MODIFICATION OF THE LEES METHOD
IN CALCULATIONS OF HEAT FLUX
FROM A SPHERICAL PARTICLE
AT ARBITRARY KNUDSEN NUMBERS

A. A. Yushkanov[1] and S. A. Savkov[2]   UDC 533.72

Currently, different versions of moment methods including the Lees method and that of half-space moments are widely used to solve the problems of kinetic gas theory. A common feature of these methods is that the distribution function is sought as a sum of velocity polynomials, the coefficients of which can be determined by solving a set of moment equations. The latter are deduced by multiplying the kinetic equation by the corresponding polynomials and then integrating it over the velocity.

In the method of half-space moments the same set of discontinuous velocity functions is employed as polynomials in the distribution function and in the derivation of the moment equations. This makes the method logically closed and allows a more correct description of the character of distribution function changes due to the interaction of gas molecules with each other and with the aerosol particles involved. However, the correct description of gas behavior in a number of cases calls for too great a number of moments, which substantially complicates the solution of the problem and makes it simply impossible to solve sometimes.

In the Lees method the distribution function can also be expressed in terms of the discontinuous velocity polynomials. However, the moment equations are deduced using continuous functions. Some of these are chosen so that the corresponding moment equations could represent one of the conservation laws. The missing moments have to be given artificially. The fact that in a given method the conservation laws are satisfied automatically, allows one to obtain satisfactory results by taking the distribution function rather approximately. However, the real pattern of distribution function relaxation is substantially distorted because the information between the cones of particle influence, i.e., the mixing of distribution functions for molecules falling and reflected from the surface, can be transferred not only by a collision integral, which is typical of the method of half-space moments, but also artificially by multiplying this integral by a continuous velocity function. For the same reasons the Lees method does not allow a correct description of the influence of mass and heat fluxes throughout the cones, which, for a number of problems, is of its particular interest.

The present paper reports a procedure (the reverse of the Lees method) of solving a kinetic equation which combines the advantages of both the half-space moments and the Lees methods, i.e., the distribution function is expressed in terms of the continuous velocity functions used in the direct method to derive the moment equations and the kinetic equation is multiplied by the corresponding discontinuous ones. First, this approach makes it possible to decrease the number of moments and moment equations necessary to satisfy the conservation laws automatically. Second, it allows a correct description of the character of distribution function changes due to the interaction of gas molecules with each other and with the particle surface.

For example, consider now the problem of calculating the heat flux from a spherical particle with radius R uniformly heated to a temperature T_ω in gas in which a constant temperature T_0 is maintained at infinity. Assume that the temperature difference $\Delta T = T_\omega - T_0$ is small enough to linearize the problem.

At each point of space the particle is connected with three invariant "cones" involving the rate of molecules flying toward the particle, from it, and past it (regions I–III in Fig. 1). The cone boundaries are
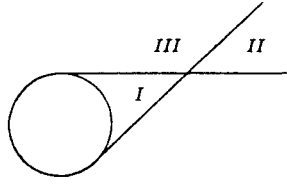

Fig. 1

crossed by gas molecules only upon collisions with each other. Since regions I and III merge when this and similar problems are solved by the conventional Lees method (see, e.g., [1–3]), it is natural to start our considerations with this case.

Introduce a spherical system of coordinates with their origin at the particle center. The state of the gas around the particle is described by the kinetic Boltzmann equation [4]:

$$\mathbf{V} \cdot \nabla f = J_{st} \tag{1}$$

($\mathbf{V}$ is the eigenvelocity of gas molecules; f is the velocity distribution function of the molecules; J_{st} is the collision integral).

Further, we restrict ourselves to the BGK-model of collision integrals [5]:

$$J_{st} = \frac{1}{\tau}(f_{eq} - f)\left(\frac{2kT}{m}\right)^{1/2}.$$

Here

$$\tau = \frac{3\lambda}{\sqrt{\pi}} = \frac{\ae}{5n}\left(\frac{8m}{k^3 T}\right)^{1/2}; \quad f_{eq} = n\left(\frac{m}{2\pi kT}\right)^{3/2}\exp\left(-\frac{mv^2}{2kT}\right)$$

is the local equilibrium distribution function; λ is the mean free path of the gas molecules; $\ae$ is its heat conductivity.

Due to the problem linearity, there is a rather small difference between the distribution function and the distribution at infinity:

$$f = f_0(1 + \Phi), \quad f_0 = n_0\left(\frac{m}{2\pi kT_0}\right)^{3/2}\exp\left(-\frac{mv^2}{2kT_0}\right)$$

(m and n are the mass and concentration of the gas molecules; k is the Boltzmann constant).

Thus, the problem reduces to the determination of the Φ correction for the equilibrium distribution function f_0.

The conventional Lees method uses a two-flow distribution function:

$$\Phi^{\pm} = a_1^{\pm} + C^2 a_2^{\pm},$$

where the "+" sign refers to the distribution function for molecules flying from the particle, the velocity vector of which is within region II (Fig. 1); the "−" sign refers to molecules whose velocity vector is beyond the given region. For convenience, let us introduce the auxiliary function:

$$\eta^+ = \begin{cases} 1 & \text{at} \quad C_r < C\sqrt{1 - (R/r)^2}, \\ 0 & \text{at} \quad C_r > C\sqrt{1 - (R/r)^2}, \end{cases} \quad \mathbf{C} = \mathbf{V}\sqrt{m/2kT}.$$

Thus the distribution function to be determined can be written in the form

$$\Phi = \Phi^+\eta^+ + \Phi^-(1 - \eta^+). \tag{2}$$

The coefficients $a_i^{\pm}$ can be determined from a set of moment equations obtained by multiplying the kinetic equation by 1, C_r, C^2, $C_r C^2$ and integrating it over the velocity. Accordingly, in the reverse procedure

the distribution function must be sought in the form

$$\Phi = a_1 + C_r a_2 + C^2 a_3 + C_r C^2 a_4. \tag{3}$$

The moment equations must be derived using η^+, $(1 - \eta^+)$, $C^2\eta^+$, and $C^2(1 - \eta^+)$.

Multiplying the kinetic equation involving distribution function (3) by the above moments and integrating it over the velocity we obtain the following set of differential equations:

$$\pm \frac{1}{\sqrt{\pi}} \frac{R^2}{r^2} \frac{d}{dr}\left(\frac{1}{2} a_1 + a_3\right) + \left(1 \mp \left(1 - \frac{R^2}{r^2}\right)^{3/2}\right) \frac{d}{dr}\left(\frac{1}{4} a_2 + \frac{5}{8} a_4\right)$$

$$+ \frac{1}{r}\left(2 \mp 3\left(1 - \frac{R^2}{r^2}\right)^{1/2} \pm \left(1 - \frac{R^2}{r^2}\right)^{3/2}\right)\left(\frac{1}{4} a_2 + \frac{5}{8} a_4\right) = \pm \frac{1}{\sqrt{\pi}} \frac{R^2}{r^2} \frac{a_4}{4\tau},$$

$$\pm \frac{1}{\sqrt{\pi}} \frac{R^2}{r^2} \frac{d}{dr}(a_1 + 3a_3) + \left(1 \mp \left(1 - \frac{R^2}{r^2}\right)^{3/2}\right) \frac{d}{dr}\left(\frac{5}{4} a_2 + \frac{35}{16} a_4\right) \tag{4}$$

$$+ \frac{1}{r}\left(2 \mp 3\left(1 - \frac{R^2}{r^2}\right)^{1/2} \pm \left(1 - \frac{R^2}{r^2}\right)^{3/2}\right)\left(\frac{5}{4} a_2 + \frac{35}{16} a_4\right) = \mp \frac{1}{\sqrt{\pi}} \frac{R^2}{r^2} \frac{a_4}{2\tau}.$$

The solution decaying at infinity is of the form

$$a_1 = K\left(-\frac{5}{2} \frac{R^2}{r\tau} - \frac{5}{4}\sqrt{\pi}\left(\frac{1}{3}\left(1 - \frac{R^2}{r^2}\right)^{\frac{3}{2}} - 2\left(1 - \frac{R^2}{r^2}\right)^{\frac{1}{2}} + 2\mathrm{Ln}\left(1 + \left(1 - \frac{R^2}{r^2}\right)^{\frac{1}{2}}\right) + \frac{5}{3} - 2\mathrm{Ln}\,2\right)\right), \tag{5}$$

$$a_2 = -\frac{5}{2} \frac{R^2}{r^2} K, \quad a_3 = -\frac{1}{2} a_1 - \frac{1}{4} \frac{R^2}{r\tau} K, \quad a_4 = \frac{R^2}{r^2} K.$$

The integration constant K can be found through the condition of gas molecule reflection from the particle surface:

$$f^+ = \Omega f^- \qquad \text{at} \quad r = R. \tag{6}$$

In this case, f^- and f^+ are the distribution functions for molecules falling and reflected from the particle; Ω is the operator describing the reflection law.

Condition (6) must also be written in moment form. To do this, it must be introduced into kinetic equation (1). Then, the derivation of moment equations (4) will automatically give the corresponding moment boundary conditions. Formally, this means (see, e.g., [6]) that equality (6) must be written in the form $C_r f^+ = C_r \Omega f^-$, multiplied successively by η^+ and $C^2\eta^+$, and integrated over the velocity. As a result, we get a set of moment conditions on the particle surface:

$$\int \eta^+ C_r (a_1 + C_r a_2 + C^2 a_3 + C_r C^2 a_4) \exp(-C^2)\, d\mathbf{C} = \int \eta^+ C_r \Omega f^-\, d\mathbf{C},$$

$$\int \eta^+ C^2 C_r (a_1 + C_r a_2 + C^2 a_3 + C_r C^2 a_4) \exp(-C^2)\, d\mathbf{C} = \int \eta^+ C^2 C_r \Omega f^-\, d\mathbf{C}.$$

Note that the arbitrary law of gas molecule reflection from the particle surface can be considered only by using discontinuous velocity functions to obtain the moment equations. Thus, the conventional Lees method considers only the conditions of specular-diffusion reflection.

In the analysis we restrict ourselves to the law of a purely diffusive reflection:

$$\Omega f^- = f_\omega \quad \left(f_\omega = f_0\left(1 + \frac{\Delta n}{n_0} + \left(C^2 - \frac{3}{2}\right)\frac{\Delta T}{T_0}\right)\right).$$

In this case the conditions on the particle surface take the form

$$\frac{1}{\sqrt{\pi}}\left(\frac{1}{2} a_1 + a_3\right) + \left(\frac{1}{4} a_2 + \frac{5}{8} a_4\right) = \frac{1}{4\sqrt{\pi}}\left(2\frac{\Delta n}{n_0} + \frac{\Delta T}{T_0}\right), \tag{7}$$

$$\frac{1}{\sqrt{\pi}}(a_1 + 3a_3) + \left(\frac{5}{8} a_2 + \frac{35}{16} a_4\right) = \frac{1}{\sqrt{\pi}}\left(\frac{\Delta n}{n_0} + \frac{3}{2}\frac{\Delta T}{T_0}\right).$$

Substituting (5) into (7) and solving the set of equations with respect to K, we arrive at

$$K = \frac{1}{\frac{R}{\tau} + \frac{5}{4}\sqrt{\pi}\left(\frac{4}{3} - \ln 2\right)}\frac{\Delta T}{T_0}.$$

The radial component of the heat flux can be determined from the relation

$$q_r = \int f \frac{mV^2}{2} V_r \, d\mathbf{V} = n\left(\frac{2k^3T^3}{m}\right)^{1/2} Q_r, \tag{8}$$

where

$$Q_r = \frac{1}{\frac{4}{5}\frac{R}{\tau} + \sqrt{\pi}\left(\frac{4}{3} - \ln 2\right)}\frac{R^2}{r^2}\frac{\Delta T}{T_0}.$$

The direct Lees method for distribution function (2) gives

$$Q_r = \frac{1}{\frac{4}{5}\frac{R}{\tau} + \sqrt{\pi}}\frac{R^2}{r^2}\frac{\Delta T}{T_0}. \tag{9}$$

For a large particle ($R/\tau \to \infty$) the results of direct and reverse methods coincide and lead to the well-known gas-dynamic solution [7]

$$Q_r = \frac{5}{4}\tau\frac{R}{r^2}\Delta T, \quad q_r = æ\frac{R}{r^2}\Delta T. \tag{10}$$

For a moderately large particle the heat flux can be represented as

$$q_r = æ\frac{R}{r^2}\Delta T \frac{1}{1 + C_t\lambda/R}. \tag{11}$$

Here C_t is the coefficient of the temperature jump, which obeys the relation

$$\delta T = \frac{\lambda}{R} C_t \frac{dT}{dr}.$$

Comparing (8) and (11) we obtain $C_t = (5/4)(\tau/\lambda)\sqrt{\pi}(4/3 - \ln 2) = 2.401$, which differs by 9% from the exact solution 2.19 [8], calculated for this model of the collision integral, whereas for the direct method $C_t = 3.75$.

In the free molecular regime ($R/\tau \to 0$) the reverse method yields a heat flux value that is 1.5 times as large as that of the direct one. This can be caused by the insufficient number of retained moments in both the direct and reverse methods.

Of particular interest is a consideration of all three influence cones. In this case, the correction for the distribution function must be sought in the form

$$\Phi = \left(\frac{3}{2} - C^2\right)a_1 + \left(\frac{5}{2} - C^2\right)\left(C_r a_2 + C_r^2 a_3\right) + \left(\frac{7}{2} - C^2\right)C_r^3 a_4. \tag{12}$$

The moment equations must be obtained using

$$(2 - C^2)\eta^{\pm}, \quad \left(\frac{5}{2} - C^2\right)(1 - \eta^+ - \eta^-) \quad \text{и} \quad C_r\left(\frac{5}{2} - C^2\right)(1 - \eta^+ - \eta^-).$$

In this case, η^- is an auxiliary function describing molecules flying to the particle, the velocity vector of which lies within region I (Fig. 1):

$$\eta^- = \begin{cases} 1 & \text{at} \quad C_r < -C\sqrt{1 - (R/r)^2}, \\ 0 & \text{at} \quad C_r > -C\sqrt{1 - (R/r)^2}. \end{cases}$$
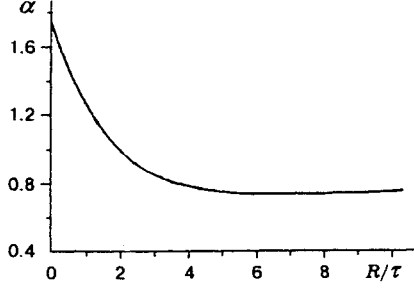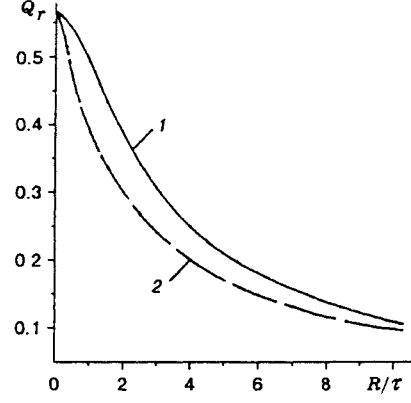
Fig. 2

Fig. 3

Multiplying the kinetic equation by the above moments and integrating it over the velocity, we obtain the following set of differential equations:

$$
\pm \frac{1}{\sqrt{\pi}} \frac{R^2}{r^2} \frac{da_1}{dr} + \frac{5}{8}\left(1 - \left(1 - \frac{R^2}{r^2}\right)^{3/2}\right)\frac{da_2}{dr} \pm \frac{7}{4\sqrt{\pi}} \frac{R^2}{r^2}\left(2 - \frac{R^2}{r^2}\right)\frac{da_3}{dr}
$$

$$
+ \frac{21}{16}\left(1 - \left(1 - \frac{R^2}{r^2}\right)^{5/2}\right)\frac{da_4}{dr} + \frac{5}{8}\left(2 - 3\left(1 - \frac{R^2}{r^2}\right)^{1/2} - \left(1 - \frac{R^2}{r^2}\right)^{3/2}\right)\frac{a_2}{r}
$$

$$
\pm \frac{7}{2\sqrt{\pi}} \frac{R^4}{r^4} \frac{a_3}{r} + \frac{63}{16}\left(\frac{2}{3} - \frac{5}{3}\left(1 - \frac{R^2}{r^2}\right)^{3/2} - \left(1 - \frac{R^2}{r^2}\right)^{5/2}\right)\frac{a_4}{r}
$$

$$
= \frac{1}{\tau}\frac{R^2}{r^2}\left(\mp \frac{a_2}{\sqrt{\pi}} - \frac{5}{8}\left(1 - \frac{R^2}{r^2}\right)^{1/2} a_3 \mp \frac{5}{4}\left(2 - \frac{R^2}{r^2}\right)\frac{a_4}{\sqrt{\pi}}\right), \tag{13}
$$

$$
\frac{5}{4}\left(1 - \frac{R^2}{r^2}\right)^{3/2}\frac{da_2}{dr} + \frac{5}{4}\left(3\left(1 - \frac{R^2}{r^2}\right)^{1/2} - \left(1 - \frac{R^2}{r^2}\right)^{3/2}\right)\frac{a_2}{r}
$$

$$
+ \frac{21}{8}\left(1 - \frac{R^2}{r^2}\right)^{5/2}\frac{da_4}{dr} + \frac{63}{8}\left(\frac{5}{3}\left(1 - \frac{R^2}{r^2}\right)^{3/2} - \left(1 - \frac{R^2}{r^2}\right)^{5/2}\right)\frac{a_4}{r} = \frac{1}{\tau}\frac{R^2}{r^2}\frac{5}{8}\left(1 - \frac{R^2}{r^2}\right)^{1/2} a_3,
$$

$$
\frac{5}{4}\frac{da_1}{dr} + \frac{27}{8}\left(1 - \frac{R^2}{r^2}\right)\frac{da_3}{dr} + \frac{9}{2}\left(1 + \frac{3}{2}\frac{R^2}{r^2}\right)\frac{a_3}{r} = -\frac{5}{4}\frac{a_2}{\tau} - \left(1 - \frac{R^2}{r^2}\right)\frac{21}{8}\frac{a_4}{\tau}.
$$

For this system the moment boundary condition on the particle surface is of the form

$$
\frac{a_1}{\sqrt{\pi}} + \frac{5}{8}a_2 + \frac{7}{4}\frac{a_3}{\sqrt{\pi}} + \frac{21}{16}a_4 = -\frac{1}{\sqrt{\pi}}\frac{\Delta T}{T_0}. \tag{14}
$$

The set of differential equations (13) with condition (14) on the particle surface has been solved numerically. The initial values of a_i have been chosen by the shooting method to cut off a solution exponentially increasing at infinity. This gives the expression for the heat flux:

$$
Q_r = \frac{1}{\frac{4}{5}\frac{R}{\tau} + \alpha}\frac{R^2}{r^2}\frac{\Delta T}{T_0}. \tag{15}
$$

The dependence of parameter α on the particle size is depicted in Fig. 2. For comparison, Fig. 3 shows the values of the dimensionless heat flux Q_r calculated for distribution function (12) (curve 1) and the data of the conventional Lees method (curve 2).

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For a small particle ($R/\tau \to 0$) the α value moves toward $\sqrt{\pi}$, which coincides with the results of the direct method for distribution function (2).

In the gas-dynamic regime ($R/\tau \to \infty$), formula (15) leads to (10). In this limit $\alpha = \sqrt{\pi}/2$. Accordingly, $C_t = 1.875$, which coincides with the well-known Maxwell value and differs by 14% from the exact value.

The data obtained testify to a sufficient reliability of the method and offer hope that it could be used for solving more complex problems.

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