A MATHEMATICAL EXPERIMENT FOR COMPUTING TRANSPORT COEFFICIENTS

AERODYNAMICS

1968

SovietRxiv

Abstract

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UDC 533.6.011.8

AERODYNAMICS

V. I. VLASOV, S. L. GORELOV, M. N. KOGAN

A MATHEMATICAL EXPERIMENT FOR COMPUTING TRANSPORT COEFFICIENTS

(Presented by Academician A. A. Dorodnitsyn, 13 VII 1967)

Macroscopic equations describing the motion of a medium under various conditions can be obtained phenomenologically (^{1,2}). In particular, the relation between the stress tensor and heat flux and the corresponding gradients of hydrodynamic quantities, necessary for deriving equations for flows close to equilibrium (equations of the Navier–Stokes type), can be found by the methods of the thermodynamics of irreversible processes. However, phenomenological theories do not make it possible to find the transport coefficients; they can be obtained from experiment, but often, especially at high temperatures, carrying out such experiments is difficult.

To determine transport coefficients, kinetic theory (the Boltzmann equation) is used. For monatomic gases this theory gives fairly simple expressions for the transport coefficients (^{3,4}). For real gases, if the internal degrees of freedom are treated quantum-mechanically (^{5,6}), the probabilities of direct and reverse transitions are equal, and the collision integral in the Boltzmann equation assumes a symmetric form convenient for investigation. With such an approach a number of interesting results have been obtained; however, to compute transport coefficients it is necessary to know the differential collision cross sections, which constitutes a difficult independent problem. On the other hand, the process of excitation of the internal degrees of freedom of molecules in collisions can be described within the framework of classical mechanics (^{9}); in this case the interaction of atoms both within a molecule and between molecules can be approximated by laws of the Morse type or by others with a small number of constants determined from experiment. However, with such a description the direct and reverse processes are not equivalent and the collision integral becomes substantially more complicated, which makes solving the Boltzmann equation difficult.

In the present work an example is given of carrying out a mathematical experiment, for the realization of which only knowledge of the law of interaction of the molecules is required. Although the Monte Carlo method considered is equivalent to solving the Boltzmann equation, it does not require writing out the equation itself or investigating the properties of the collision integral. Monte

Carlo methods have also been applied previously to solving the Boltzmann equation (^{5,7,8}), but they do not make it possible to obtain transport coefficients, since in states close to equilibrium the transport processes are determined by small deviations from equilibrium, so that errors arising in the calculation of the equilibrium part, which is inessential for transport properties, become decisive.

To illustrate the method, let us consider the simplest case of a monatomic gas consisting of spherical molecules whose cross section σ varies inversely proportional to their relative speed g:

$$\sigma = \sigma_0/g, \qquad \sigma_0 = \text{const.} \tag{1}$$

Suppose we have a flow close to equilibrium. From phenomenological considerations one can write expressions for the stress tensor and heat flux:

$$P_{ij} = p\delta_{ij} - \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - {}^2/_3\delta_{ij}\frac{\partial u_k}{\partial x_k}\right), \qquad q_i = -\lambda\frac{\partial T}{\partial x_i}. \tag{2}$$

The problem consists in finding μ and λ. For flows close to equilibrium, the distribution function of the molecular velocities $\vec{\xi}$ can be written in the form

$$f(x,\vec{\xi}) = f_0(x,\vec{\xi})[1+\varphi(x,\vec{\xi})], \qquad f_0 = n(m/2k\pi T)^{3/2}\exp(-m\vec{\xi}^{\,2}/2kT), \tag{3}$$

where f_0 is the locally equilibrium function, and φ is a small correction, usually determined by solving the Boltzmann equation by the Chapman–Enskog method [3]. The expressions for the coefficients μ and λ for such molecules are known:

$$\mu = 2kT/\sigma_0, \qquad \lambda = 15k^2T/2m\sigma_0, \tag{4}$$

where k is Boltzmann' s constant.

Let us now determine these coefficients by means of a mathematical experiment. Consider, for example, the coefficient of thermal conductivity. Suppose we have a stationary gas ($u_i = 0$) with a prescribed constant temperature gradient along the x-axis. According to the Navier–Stokes equations, $q_x = \text{const}$ and $p = nkT = \text{const}$. Suppose we are interested in the value of λ at the temperature T_0. Choose the origin of coordinates in the plane $T = T_0$ and consider a layer $\pm d/2$ of thickness of the order of the mean free path l (we note that μ and λ are of order l). Neglecting quantities of order l^2, the distribution function in the layer can be written in the form

$$f(x,\vec{\xi}) = f_{00}\left[1 + x\left(m\vec{\xi}^{\,2}/2kT_0 - {}^5/_2\right)\partial\ln T/\partial x + \varphi(0,\vec{\xi})\right], \tag{5}$$

Fig. 1

Figure 1: Fig. 1

where $f_{00} = f_0(0, \vec{\xi})$.

If the function $\varphi(0, \vec{\xi})$ is known, then λ is found from the relation:

$$-\lambda(T_0)\frac{\partial T}{\partial x} = q_x = \int \frac{m\vec{\xi}^{\,2}}{2}\,\xi_x f(0, \vec{\xi})\, d\vec{\xi} = \int \frac{m\vec{\xi}^{\,2}}{2}\,\xi_x f_{00}\varphi(0, \vec{\xi})\, d\vec{\xi}. \tag{6}$$

Suppose that throughout the layer the molecules are distributed with density f_{00}, and suppose that a test molecule traverses the layer along some trajectory L_i. Let us find the probability w_0 that the molecule will pass along this trajectory. The probability that the molecule flies out from one of the boundaries with velocity $\vec{\xi}$ is equal to $f_{00}(\vec{\xi})$; the probability of traversing the given distance r is $p_0(r, \vec{\xi})$ (the probability density of the free path r, corresponding to the function $f_{00}(\vec{\xi})$); the probability of collision with a molecule flying with velocity $\vec{\xi}_1$ is proportional to $g\sigma(g)f_{00}(\vec{\xi}_1)$, where $g = |\vec{\xi} - \vec{\xi}_1|$ is the relative velocity, etc. Obviously, the probability for the molecule to traverse the layer along the given trajectory is equal to (since the events are independent)

$$w_0 = f_{00}(\vec{\xi})p_0(r, \vec{\xi})g\sigma(g)f_{00}(\vec{\xi}_1)\ldots \tag{7}$$

Now suppose that throughout the layer the molecules are distributed with the function $f(x, \vec{\xi})$. Then the probability w for the molecule to traverse the same trajectory L_i is equal to:

$$w = f(x, \vec{\xi})p(r, \vec{\xi})g\sigma(g)f(x, \vec{\xi}_1)\ldots \tag{8}$$

If the heat flux carried by a molecule along the given trajectory L_i is denoted by Δq_i, then the heat flux, averaged over a large number of

the trajectories N for the function f_{00}, to within random fluctuations, is equal to

$$\frac{1}{N}\sum_{i=1}^{N}\Delta q_i = 0. \tag{9}$$

Among the set of all trajectories for the function f, each trajectory L_i occurs w/w_0 times more often than for f_{00}; therefore, to obtain the heat flux q_x, the heat flux carried along each trajectory in accordance with f_{00} must be multiplied by w_i/w_{0i}:

Fig. 1

$$q_x = \frac{1}{N}\sum_{i=1}^{N} \Delta q_i \, \frac{w_i}{w_{0i}}. \tag{10}$$

To eliminate the errors introduced by f_{00}, one must subtract (9):

$$q_x = \frac{1}{N}\sum_{i=1}^{N} \left(\frac{w_i}{w_{0i}} - 1\right) \Delta q_i. \tag{11}$$

Let us consider w/w_0:

$$\frac{w}{w_0} = \frac{f(x,\vec{\xi})}{f_{00}(\vec{\xi})} \, \frac{p(r,\vec{\xi})}{p_0(r,\vec{\xi})} \, \frac{f(x,\vec{\xi}_1)}{f_{00}(\vec{\xi}_1)} \cdots . \tag{12}$$

Linearizing this expression and noting that $\varphi(0,\vec{\xi})$ can, according to (6), be represented as $\bar{\varphi}(\vec{\xi})\,\partial T/\partial x$, we obtain

$$w/w_0 = 1 + A\,\partial T/\partial x, \tag{13}$$

where A is the sum of the coefficients of $\partial T/\partial x$ in the factors of product (12). (We note that only one unknown function $\varphi(\vec{\xi})$ enters these coefficients.)

Substituting (13) into (11) and canceling by $\partial T/\partial x$, we obtain (taking (6) into account)

$$\lambda(T_0) = -\frac{1}{N}\sum_{i=1}^{N} A_i \Delta q_i. \tag{14}$$

We find the function $\bar{\varphi}(\vec{\xi})$ by the method of successive approximations. Write (6) in the form of a sum:

$$q_x = \frac{\partial T}{\partial x} \sum_{ijk} \frac{m\xi_{ijk}^2}{2} \, \xi_{xi} f_{00}(\xi_{ijk}) \bar{\varphi}(\xi_{iju}) \, \Delta\xi_{ijk} = \sum_{ijk} q_{xiji}. \tag{15}$$

Then

$$\bar{\varphi}(\xi_{ijk}) = 2q_{xijk} \left[m\xi_{ijk}^2 \xi_{xi} f_{00}(\xi_{ijk}) \Delta\xi_{ijk} \partial T/\partial x\right]^{-1}. \tag{16}$$

For the initial approximation we set, for example, $\varphi = 0$. The calculation is continued until $q^{(n)} = q_x^{(n-1)}$ to the prescribed accuracy (where the superscript denotes the iteration number).

Fig. 2

Figure 2: Fig. 2

In the same way we also obtain the viscosity coefficient μ. Figure 1 presents several iterations in the calculation of the heat flux q (normalized to the theoretical value (4)). As the initial approximation, $\varphi = \varphi_{\text{theor}}$ was chosen, obtained from the solution of the Boltzmann equation by the Chapman-Enskog method (^{3,4}).

Fig. 2

Figure 2 presents several iterations in the calculation of the viscosity coefficient, normalized to the theoretical value. As the initial approximation, $\varphi = 0$ was chosen.

As can be seen from these graphs, the method converges and is stable. The determination of the transport coefficients has been reduced to the calculation of elementary mechanical processes. In the case of diatomic molecules, much more machine time will be required, since at each collision it will be necessary to solve the problem of the collision of four bodies.

Received
11 VII 1967

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