GENERALIZATION OF THE KROOK KINETIC RELAXATION EQUATION

E. M. Shakhov

Izv. AN SSSR. Mekhanika Zhidkosti i Gaza, Vol. 3, No. 5, pp. 142-145, 1968

One of the most significant achievements in rarefied gas theory in the last 20 years is the Krook model for the Boltzmann equation [1]. The Krook model relaxation equation retains all the features of the Boltzmann equation which are associated with free molecular motion and describes approximately, in a mean-statistical fashion, the molecular collisions. The structure of the collisional term in the Krook formula is the simplest of all possible structures which reflect the nature of the phenomenon. Careful and thorough study of the model relaxation equation [2-4], and also solution of several problems for this equation, have aided in providing a deeper understanding of the processes in a rarefied gas. However, the quantitative results obtained from the Krook model equation, with the exception of certain rare cases, differ from the corresponding results based on the exact solution of the Boltzmann equation. At least one of the sources of error is obvious. It is that, in going over to a continuum, the relaxation equation yields a Prandtl number equal to unity, while the exact value for a monatomic gas is 2/3.

In a comparatively recent study [5] Holway proposed the use of the maximal probability principle to obtain a model kinetic equation which would yield in going over to a continuum the expressions for the stress tensor and the thermal flux vector with the proper viscosity and thermal conductivity.

In the following we propose a technique for constructing a sequence of model equations which provide the correct Prandtl number. The technique is based on an approximation of the Boltzmann equation for pseudo-Maxwellian molecules using the method suggested by the author previously in [6]. For arbitrary molecules each approximating equation may be considered a model equation. A comparison is made of our results with those of [5].

§1. Consider the Boltzmann equation in the absence of external forces

$$\frac{\partial f}{\partial t}+\xi_i\frac{\partial f}{\partial x_i}=\nu(f^+-f)\equiv J(f),\qquad \nu=\int f_1 g\sigma\,d\xi_1,$$
$$g=|\xi-\xi_1|,\qquad f^+=\frac{J^+}{\nu},\qquad J^+=\int f'f_1'g\,d\sigma\,d\xi_1. \tag{1.1}$$

Here ν is the collision frequency, J^+ is the reverse collision integral, σ is the collision section; summation over repeating subscripts is assumed.

In the following we restrict ourselves to pseudo-Maxwellian molecules, i.e., we shall consider σ and $d\sigma$ to be inversely proportional to the relative velocity of the colliding molecules. In this case the collision frequency is independent of the molecular velocity. Along with (1.1) we consider the equation

$$\frac{\partial F}{\partial t}+\xi_i\frac{\partial F}{\partial x_i}=\frac{1}{\tau}(F^+-F), \tag{1.2}$$

in which F^+ is assumed to depend on the thermal velocities and some combination of macroscopic parameters; the form of this relationship is defined later.

We shall term (1. 2) an approximating equation for the Boltzmann equation (1.1) if some number of first moment equations of the exact and approximating equations coincide, i.e., if the conditions

$$\int\frac{1}{\tau}(F^+-F)\psi\,d\xi=\int J(F)\psi\,d\xi,$$
$$\psi=\psi(\xi)=1,\ \xi_i,\ \xi_i\xi_j,\ \xi_i\xi_j\xi_k,\ \ldots \tag{1.3}$$

are met, or

$$\psi=\psi(c)=1,\ c_i,\ c_ic_j,\ c_ic_jc_k,\ \ldots,\qquad c_i=\xi_i-\int\xi_iF\,d\xi.$$

More precisely, we shall call (1.2) the n-th approximating equation for (1.1) if the conditions (1.3) are satisfied for all ψ which include power-law monomials of n-th order.

The approximating equation which satisfies the conditions (1.3) for the set of ψ including not all power-law monomials of third order, but only convolutes of the form $\xi_i\xi^2$, may be termed an approximating kinetic equation in the 13-moment approximation, since the combination of macroparameters appearing in F^+ is defined by the first 13 moments of the distribution function. We set the collision frequency $1/\tau$ of (1.2) equal to the collision frequency ν of (1.1).

The form of F^+ as a function of the molecular velocities and the macroparameters is not defined by the conditions (1.3). For simplicity, following [6], we take F^+ in the form

$$F^+=F^{(0)}\{a^{(0)}+a_i^{(1)}c_i+a_{ij}^{(2)}c_ic_j+a_{ijk}^{(3)}c_ic_jc_k+\ldots\},$$
$$F^{(0)}=\frac{\rho}{(2\pi RT)^{3/2}}e^{-c^2/2RT},\qquad c^2=c_ic_i,\qquad c_i=\xi_i-u_i. \tag{1.4}$$

Here $F^{(0)}$ is a locally Maxwellian distribution function, and u_i is the gas mass velocity. The combination of coefficients $a(x_i, t)$ is defined by (1.3).

If we restrict ourselves to a finite number of terms of the series, then we shall have the corresponding approximation for the reverse collision integral. Considering for the moment the second approximation, for which F^+ includes all the power-law monomials up to and including second order, and referring to (1.3) with $\psi = 1, c_i, c_ic_j$, we obtain $a^{(0)}=a_i^{(1)}=a_{ij}^{(2)}=0$ in view of the choice of $F^{(0)}$ and τ. Thus, in the second approximation, when the moment equations up to and including second order agree with the exact equations, we obtain as the approximating equation for the Boltzmann equation the Krook model

$$\frac{\partial F}{\partial t}+\xi_i\frac{\partial F}{\partial x_i}=\frac{1}{\tau}(F^{(0)}-F). \tag{1.5}$$

In the next, third approximation we restrict ourselves to representing F^+ by convoluted Hermitian polynomials. We set

$$F^+=F^{(0)}\Big\{a^{(0)}+a_i^{(1)}c_i+$$
$$+a_{ij}^{(2)}\Big(\frac{c_ic_j}{RT}-\delta_{ij}\Big)+a_i^{(3)}c_i\Big(\frac{c^2}{2RT}-\frac{5}{2}\Big)\Big\}. \tag{1.6}$$

To determine the combination $a(x_i, t)$ we use also the corresponding orthogonal polynomials. We obtain

$$a^{(0)}=a_i^{(1)}=a_{ij}^{(2)}=0,$$
$$a_i^{(3)}=\frac{1-\Pr}{5}\frac{S_i}{pRT},\qquad S_i=\int c_ic^2F\,d\xi.$$

Thus the approximating equation of the incomplete third (or 13-moment) approximation has the form

$$\frac{\partial F}{\partial t}+\xi_i\frac{\partial F}{\partial x_i}=\frac{1}{\tau}(F^+-F),$$
$$F^+=F^{(0)}\Big[1+\frac{1-\Pr}{5}\frac{S_ic_i}{pRT}\Big(\frac{c^2}{2RT}-\frac{5}{2}\Big)\Big]. \tag{1.7}$$

As $\tau \to 0$ the moment equations for this equation yield the expressions for the stresses and the thermal flux with the correct values of the viscosity and heat conductivity.

§2. Obviously the approximation process may be continued. The structure of the approximating equations obtained in any approximation is such that is is possible to construct a numerical solution method without storing the distribution function.

Whether or not the approximation approaches the exact solution of the Boltzmann equation with increasing number of terms in the representation of F+ depends on the convergence of series (1.4). The condition for convergence in the mean for this series amounts to existence of the integral

$$\int \frac{[J^+(F)]^2}{F^{(0)}} d\xi.$$

Thus, together with the previously adopted representation for the distribution function as a series in Hermitian polynomials, multiplied by a locally Maxwellian distribution function [7, 4], we propose to use a similar expansion for the reverse collision integral.

The assumption that it is possible to expand J^+ is natural from the physical point of view. Indeed, the reverse collision integral describes the velocity distribution of only those molecules which have experienced collisions at a given point of physical space; therefore for its approximation it is natural to use a representation with separated variables, i.e., in terms of molecular velocities for fixed x_i and t, where the leading term of this expansion must be a locally Maxwellian function because of the nature of the process. Unlike J^+, the distribution function contains a significant component associated with free molecular motion, i.e., that component in which the variables are not separated but occur in combination. Even for the problem of relaxation in a one-dimensional space the respresentation of the distribution function in the form

$$F = F^{(0)}(1 + a_i c_i + a_{ij} c_i c_j + a_{ijk} c_i c_j c_k + \ldots) \tag{2.1}$$

does not yield the true behavior of the distribution function in time, since in accordance with (2.1) the number of molecules with small velocities differs little from the equilibrium value over the time of the process regardless of the initial conditions.

Continuity of the reverse collision integral means that we might expect not only convergence in the mean, but even uniform and quite rapid convergence of (1.4) in a finite region of velocity space.

§3. The technique proposed above for obtaining the approximate kinetic equations with a collision frequency which is independent of the relative velocity of the colliding molecules differs significantly from that proposed in [5] in that it offers an improvement of the solution by using moment relations (1.3) of higher and higher order. If we restrict ourselves to second-order moments, then by selecting the collision frequency, as in [5], we can also obtain an approximate kinetic equation which provides the correct Prandtl number. This equation will agree with that of [5] for conditions sufficiently close to equilibrium, i.e., when the ellipsoidal distribution can be linearized relative to the Maxwellian.

The choice of F^+ in the form (1.4), as noted before, was based on considerations of simplicity. We could, following [5], use the principle of the most probable distribution, defining the moments of this distribution in terms of the distribution function moments from conditions (1.3), which reduce to a system of transcendental equations. The combination of the principle of most probable distribution and the moment relations for the collision integral yields in principle the possibility of constructing a sequence of model equation. In particular, along with the second-order moments of the most probable distribution, as suggested in [5], we could introduce the third-order moments. When trying to provide the correct expression for the heat flux (third-order moment) and consequently the Prandtl number, this procedure appears more natural than the choice of the collision frequency. In this case we would again obtain as the most probable distribution an exponential distribution, but now containing power-law monomials of third order in the exponent. Consequently, for high velocities the integrals will deverge, i.e., we will run into the same difficulty as in using the most-probable-distribution principle for quasi-equilibrium flows [4, 8]. To overcome this difficulty it is necessary to either always restrict ourselves to the higher even-order moments or linearize the exponent, i.e., take F^+ in form (1.4).

§4. In conclusion we shall consider the question of equilibrium solutions of the approximate equations. Unfortunately, rigorous proof of the H-theorem for an F^+ of form (1.4) is not possible, since F^+ and consequently F, as well, may be negative. However, we can hope that in most cases the coefficients of the expansion (1.4) will be sufficiently small and F will be negative only in the region of large values of the velocities, where the distribution function itself is small.

We consider the case of small deviations from equilibrium in a homogeneous space and restrict ourselves to analysis of (1.7), which is the simplest of the model kinetic equations providing the correct Prandtl number, with Pr = 2/3.

Multiplying both sides of (1.7) by ln F and integrating over the entire velocity space, we obtain after an obvious transformation of the right side

$$\frac{\partial H}{\partial t} = -\frac{1}{\tau} \int (F - F^+) \ln \frac{F}{F^+} d\xi + $$
$$+ \frac{1}{\tau} \int (F^+ - F) \ln F^+ d\xi,$$
$$H = \int F \ln d\xi. \tag{4.1}$$

In view of the smallness of S_i, we linearize $\ln F^+$ relative to S_i; in addition, we use the moment relations (1.3). We obtain

$$\frac{\partial H}{\partial t} = -\frac{1}{\tau} \int (F - F^+) \ln \frac{F}{F^+} d\xi -$$
$$- \frac{8}{45} \frac{S_1^2 + S_3^2 + S_3^2}{\rho (2RT)^3}. \tag{4.2}$$

According to (4.2), for sufficiently small deviations from equilibrium the Boltzmann function H decreases.

For arbitrary, not small deviations from equilibrium the expansion of $\ln F^+$ is not valid; consequently the proof of the H-theorem is difficult. However, the question of the uniqueness of the Maxwellian distribution for equilibrium conditions is solved uniquely if we turn to the moment conditions (1.3). For equilibrium we must have $F = F^+$; therefore on the left in (1.3) there will be zeros. Consequently, for example, for (1.7) we obtain $S_i = 0$, i.e., for equilibrium the Maxwellian distribution is the only possible one.

REFERENCES

1. P. L. Bhatnagar, E. P. Gross and M. Krook, "A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component systems," Phys. Rev., vol. 94, p. 511, 1954.

2. M. Krook, "Continuum equations in the dynamics of rarefied gases," J. Fluid Mech., vol. 6, no. 4, pp. 523-541, 1959.

3. M. N. Kogan, "On the equations of motion of a rarefied gas," PMM, vol. 22, no. 4, 1958.

4. M. N. Kogan, Rarefied Gasdynamics [in Russian], Nauka, Moscow, 1967.

5. L. H. Holway, "New statistical models in kinetic theory: methods of construction," Phys. Fluids, vol. 9, no. 9, pp. 1658-1673, 1966.

6. E. M. Shakhov, "On the approximate kinetic equations in rarefied gas theory," Izv. AN SSSR, MZhG [Fluid Dynamics], no. 1, 1968.

7. H. V. Grad, Communications on Pure and Appl. Math., vol. 2, no. 4, 1949.

8. A. M. Kogan, "Derivation of equations of the Grad type and analysis of their relaxational properties by the entropy maximization method," PMM, vol. 29, no. 1, 1965.

29 January 1968 Moscow