for Maxwell molecules. The transport coefficients obtained are highly nonlinear functions of the shear rate. The results are compared with those previously obtained from the BGK and Boltzmann equations.

1. Introduction

The nonlinear Boltzmann equation provides an adequate framework for analysing the transport properties in a dilute gas [1]. For near equilibrium states, the Boltzmann equation may be solved for a general interaction law by the standard Chapman–Enskog or Hilbert expansions [2]. From the expressions of the average fluxes (momentum, heat, ...) one derives the hydrodynamic equations in successive approximations. Nevertheless, due to the mathematical complexity of the Boltzmann collision integral, it is a very hard task to obtain explicit results, especially for states far from equilibrium. This problem has motivated the search for mathematically simpler equations that retain the main physical properties. One of the most widely used models in the past years has been the one proposed by Bhatnagar, Gross and Krook (BGK) [3].

In the uniform shear flow (USF) state, the solution to the BGK equation for potentials of the form $r^{-\mu}$ was given first by Zwanzig [4]. In the particular case of Maxwell molecules ($\mu = 4$), the hydrodynamic fields and pressure tensor components given by the BGK equation are the same as those obtained from the Boltzmann equation [5] if one chooses the BGK-collision frequency to be a given eigenvalue of the Boltzmann collision operator. The BGK results have been extended to describe heat transport around the state of uniform shear flow [6, 7].

The BGK model, however, has some insufficiencies. For example, it does not give the correct value of the Prandtl number. In order to improve the results derived from the BGK equation, Liu has proposed recently a new kinetic model [8]. The main property of this equation is that in the cases of viscous flow and molecular flow, its solutions are the same as those given by the Boltzmann equation. For this reason Liu suggests a collision term proportional to the Chapman–Enskog first approximation, which is the solution to the linearized Boltzmann equation. The Liu model has been solved by using the Hilbert method for $r^{-\mu}$ potentials up to the Burnett approximation [9]. The Burnett transport coefficients have been shown to be identical to those given by the Boltzmann equation for some values of the ratio of the two collision frequencies ζ/ν introduced in the Liu model. In this way, the transport coefficients obtained from the Liu model are clearly closer to the Boltzmann coefficients than the ones predicted by the BGK equation [10] for the same choices of the collision frequencies. Now, the question arises as to whether the agreement between the Boltzmann and Liu descriptions is sustained for situations far from equilibrium.

The aim of this paper is to study the coupling between the USF and a temperature gradient from the Liu kinetic model. The physical situation corresponds to a dilute gas in a non-stationary state subject to velocity and temperature gradients. In this problem, there are two parameters measuring the departure from equilibrium: the shear rate a and the thermal gradient ∇T. The motivation for considering this complex problem is that the Liu model presents identical results as those given by the BGK equation in the limit cases where $a = 0$ or $\nabla T = 0$. Thus, in the absence of a thermal gradient (pure USF), if one takes $\zeta/\nu = 8/5$ the Liu model reduces to the BGK equation and the results predicted by both models [4] are the same as those obtained from the Boltzmann equation for Maxwell molecules [5]. On the other hand, in the absence of shear flow (pure heat flow) if $\zeta/\nu = 16/15$ analogous conclusions can be obtained for the heat flux [11, 12]. In this way, one expects that the results obtained from the Liu and BGK equations will be noticeably different for transport problems where the Prandtl number plays an important role. This corresponds to situations where the system is drawn out from equilibrium by the presence of both heat and momentum transport.

The plan of the paper is as follows. In section 2, we give a short description of the solution to the Liu model in the USF state. Section 3 concerns the study of the coexistence between both velocity and temperature gradients in the case of interaction models with uniform collision frequency for which a generalized Fourier's law is found. Section 4 deals with the coupling between the USF and a weak thermal gradient for Maxwell molecules where the collision frequency is proportional to the local density. Finally, a brief discussion is made in Section 5.

2. Description of the Liu model in the USF state

We consider the Liu model kinetic equation for the one-particle distribution function $f(\mathbf{r}, \mathbf{v}; t)$ [8]

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla f = -\zeta(f - f^{\rm LE}) + f^{\rm LE}\left(1 - \frac{\zeta\eta}{nk_{\rm B}T}\right)\frac{m}{k_{\rm B}T}(V_iV_j - \tfrac{1}{3}V^2\delta_{ij})\nabla_j u_i$$
$$+ f^{\rm LE}\left(1 - \frac{2}{5}\zeta\kappa\frac{m}{nk_{\rm B}^2T}\right)\left(\frac{mV^2}{2k_{\rm B}T} - \frac{5}{2}\right)V_i\nabla_i \ln T, \qquad (1)$$

where $\zeta(\mathbf{r}, t)$ is a collision frequency similar to that of the BGK model. Here, $\mathbf{V} = \mathbf{v} - \mathbf{u}$, $k_{\rm B}$ is the Boltzmann constant, m is the mass of a particle, and $f^{\rm LE}(\mathbf{r}, \mathbf{v}; t)$ is the local equilibrium distribution function defined in terms of the local density $n(\mathbf{r}, t)$, local velocity $\mathbf{u}(\mathbf{r}, t)$, and local temperature $T(\mathbf{r}, t)$, respectively. Further, equation (1) introduces the coefficients of viscosity $\eta = (5/8)nk_{\rm B}T/\nu$, and thermal conductivity $\kappa = (15/4)k_{\rm B}\eta/m$ obtained from the

Chapman–Enskog first approximation to the Boltzmann equation [13]. Here, $\nu(\mathbf{r}, t)$ is another velocity-independent collision frequency that can depend upon the density and temperature. In the particular case of repulsive potentials of the form $r^{-\mu}$, $\nu \propto nT^{\alpha}$ with $\alpha = (1/2) - (2/\mu)$. Obviously, an identical dependence on space and time must be considered for ζ. In this paper, from now on we will restrict ourselves to that type of interaction.

The Liu model can be seen as the BGK equation (first term on the right-hand side of equation (1)) plus a term related with the Chapman–Enskog solution to the linearized Boltzmann equation. This term depends on the ratio of the collision frequencies ζ/ν. Recently it has been shown that some particular choices of this ratio lead to a good agreement between the results derived from the Liu and Boltzmann equations [9]. For instance, if one takes $\zeta = (8/5)\nu$ (in which case the term proportional to $\nabla_j u_i$ in equation (1) disappears), the Burnett transport coefficients defined in the pressure tensor expression are the same as those obtained from the Boltzmann equation. On the other hand, if $\zeta = (16/15)\nu$ (in which case the term proportional to $\nabla \ln T$ in equation (1) disappears), identical conclusions are obtained for the heat flux. This possibility of choosing the relation ζ/ν may enable us to compare results derived from both the Liu and Boltzmann equations in several transport problems.

As said in the Introduction, the USF state has been one of the problems most extensively studied in the past few years. This state is macroscopically characterized by uniform density and temperature and a flow velocity of the form $u_i = a_{ij}r_j$, $a_{ij} = a\delta_{ix}\delta_{jy}$, where a is the constant shear rate. The shearing motion generates viscous heating, so that the temperature increases monotonically in time. The main transport properties are related to the pressure tensor components. They are defined by

$$P_{ij} = m\int d\mathbf{v}\, V_iV_j f. \qquad (2)$$

According to the results obtained in the Burnett approximation [9], one expects that for $\zeta = (8/5)\nu$ the results predicted in the shear flow state by the Liu and Boltzmann equations have a good agreement. In fact, this choice reduces the Liu model to the BGK equation, and so the results derived from both models coincide with those given by the Boltzmann equation for Maxwell molecules in the USF [4, 5]. Similar conclusions may be obtained in the steady heat flow problem [11, 12] when one takes $\zeta = (16/15)\nu$. Since the goal of this paper is to analyse the transport around the shear flow, from now on we will restrict ourselves to the particular value $\zeta = (8/5)\nu$.

In the USF state it is convenient to consider the peculiar velocity given by $V_i = v_i - a_{ij}r_j$, so that the distribution function $f_0(\mathbf{V}; t) \equiv f(\mathbf{r}, \mathbf{v}; t)$ is now homogeneous. Then, under this description the Liu model (or the BGK model) becomes

$$\left(\frac{\partial}{\partial t} - a_{ij}V_j\frac{\partial}{\partial V_i}\right)f_0 = -\zeta(f_0 - f^{\rm LE}). \qquad (3)$$

In the long time limit, equation (3) admits a consistent solution [4, 14] given by

$$f_0(\mathbf{V}; t) = \int_0^t ds\, \frac{U(t)}{U(s)}\zeta(s)\, n\left(\frac{m}{2\pi k_{\rm B}T(s)}\right)^{3/2}\exp\left(-\frac{m}{2k_{\rm B}T(s)}\mathbf{V}\cdot\Gamma_{t-s}\cdot\mathbf{V}\right) \qquad (4)$$

where $U(t) = \exp[-\int_0^t ds\,\zeta(s)]$ and Γ_t is the matrix of components

$$\Gamma_{ij}(t) = \delta_{ij} + a^2 t^2 \delta_{iy}\delta_{jy} + at(\delta_{ix}\delta_{jy} + \delta_{iy}\delta_{jx}). \tag{5}$$

From equation (3) the equation of viscous heating can be obtained [4]. In the particular case of Maxwell molecules ($\alpha = 0$), the dominant contribution to the general solution is

$$T(t) = T_0 \exp(\lambda t), \tag{6}$$

T_0 being a constant, and λ being given by [14]

$$\lambda(a^*) = \tfrac{4}{3}\zeta \sinh^2[\tfrac{1}{6}\cosh^{-1}(1+9a^{*2})]$$

$$= \tfrac{1}{3}\zeta\left\{\left[1+9a^{*2}+3(2a^{*2}+9a^{*4})^{1/2}\right]^{1/3}+\left[1+9a^{*2}-3(2a^{*2}+9a^{*4})^{1/2}\right]^{1/3}-2\right\} \tag{7}$$

where $a^* = a/\zeta$ is the reduced shear rate. By inserting equation (6) into equation (4), one obtains the non-zero components of the reduced pressure tensor $P^*_{ij} = P_{ij}/p$:

$$P^*_{xy} = -\frac{3}{2}\frac{\lambda^*}{a^*}, \tag{8}$$

$$P^*_{yy} = P^*_{zz} = 1/(1+\lambda^*), \tag{9}$$

$$P^*_{xx} = (1+3\lambda^*)/(1+\lambda^*), \tag{10}$$

where $\lambda^* = \lambda/\zeta$, and $p = nk_B T$ is the hydrostatic pressure. For $\alpha \neq 0$, a closed form solution is not known and one has to look for an expansion in powers of the reduced shear rate a^*. Thus, it is easy to show that the asymptotic behaviour of the collision frequency is given by [14]

$$\zeta \approx \tfrac{2}{3}a^2\alpha t. \tag{11}$$

From this relation the dominant contribution to the temporal behaviour of the temperature can be obtained. All these results will be used in the next Sections.

3. Coupling between shear flow and temperature gradient. Uniform collision frequency

Let us assume now that the system is slightly perturbed from the USF by the presence of a thermal gradient. Under these conditions one expects that the system is essentially described by the distribution function corresponding to USF. In this way, one may suppose (to be confirmed later) that the macroscopic state is characterized by a steady local density $n(\mathbf{r})$, a linear velocity $u_i = a\delta_{ix}\delta_{jy}$ and a local temperature $T(\mathbf{r};t)$ whose temporal dependence is given by the relation (6). We write the velocity distribution function in the form

$$f(\mathbf{r},\mathbf{V};t) = f_0(\mathbf{r},\mathbf{V};t) + \delta f(\mathbf{r},\mathbf{V};t), \tag{12}$$

where f_0 is given by equation (4), but introducing the local dependence on $n(\mathbf{r})$, $\zeta(\mathbf{r};t)$ and $T(\mathbf{r};t)$. It must be noticed that the perturbation δf retains all the hydrodynamic orders in the shear rate and in the thermal gradient. By substituting

equation (12) into equation (1) and taking into account equation (3), one gets

$$\left[\frac{\partial}{\partial t} - a_{ij}V_j\frac{\partial}{\partial V_i} + (V_i + a_{ij}r_j)\frac{\partial}{\partial r_i}\right]\delta f = -\zeta(\delta f - \delta\Phi), \tag{13}$$

where

$$\delta\Phi = -\frac{1}{\zeta}(V_i + a_{ij}r_j)\left(\nabla_i n\frac{\partial}{\partial n} + \nabla_i T\frac{\partial}{\partial T}\right)f_0 - \frac{1}{2\zeta}\left(\frac{mV^2}{2k_B T} - \frac{5}{2}\right)f^{\mathrm{LE}}V_i\nabla_i \ln T. \tag{14}$$

Since the function δf must be consistent with the hydrodynamic fields proposed, the conditions

$$\int d\mathbf{V}(1,\mathbf{V},V^2)\,\delta f = 0. \tag{15}$$

must be fulfilled. The hydrodynamic balance equations derived from equation (13) show that δf does not satisfy the above conditions even to the first order in the thermal gradient. In order to obtain a consistent solution, we impose the constraints

$$\mathbf{u}\cdot\nabla n = \mathbf{u}\cdot\nabla T = 0, \tag{16}$$

$$\nabla p = 0, \tag{17}$$

$$\nabla\cdot(\nabla T) = 0, \tag{18}$$

$$\nabla\zeta = 0. \tag{19}$$

Conditions (16–19) imply basically that the coexistence between the shear flow and a temperature gradient is only possible for models with uniform collision frequency. If one considers a more realistic potential where ζ depends on $\mathbf{r}$, the local velocity field is modified by the presence of ∇T. In this Section, we will focus on two particular cases: a simple collision model with ζ constant and the so-called very-hard-particle (VHP) interaction [15] ($\alpha = 1$) for which $\zeta(t) \propto p(t)$. Despite the fact that both interaction models do not correspond to any physical potential, this study can be taken as a starting point for extending the problem to more realistic potentials. To our knowledge, no solution has been found to the Boltzmann equation for this kind of interaction models. Taking into account the relations (16–19), the solution to equation (13) in the long-time limit can be written in the form

$$\delta f = -\int_0^t dt'\,\frac{U(t)}{U(t')}\frac{p'}{4k_B}\left(\frac{m}{2\pi k_B}\right)^{3/2}\left\{T'^{-5/2}\left(\frac{m}{k_B T'}\mathbf{V}\cdot\Gamma_{t-t'}\cdot\mathbf{V} - 5\right)\mathbf{V}\cdot\nabla\ln T\right.$$
$$+\sum_{n=1}^{\infty}\frac{(t-t')^n}{n!}T'^n(\mathbf{V}\cdot\nabla\ln T)\left(\frac{d}{dT}\right)^n T'^{-5/2}\left[\left(\frac{m}{k_B T'}\mathbf{V}\cdot\Gamma_{t-t'}\cdot\mathbf{V} - 5\right)\mathbf{V}\cdot\nabla\ln T\right.$$
$$\left.\left. - 4\zeta'\right]\exp\left(-\frac{m}{2k_B T'}\mathbf{V}\cdot\Gamma_{t-t'}\cdot\mathbf{V}\right)\right\}, \tag{20}$$

where $p' \equiv p(t')$, $T' \equiv T(t')$, and $\zeta' \equiv \zeta(t')$.

Expression (20) provides a generalized expansion of the distribution function in powers of the thermal gradient. But, identically to what happens in the BGK equation [6], its velocity moments are polynomial functions of ∇T. In particular, the conditions (15) are verified and

$$\delta \mathbf{P} = \int d\mathbf{V}\, m \mathbf{V}\mathbf{V}\, \delta f = 0. \tag{21}$$

The pressure tensor does not explicitly depend on the thermal gradient. The first non-zero moment is the heat flux vector

$$\delta \mathbf{J} = \int d\mathbf{V} \frac{m}{2} V^2 \mathbf{V}\, \delta f. \tag{22}$$

This obeys a generalized linear Fourier law

$$\delta \mathbf{J} = -\Lambda(a^*)\cdot\nabla T, \tag{23}$$

where Λ is a shear-rate dependent thermal conductivity tensor. Its explicit expression is quoted in the Appendix for the ζ-constant and VHP models. It must be emphasized again that equation (23) is valid for arbitrary values of both the shear rate and the thermal gradient. For $a^* = 0$, $\Lambda_{ij} = \kappa\delta_{ij}$, with κ being the thermal conductivity coefficient defined in equation (1).

According to the results quoted in the Appendix, Λ happens to be a polynomial in a^* for the VHP model. The shear-rate dependence of this tensor must be seen as mainly formal since $a^* \to 0$ in the long-time limit. Therefore, equation (A4) gives the first terms in the Chapman–Enskog expansion in powers of the shear rate. In the ζ-constant case, Λ exhibits a much higher nonlinear dependence on a^*. It is due to the fact that for this model $a^* = a/\zeta$ is a constant so that the system has always the same departure from equilibrium. In order to carry out a comparison with the results derived from the BGK equation for the ζ-constant model [7], in figure 1 we have plotted $\Lambda^*_{kk}/3$ versus a^*. Here, $\Lambda^*_{ij} \equiv \Lambda_{ij}/\kappa$. Figure 1 shows that the agreement between both models increases as a^* decreases. For large a^*, the value predicted

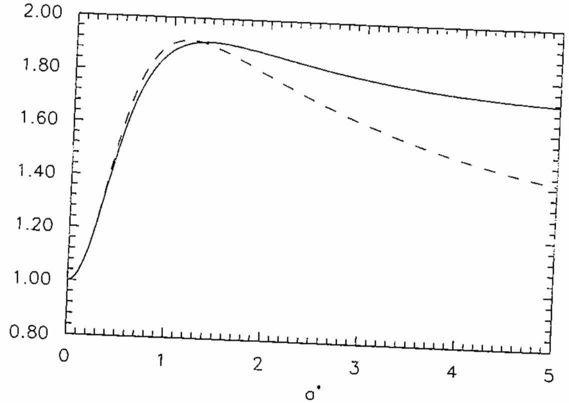

Figure 1. Shear rate dependence of the trace $\Lambda^*_{kk}/3$ of the dimensionless thermal conductivity tensor for the ζ-constant model. The solid line corresponds to the Liu model and the dashed line refers to the BGK equation.

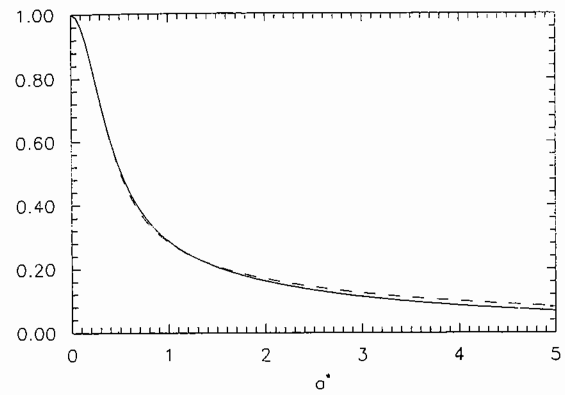

Figure 2. Shear rate dependence of the relative Prandtl number $\gamma(a^*)/\gamma(0)$. The solid line indicates the Liu result and the dashed line the corresponding BGK result.

by the Liu model is greater than the one obtained from the BGK equation. On the other hand, the general shear-rate dependence of this coefficient is quite similar in both kinetic models. For $a^* < 1{\cdot}4$, it increases as a^* while the opposite happens for $a^* > 1{\cdot}4$. It is interesting to relate the heat and momentum fluxes calculated for the ζ-constant model. Its relationship can be characterized through a shear-rate dependent Prandtl number defined by

$$\gamma(a^*) = C_p \frac{\eta}{K}, \tag{24}$$

where C_p is the specific heat, η is the nonlinear shear viscosity given from equation (8) by the relation

$$P_{xy} = -\eta a, \tag{25}$$

and $K \equiv \Lambda_{kk}/3$ can be identified as the nonlinear thermal conductivity coefficient. In figure 2, we have plotted the ratio $\gamma(a^*)/\gamma(0)$ as a function of the shear rate a^*. Here, $\gamma(0) = 2/3$ is the usual Prandtl number defined from the Liu model in the zero shear rate limit. It is shown that the Prandtl number monotonically decreases with respect to its equilibrium value as a^* increases. Further, the values predicted from the Liu model are practically identical to those given from the BGK equation.

4. Perturbation expansion for Maxwell molecules

The equations governing the USF state are characterized by a spatially uniform collision frequency ζ. When this state is slightly perturbed by the presence of a temperature (or density) gradient, ζ is not uniform and this gives rise to a modification in the linear velocity field. As we have shown in the previous Section, the coexistence between both linear gradients is only allowed for very simple interaction models. In this Section we extend the above description to more realistic potentials.

Specifically, we deal with the Maxwell interaction ($\alpha = 0$), for which the collision frequency is proportional to the local density.

Following the scheme presented in [7], we take the USF as the reference state and we perturb around it considering the thermal (or density) gradient as a small perturbation. The transport coefficients derived from this method are highly nonlinear functions of the shear rate. Thus, we propose the following expansion for the hydrodynamic fields:

$$n(\mathbf{r};t) = n_0(\mathbf{r}) + n_2(\mathbf{r};t) + \dots, \tag{26}$$

$$p(\mathbf{r};t) = p_0(\mathbf{r};t) + p_2(\mathbf{r};t) + \dots, \tag{27}$$

$$u_i(\mathbf{r};t) = a_{ij}r_j + u_{1i}(\mathbf{r};t) + \dots, \tag{28}$$

where the subindex denotes the corresponding order in ∇n_0, taken as perturbation parameter. Analogously, the velocity distribution function can be written as

$$f(\mathbf{r},\mathbf{V};t) = f_0(\mathbf{r},\mathbf{V};t) + f_1(\mathbf{r},\mathbf{V};t) + f_2(\mathbf{r},\mathbf{V};t) + \dots, \tag{29}$$

where each approximation f_k is of order k in ∇n_0 (or ∇T_0), but it keeps all the hydrodynamic orders in a^*. If ζ is uniform, $n_k = p_k = u_{ki} = 0$, for $k \geq 1$ and all results reduce to the ones obtained in Section 3. It must be noticed that the symmetry of the functions f_k justifies the parity of the terms defined in equations (26–28). Further details of this method can be found in [7].

Solving recursively, and using from now on the notation used in [7], the kinetic equation for f_1 is given by

$$\left(\frac{\partial}{\partial t} - a_{ij}V_j\frac{\partial}{\partial V_i} + \zeta_0\right) f_1 = -\mathbf{V}\cdot\nabla f_0 + \zeta_0 f_1^{\mathrm{LE}} - \frac{1}{2} f_0^{\mathrm{LE}}\left(\frac{mn_0}{2p_0}V^2 - \frac{5}{2}\right)\mathbf{V}\cdot\nabla \ln\left(\frac{p_0}{n_0 k_{\mathrm{B}}}\right), \tag{30}$$

where we have introduced the functions

$$f_0^{\mathrm{LE}} = n_0\left(\frac{mn_0}{2\pi p_0}\right)^{3/2} \exp\left(-\frac{mn_0}{2p_0}V^2\right), \tag{31}$$

$$f_1^{\mathrm{LE}} = \frac{mn_0}{p_0}\mathbf{u}_1\cdot\mathbf{V} f_0^{\mathrm{LE}}, \tag{32}$$

and $\mathbf{u}_1$ is given by equation (33) of [7]. In the long-time limit, the solution to equation (30) is

$$\begin{aligned} f_1(\mathbf{r},\mathbf{V};t) = {} & \zeta_0\int_0^\infty ds\, \exp(-\zeta_0 s)\exp\left(asV_y\frac{\partial}{\partial V_x}\right)[f_1^{\mathrm{LE}}(t-s) - s\mathbf{V}\cdot\nabla f_0^{\mathrm{LE}}(t-s)] \\ & + (\mathbf{V}\cdot\nabla\zeta_0)\int_0^\infty ds\,\exp(-\zeta_0 s)\exp\left(asV_y\frac{\partial}{\partial V_x}\right)\left(\frac{\zeta s_0^2}{2} - s\right) f_0^{\mathrm{LE}}(t-s) \\ & - \frac{1}{2}\int_0^\infty ds\,\exp(-\zeta_0 s)\exp\left(asV_y\frac{\partial}{\partial V_x}\right) \\ & \times f_0^{\mathrm{LE}}(t-s)\left(\frac{mn_0}{2p_0}V^2 - \frac{5}{2}\right)\mathbf{V}\cdot\nabla\ln\left(\frac{p_0}{n_0 k_{\mathrm{B}}}\right), \end{aligned} \tag{33}$$

where p_0 must be evaluated in $t - s$. From equation (31), it is easy to see that the first non-trivial moment is the heat flux. It can be expressed in the form

$$J_{1i} = -\lambda_{ij}\nabla_j T_0 - \theta_{ij}\nabla_j p_0\, a, \tag{34}$$

where the tensors λ_{ij}, θ_{ij} are given by equations (A 6) and (A 7) of the Appendix respectively. They are highly nonlinear functions of the shear rate a^*. For $a^* = 0$, Fourier's linear law is obtained again. The components of these tensors define a set of shear-rate dependent transport coefficients. For the sake of simplicity, we will restrict our discussion to the particular case of parallel gradients. In this case the relevant coefficients are λ_{yy} and θ_{xy}. The coefficient λ_{yy} can be identified as a generalized thermal conductivity, while θ_{xy} is a generalization of a Burnett coefficient. In fact, their exact zero shear rate values are given by

$$\lambda_{yy} = \frac{15}{4}\frac{p_0 k_{\mathrm{B}}}{m\zeta_0}, \tag{35}$$

$$\theta_{xy} = -\frac{35}{4}\frac{p_0}{mn_0\zeta_0}, \tag{36}$$

which coincide with the ones predicted from the Hilbert expansion [9].

Marchetti and Dufty [16] have studied the shear-rate dependence of transport coefficients analogous to λ_{yy} and θ_{xy}. Their results were derived from the Boltzmann equation by using non-equilibrium time correlation functions. They showed their results in a single eigenvalue approximation. In order to carry out a closer comparison betwen the results derived from kinetic models (Liu and BGK equations) with the ones corresponding to the Boltzmann equation, we define the

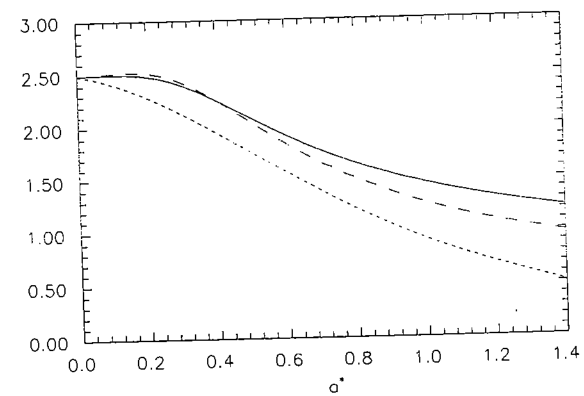

Figure 3. Shear rate dependence of the dimensionless coefficient $\lambda^*(a^*)$ for the Liu model (———), the BGK equation (— — —), and the Boltzmann equation (- - -).

dimensionless coefficients

$$\lambda^*(a^*) = \frac{2}{3}\frac{m\zeta_0}{p_0 k_B}\lambda_{yy}(a^*), \tag{37}$$

$$\theta^*(a^*) = \frac{28}{35}\frac{p_0}{mn_0\zeta_0}\theta_{xy}(a^*), \tag{38}$$

where the corresponding numerical values are chosen to adjust all the results in the limit of exact zero shear rate. Figure 3 shows the shear-rate dependence of λ^*. According to the Liu results, we see that the generalized thermal conductivity decreases relative to its Navier–Stokes value for all shear rates. An identical behaviour is also exhibited in the Boltzmann description. However, in the BGK equation there exists a small region of shear rates ($a^* < 0{\cdot}3$) for which the opposite happens. For large a^*, the BGK predictions are closer to the Boltzmann values than the ones given by the Liu model. Analogous conclusions can be drawn for the coefficient θ^*. Its dependence on a^* is illustrated in figure 4. However, the discrepancy between both kinetic models is smaller than the one obtained for the thermal conductivity case. Furthermore, for large shear rates all the predictions (Boltzmann and kinetic models) are very similar. It must be noticed that the shear rate dependence of the Boltzmann coefficients is only qualitatively correct since it has been obtained in the single eigenvalue approximation. One expects that this dependence will not be far from the exact description.

5. Discussion

In this paper we have addressed the problem of coupling between the shear flow and a temperature gradient in a non-steady state. The analysis was done from a kinetic model recently proposed: the Liu model. This model has been

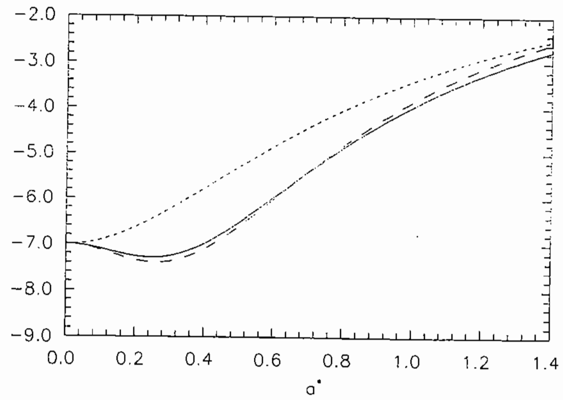

Figure 4. The same as in figure 3 but now for the dimensionless coefficient θ^*.

suggested for the improvement of some insufficiencies of the well-known BGK equation. In particular, it gives the correct value of the Prandtl number. In the same way as our previous BGK results [6, 7], the coexistence between both velocity and temperature gradients is only possible for interaction models with uniform collision frequency ζ. In any other case, the shear flow is disturbed by the action of the thermal gradient ∇T. We considered two interaction models: a simple model with constant ζ and the so-called VHP interaction model for which $\zeta(t) \propto p(t)$. Whereas the pressure tensor is not explicitly affected by the presence of ∇T, the heat flux verifies a generalized Fourier law where a thermal conductivity tensor Λ can be identified. This tensor depends on the shear rate a^*. In addition, a shear-rate Prandtl number $\gamma(a^*)$ was explicitly obtained. The dependence on shear rate of Λ_{kk} and γ was examined for the ζ-constant model. Results showed a good agreement with those previously obtained from the BGK equation [7], especially for small shear rates.

In the case of more realistic potentials where ζ is not uniform, a perturbation method was proposed. The main feature of this expansion is that the zeroth-order approximation corresponds to the USF distribution function which keeps all the hydrodynamic orders in a^*. The transport equations derived are a generalization of the usual Euler, Navier–Stokes, Burnett, ... equations, but now the transport coefficients nonlinearly depend on the shear rate. Although the expansion is restricted to the Maxwell interaction, the extension to other intermolecular potentials can be possible. Here, the irreversible fluxes were evaluated up to first order in the thermal gradient. Modifications of Fourier's heat law are obtained in terms of transport coefficients that depend on the shear rate. This dependence was illustrated for several transport coefficients and compared with previous results given by the Boltzmann [16] and BGK [7] equations.

The study made in this paper from the Liu model encourages our objective of analysing other non-equilibrium states for which a BGK description has been done. In particular, we will study the coupling between velocity and temperature gradients in a steady state for comparing with the results obtained from the BGK equation [17].

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Appendix

Since the procedures to arrive at equations (23) and (34) are identical to the ones employed in [6] and [7] for the same problem within the BGK equation, we only sketch and quote some of the steps in this appendix and refer the interested reader to [6] and [7] for further details.

In the case of interaction models with uniform collision frequency, the thermal conductivity tensor $\Lambda(a^*)$ is given by

$$\Lambda(a^*) = \frac{nk_B^2}{2mT}\int_0^t dt' \frac{U(t)}{U(t')}[\zeta'(t-t') + \tfrac{1}{2}]T'^2\Omega_{t-t'}, \tag{A 1}$$

where the components of the tensor $\boldsymbol{\Omega}$ are

$$\Omega_{ij}(t) = (5 + 10a^2t^2 + 3a^4t^4)\delta_{ix}\delta_{jx} + (5 + 3a^2t^2)\sigma_{iy}\delta_{jy} + (5 + a^2t^2)\delta_{iz}\delta_{jz} - at(7 + 3at)(\delta_{ix}\delta_{jy} + \delta_{iy}\delta_{jx}). \tag{A 2}$$

In order to evaluate the expression (A 1), one must take into account the explicit temporal dependence of the temperature and the collision frequency. We consider two cases: a simple model where ζ is constant and the VHP model.

In the ζ-constant model, the temperature is given by equation (6) and ζ is a constant. Therefore, in the long-time limit one obtains

$$\begin{aligned}\Lambda_{ij} &= \frac{nk_B^2T}{2m\zeta}\int_0^\infty d\tau\, \exp[-\tau(1+2\lambda^*)]\,(\tau+\tfrac{1}{2})\Omega_{ij}(\tau/\zeta)\\ &= \kappa\Big\{\big[(1+\tfrac{2}{3}\lambda^*)\beta^2 + \tfrac{4}{3}(7+2\lambda^*)a^{*2}\beta^4 + \tfrac{24}{5}(11+2\lambda^*)a^{*4}\beta^6\big]\delta_{ix}\delta_{jx}\\ &\quad + \big[(1+\tfrac{2}{3}\lambda^*)\beta^2 + \tfrac{2}{5}(11+10\lambda^*)a^{*2}\beta^4\big]\delta_{iy}\delta_{jy}\\ &\quad + \big[(1+\tfrac{2}{3}\lambda^*)\beta^2 + \tfrac{8}{15}(4+5\lambda^*)a^{*2}\beta^4\big]\delta_{iz}\delta_{jz}\\ &\quad - \big[\tfrac{7}{15}(9+10\lambda^*)a^*\beta^3 + \tfrac{6}{5}(13+10\lambda^*)a^{*3}\beta^5\big](\delta_{ix}\delta_{jy}+\delta_{iy}\delta_{jx})\Big\}.\end{aligned} \tag{A 3}$$

Here, $\beta = 1/(1+2\lambda^*)$ and κ is the thermal conductivity coefficient defined from equation (1).

In our problem, the VHP interaction is defined by a collision frequency proportional just to the pressure, i.e., $\alpha = 1$. For long times, one has that $T(t) \propto t$, and $\zeta(t) \approx (2/3)a^2t$. Inserting these temporal behaviours into equation (A 1), in the long-time limit the asymptotic behaviour of the thermal conductivity tensor is given by

$$\begin{aligned}\Lambda_{ij} = \kappa\Big[&(1+\tfrac{28}{3}a^{*2}+\tfrac{264}{5}a^{*4})\delta_{ix}\delta_{iy} + (1+\tfrac{14}{5}a^{*2})\delta_{iy}\delta_{jy}\\ &+ (1+\tfrac{14}{15}a^{*2})\delta_{iz}\delta_{jz} - (\tfrac{7}{3}+\tfrac{54}{5}a^{*2})a^*(\delta_{ix}\delta_{jy}+\delta_{iy}\delta_{jx})\Big].\end{aligned} \tag{A 4}$$

In the case of Maxwell molecules, proceeding in a similar way to the calculations made in [7], the heat flux can be written as

$$J_{1i} = -\lambda_{ij}\nabla_jT_0 - \theta_{ij}\nabla_jp_0a, \tag{A 5}$$

where

$$\begin{aligned}\lambda_{ij} = \frac{p_0k_B}{m\zeta_0}\Big\{&\frac{1}{16}\frac{\partial^2}{\partial\lambda_0^{*2}}B_{ij} - \frac{\hat{\lambda}_0^*}{\lambda_0^*}\Big\{\Big(\frac{A_{ik}}{2}-\frac{3}{2}\delta_{ik}-P_{0ik}^*\Big)\Big[\Big(\delta_{kl}-\frac{a_{kl}^*}{\lambda_0^*}\Big)\\ &\Big(\frac{\partial}{\partial\lambda_0^*}P_{0lj}^* - \frac{\lambda_0^*}{\hat{\lambda}_0^*}\frac{\partial}{\partial\lambda_0^*}P_{0lj}^* - \frac{1}{\lambda_0^*}P_{0lj}^*\Big) + \frac{a_{kl}^*}{\lambda_0^{*2}}P_{0lj}^*\Big]\\ &+\frac{1}{4}\Big(\delta_{kl}-\frac{a_{kl}^*}{\lambda_0^*}\Big)P_{0lj}^*\frac{\partial}{\partial\lambda_0^*}A_{ik} - \frac{\lambda_0^*}{4}\frac{\partial^2}{\partial\lambda_0^{*2}}A_{ik}\Big\}\\ &-\frac{1}{8}\hat{\lambda}_0^*\frac{\partial}{\partial\lambda_0^*}A_{ij} + \frac{1}{4}A_{ij}\Big\}\end{aligned} \tag{A 6}$$

$$\theta_{ij} = \frac{p_0}{mn_0\zeta_0a}\Big[\frac{1}{\lambda_0^*}\Big(\frac{A_{ik}}{2}-\frac{3}{2}\delta_{ik}-P_{0ik}^*\Big)\Big(\delta_{kl}-\frac{a_{kl}^*}{\lambda_0^*}\Big)P_{0lj}^* - \frac{1}{2}\frac{\partial}{\partial\lambda_0^*}B_{ij} + \frac{1}{4}A_{ij}\Big]. \tag{A 7}$$

Here,

$$\hat{\lambda}_0^* = \lambda_0^* - \frac{4}{3}\frac{\sinh[(1/3)\cosh^{-1}(1+9a^{*2})]}{(2+9a^{*2})^{1/2}}a^*, \tag{A 8}$$

the non-zero components of $\mathbf{P}_0$ are given by equations (8–10), and the tensors $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$ are defined by equations (A 12) and (A 13) of [7], respectively.

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