COUPLING BETWEEN SHEAR FLOW AND TEMPERATURE GRADIENT FOR THE VERY HARD PARTICLES INTERACTION

V. GARZÓ [1] and J. DE LA RUBIA
Departamento de Termología, Facultad de Físicas, Universitat de València, Burjassot, Spain

Received 3 July 1986; in final form 10 October 1986

We have constructed a solution of the BGK model kinetic equation to describe a system subject to uniform shear flow and a thermal gradient. The coexistence between both gradients is maintained in the system if the collision frequency is spatially uniform. In our model this particular case corresponds to the so-called VHP interaction.

1. Introduction

One of the macroscopic systems extensively studied in the past few years is that corresponding to the plane Couette flow between two parallel plates in relative motion. Due to its simplicity, this system has been analyzed using non-equilibrium statistical mechanics as well as simulation methods [1]. Specifically, in the case of Maxwell's molecules (those with an inverse fourth power potential) and using Boltzmann's equation (BE), an explicit expression has been given for the stress tensor as a function of shear rate [2]. However, for most other types of potential the BE is too difficult to solve. Hence, the search for simplified versions of the BE. Among these and probably the best known, is the BGK model. Using this model, Zwanzig [3] studied the problem of a uniform shear flow and found a closed equation for the pressure tensor for potentials of the form $r^{-\mu}$. Recently, a consistent solution of the BGK equation has also been achieved in the case of a system subject to a non-uniform temperature gradient [4].

The aim of this paper is to give an analysis, based on the BGK equation, of the transport properties of a system, in which a uniform shear flow coexists with a weak temperature gradient. The study of the coupling between these two gradients has been treated previously using kinetic theory [5] and fluctuating hydrodynamics [6]. In both cases, under suitable boundary conditions, the study could be carried out under steady-state conditions. However, in our analysis the increase of temperature with time, due to the heat generated because of the viscous heating term, is taken into account. This represents a substantial difference from previous work.

From our model, our conclusion is that a coexistence between both gradients is only possible in the particular case that the collision frequency is spatially uniform. This case in our model corresponds to the so-called VHP interaction, for which exact solutions of the BE [7] and the BGK model [8] are known. The proposed solution appears as a power expansion of the temperature gradient, but its first moments are given as polynomials in the thermal gradient. Specifically, the pressure tensor does not depend explicitly on temperature gradient (∇T) and the heat flux is a linear function of ∇T. A generalized thermal conductivity can be defined which depends of the shear rate. When considering more realistic potentials, a formal solution is suggested analogous to that of Chapman–Enskog.

2. Uniform shear flow

We consider the BGK model kinetic equation for the one-particle distribution function $f(\boldsymbol{r}, \boldsymbol{v}; t)$

[1] To whom correspondence should be addressed.

0 009-2614/86/$ 03.50 © Elsevier Science Publishers B.V. (North-Holland Physics Publishing Division)

$$(\partial/\partial t+\boldsymbol{v}\cdot\boldsymbol{\nabla})f=-\zeta(f-f_{\mathrm{LE}})\ , \tag{1}$$

where f_{LE} is a function of the local equilibrium and ζ is the collision frequency. For repulsive potentials of the form $r^{-\mu}$, ζ depends on the density n and the temperature T:

$$\zeta \propto nT^{\alpha}\ , \tag{2}$$

with $\alpha=(\mu-4)/2\mu$. In the case of uniform shear flow, eq. (1) admits a solution characterized by a uniform density and temperature,

$$f_0(\boldsymbol{r},\boldsymbol{v};t)=\int_0^t \mathrm{d}s\,\frac{U(t)}{U(s)}\,\zeta(s)\,n_0\left(\frac{m}{2\pi k_{\mathrm{B}}T_0(s)}\right)^{3/2}\exp\left(-\frac{m}{2k_{\mathrm{B}}T_0(s)}\,\boldsymbol{V}\cdot\boldsymbol{\Gamma}_{t-s}\cdot\boldsymbol{V}\right), \tag{3}$$

where the initial distribution contribution has been neglected since we are considering long times.

In (3), considering local velocity fields of the form $u_i=\epsilon\delta_{ix}\delta_{jy}r_j$, we have introduced the quantities $\boldsymbol{V}=\boldsymbol{v}-\boldsymbol{u}$, $U(t)=\exp(-\int_0^t\mathrm{d}s\,\zeta(s))$ and $\boldsymbol{\Gamma}_t$ is the matrix of components

$$\Gamma_{ij}=\delta_{ij}+\epsilon^2t^2\delta_{iy}\delta_{jy}+\epsilon t(\delta_{ix}\delta_{jy}+\delta_{iy}\delta_{jx})\ .$$

The temperature increases with time according to the equation of viscous heating [3]. In this way for potentials of the form $r^{-\mu}$, the temporal variation of ζ will be

$$(\mathrm{d}/\mathrm{d}t+\zeta)^2\zeta^{1/\alpha-1}\mathrm{d}\zeta/\mathrm{d}t=\tfrac{2}{3}\epsilon^2\alpha\zeta^{1/\alpha+1}\ , \tag{4}$$

where $\alpha=0$ (Maxwell gas) has been excluded. If we suppose that ζ behaves as a power of t, the solution of (4) for long times is given by

$$\zeta(t)=\tfrac{2}{3}\epsilon^2\alpha t+A\ ,$$

where A is a constant which depends on the initial conditions. This expression will be used later.

Since the shear rate required for non-Newtonian effects (the stress tensor depends non-linearly on the shear rate) is unrealistically large, analysis of such effects are realized by computer simulation methods. A review of such methods can be found in ref. [1].

3. Uniform shear flow plus temperature gradient. Very-hard-particle (VHP) interaction

Let us suppose that we perturb the above state by introducing a weak thermal gradient. Under such conditions, we expect the macroscopic state to be characterized by a steady local density $n(\boldsymbol{r})$, a linear velocity $u_i=\epsilon\delta_{ix}\delta_{jy}r_j$ and a local temperature gradient $T_0(\boldsymbol{r},t)$, whose temporal dependence is fixed according to the heating equation (4). In other words, because this state is the uniform shear flow state slightly perturbed, we shall write the distribution function of the system in the form

$$f(\boldsymbol{r},\boldsymbol{v};t)=f_0(\boldsymbol{r},\boldsymbol{v};t)+\delta f(\boldsymbol{r},\boldsymbol{v};t)\ , \tag{5}$$

where f_0 is given by eq. (3), but introducing the local dependence of $n(\boldsymbol{r})$, $T_0(\boldsymbol{r},s)$ and $\zeta(\boldsymbol{r},s)$. Evidently, there will be certain restrictions in order for the BGK equation to admit such a state.

In order to solve (1) for this hydrodynamic state, we need some boundary conditions. Nevertheless, we are interested in transport properties in the bulk system, far away from the boundaries. Consequently, one would hope to get the right answer by looking for a consistent solution to eq. (1), regardless of the details of the boundary conditions. This is the spirit in which eq. (3) was obtained.

Inserting (5) into the BGK equation and taking into account that f_0 is a solution when the spatial dependence of the velocity is considered, we obtain for $\delta f(\boldsymbol{r},\boldsymbol{v};t)$ the expression

$$\delta f(\boldsymbol{r},\boldsymbol{v};t)=\int_0^t \mathrm{d}s\left(\mathrm{e}^{-t\boldsymbol{v}\cdot\boldsymbol{\nabla}}\frac{\tilde{U}(\boldsymbol{r},t)}{\tilde{U}(\boldsymbol{r},s)}\mathrm{e}^{s\boldsymbol{v}\cdot\boldsymbol{\nabla}}-\frac{U(\boldsymbol{r},t)}{U(\boldsymbol{r},s)}\right)\zeta(\boldsymbol{r},s)\,f^{t}_{\mathrm{LE}}(\boldsymbol{r},\boldsymbol{v};s)\,, \tag{6}$$

where the quantity

$$\tilde{U}(\boldsymbol{r},t)=\exp\left(-\int_0^t \mathrm{d}s\,\mathrm{e}^{s\boldsymbol{v}\cdot\boldsymbol{\nabla}}\zeta(\boldsymbol{r},s)\right)$$

has been introduced and $f^{t}_{\mathrm{LE}}(\boldsymbol{r},\boldsymbol{v};s)$ is given by

$$f^{t}_{\mathrm{LE}}(\boldsymbol{r},\boldsymbol{v};s)=n(\boldsymbol{r})\left(\frac{m}{2\pi k_{\mathrm{B}}T(\boldsymbol{r},s)}\right)^{3/2}\exp\left(-\frac{m}{2k_{\mathrm{B}}T(\boldsymbol{r},s)}\boldsymbol{V}\cdot\boldsymbol{\Gamma}_{t-s}\cdot\boldsymbol{V}\right). \tag{7}$$

The operator $\boldsymbol{\nabla}$ which appears in (6) takes the form

$$\boldsymbol{\nabla}n\,\partial/\partial n+\boldsymbol{\nabla}T\,\partial/\partial T\,,$$

since its action on $\boldsymbol{u}(\boldsymbol{r})$ has already been totally transferred through $f^{t}_{\mathrm{LE}}(\boldsymbol{r},\boldsymbol{v};s)$. In order that the function δf be consistent with the hydrodynamic state proposed, it is necessary that

$$\delta n=\int \mathrm{d}\boldsymbol{v}\,\delta f=0\,,\quad \delta(n\boldsymbol{u})=\int \mathrm{d}\boldsymbol{v}\,\boldsymbol{v}\,\delta f=0\,,\quad \delta(nk_{\mathrm{B}}T)=\int \mathrm{d}\boldsymbol{v}\,\tfrac{1}{3}m|\boldsymbol{v}-\boldsymbol{u}|^2\,\delta f=0\,. \tag{8}$$

However, δf does not satisfy these conditions even to first order in the thermal gradient (Navier–Stokes). Consequently we impose certain restrictions in order to obtain a consistent solution. By simple inspection of the macroscopic balance equations, these conditions are

$$\boldsymbol{u}\cdot\boldsymbol{\nabla}n=\boldsymbol{u}\cdot\boldsymbol{\nabla}T=0\,,\quad \boldsymbol{\nabla}p=\boldsymbol{0}\,,$$

$$\boldsymbol{\nabla}(\boldsymbol{\nabla}T)=\mathbf{0}\,,\quad \boldsymbol{\nabla}\zeta=\boldsymbol{0}\,, \tag{9}$$

where $p=nk_{\mathrm{B}}T$ is the hydrostatic scalar pressure.

This means that we are going to impose an orthogonal constant temperature gradient to the velocity $\boldsymbol{u}$ which is coupled with the density gradient in such a way that the pressure is uniform. In addition we are supposing a molecular interaction model with a uniform collision frequency. If $\alpha=1$ in eq. (2), $\zeta(t)\propto p(t)$ which is uniform in our model. This particular case corresponds to the so-called very-hard-particle (VHP) interaction. If we consider a more realistic potential with ζ depending on $\boldsymbol{r}$, the uniform shear flow would be perturbed by the presence of $\boldsymbol{\nabla}T$ and the velocity profile would no longer be linear. In any case, the solution obtained from (6) for the hydrodynamic state proposed would be approximate. However our study is confined to the VHP model. In this model δf takes the form

$$\delta f(\boldsymbol{r},\boldsymbol{v};t)=\int_0^t \mathrm{d}s\,\frac{U(t)}{U(s)}\,\zeta(s)\,\frac{p(s)}{k_{\mathrm{B}}}\left(\frac{m}{2\pi k_{\mathrm{B}}}\right)^{3/2}$$

$$\times\sum_{n=1}^{\infty}\frac{(s-t)^n}{n}\,(\boldsymbol{V}\cdot\boldsymbol{\nabla}T)^n\left(\frac{\mathrm{d}}{\mathrm{d}T}\right)^n[T(s)]^{-5/2}\exp\left(-\frac{m}{2k_{\mathrm{B}}T(s)}\,\boldsymbol{V}\cdot\boldsymbol{\Gamma}_{t-s}\cdot\boldsymbol{V}\right), \tag{10}$$

where we have suppressed the explicit dependence on $\boldsymbol{r}$. In spite of this, δf is given by an expansion in powers of $\boldsymbol{\nabla}T$ and its first moments are given by polynomic functions of $\boldsymbol{\nabla}T$. Specifically, $\delta n=\delta(nu_i)=\delta p=0$, and this shows the consistency of the solution. Additionally

$$\delta\mathbf{P}=\int \mathrm{d}\boldsymbol{v}\,m\boldsymbol{V}\boldsymbol{V}\,\delta f=\mathbf{0}\,. \tag{11}$$

There is no coupling between the shear rate and the temperature gradient in the pressure tensor. The first moment different from zero corresponds to the heat flux. This is a linear function of the temperature gradient. So, $\delta \boldsymbol{J}=-\boldsymbol{\Lambda}\cdot\nabla T$, where $\boldsymbol{\Lambda}$ is the generalized thermal conductivity tensor defined by

$$\boldsymbol{\Lambda}(\epsilon)=\frac{nk_B^2}{2mT(t)}\int_0^t ds\,\frac{U(t)}{U(s)}\,\zeta(s)\;(t-s)[T(s)]^2\boldsymbol{\Delta}_{t-s} \tag{12}$$

and $\boldsymbol{\Delta}\equiv(\mathrm{tr}\,\boldsymbol{\Gamma}^{-1})\boldsymbol{\Gamma}^{-1}+2\boldsymbol{\Gamma}^{-1}\boldsymbol{\Gamma}^{-1}$. Introducing the variables $x=\frac{1}{3}\epsilon^2t^2$ and $y=\frac{1}{3}\epsilon^2(t^2-s^2)$, the tensor $\boldsymbol{\Lambda}(\epsilon)$ for long times is

$$\boldsymbol{\Lambda}(\epsilon)=\frac{5}{2}\frac{k_Bp(t)}{m\zeta(t)}\lim_{x\to\infty}\int_0^x dy\;(x-y)[1-(1-y/x)^{1/2}]\tfrac{2}{5}e^{-y}\boldsymbol{\Delta}_{(3x)^{1/2}\epsilon^{-1}[1-(1-y/x)^{1/2}]}\,, \tag{13}$$

where we have taken into account the time behaviour of $T(t)$ and $\zeta(t)$. In order to evaluate this integral we need the result

$$\lim_{x\to\infty}(2x)^n\int_0^x dy\;(x-y)[1-(1-y/x)^{1/2}]^{n+1}e^{-y}=\tfrac{1}{2}(n+1)!\,, \tag{14}$$

and then, the tensor $\boldsymbol{\Lambda}$ is finally

$$\Lambda_{ij}(\epsilon^*)=\frac{5}{2}\frac{nk_B^2T(t)}{m\zeta(t)}\;[(1+12\epsilon^{*2}+72\epsilon^{*4})\delta_{ix}\delta_{jx}+(1+\tfrac{18}{5}\epsilon^{*2})\delta_{iy}\delta_{jy}+(1+\tfrac{6}{5}\epsilon^{*2})\delta_{iz}\delta_{jz}$$

$$-(\tfrac{14}{5}\epsilon^*+\tfrac{72}{5}\epsilon^{*3})(\delta_{ix}\delta_{jy}+\delta_{iy}\delta_{jx})] \tag{15}$$

with $\epsilon^*\equiv\epsilon/\zeta$. The generalized thermal conductivity tensor is thus a polynomial in the dimensionless shear rate ϵ^*. The dependence of $\boldsymbol{\Lambda}(\epsilon^*)$ on ϵ^* is mainly formal, since in the limit $t\to\infty$, $\epsilon^*\to 0$. Consequently, eq. (15) gives the first terms of the Chapman–Enskog expansion of $\boldsymbol{\Lambda}(\epsilon^*)$. This explains the polynomial dependence obtained. In the case $\epsilon\to 0$, the results corresponding to a steady-state heat flux are again obtained [4].

Experimental measurements on the viscosity of liquids in the presence of thermal gradients have been made [9]. However, the lack of experimental data on thermal conductivity in the presence of a shear rate, make a comparison of our results impossible at the present time.

In the case of weak shears and temperature gradients (linearized hydrodynamics), the viscous heating can be neglected so the transport coefficients do not depend on time. Under these conditions, in accordance with eqs. (3), (11) and (15), we obtain the Navier–Stokes hydrodynamics equations with shear viscosity $\eta=nk_BT/\zeta$, and thermal conductivity $\lambda=\frac{5}{2}nk_B^2T/m\zeta$. This is in agreement with the Chapman–Enskog expansion of the BGK equation.

4. Remarks

We have studied the coupling between the shear flow and a temperature gradient in the BGK kinetic model of the Boltzmann equation. Such a coexistence is only possible in the particular case of a uniform collision frequency, which in our model corresponds to the so-called VHP interaction. In any other case, the shear flow cannot be maintained in the system because it is perturbed by the imposed temperature gradient. For this interaction model, the momentum (pressure tensor) and heat fluxes have been evaluated for long times. Whereas the pressure tensor does not depend explicitly on the temperature gradient ∇T, the heat flux is a linear function of ∇T. We have obtained a generalized (linear) Fourier law and defined a generalized thermal conductivity tensor that depends on the dimensionless shear rate ϵ^*.

Despite the fact that the model studied does not correspond to any real physical potential, we think that this study can be useful as a starting point for the analysis of more realistic systems. Specifically, we are elaborating a kinetic model for the case of Maxwell molecules based on a perturbative expansion around the uniform shear flow distribution $f_0(\boldsymbol{r}, \boldsymbol{v}; t)$. The results will be published elsewhere.

References

[1] W.G. Hoover, Ann. Rev. Phys. Chem. 34 (1983) 103;
D.J. Evans and G.P. Morriss, Computer Phys. Rept. 1 (1984) 299;
J.W. Dufty, A. Santos, J.J. Brey and R.F. Rodriguez, Phys. Rev. A33 (1986) 459.
[2] E. Ikenberry and G. Truesdell, J. Rat. Mech. Anal. 5 (1956) 55;
M.C. Marchetti and J.W. Dufty, J. Stat. Phys. 32 (1983) 255, A2.
[3] R. Zwanzig, J. Chem. Phys. 71 (1979) 4416.
[4] A. Santos, J.J. Brey and V. Garzó, Phys. Rev. A, to be published.
[5] M. Garcia Sucre and D. Moronta, Phys. Rev. A26 (1982) 1713;
J.C. Nieuwoudt, T.R. Kirkpatrick and J.R. Dorfman, J. Stat. Phys. 34 (1984) 203.
[6] A. Perez-Madrid and J.M. Rubí, Phys. Rev. A33 (1986) 2716.
[7] M. Ernst, Phys. Rept. 78 (1981) 117.
[8] J.J. Brey and A. Santos, J. Stat. Phys. 37 (1984) 123.
[9] F.S. Gaeta, P. Migliardo and F. Wanderling, Phys. Rev. Letters 31 (1973) 1181.