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## MOLECULAR-KINETIC GENERALIZATION OF THE HEAT-TRANSFER EQUATION

V. L. Kolpashchikov and A. A. Baranov

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Starting from microscopic theory, the authors generalize the heat-conduction equation to the case where the gradients in molecular transport velocities vary appreciably over a mean free path.

To obtain a hydrodynamic description of a rarefied gas as a continuous medium one usually begins from the Boltzmann equations and uses the method of successive approximations to derive the equations of an ideal compressible fluid, the Navier-Stokes equations, the Barnett equations and the super-Barnett equations. However, in the work of Predvoditelev [1, 2] and Truesdell [3, 4] it was noted that equations of higher order than the Navier-Stokes equations still give a poor description of the behavior of a rarefied gas (at least no better than the Navier-Stokes equations). Several different approaches from this basis have been suggested. For example, in the work of Vallander [5, 6] a method was suggested for generalizing the Boltzmann equation, with subsequent transition to equations of hydrodynamic type. Several modifications of the Navier-Stokes equations have been proposed by Ladyzhenskaya [7].

Predvoditelev [1] generalized the Navier-Stokes hydrodynamic equations, using the Maxwell method [8] and starting from the molecular-kinetic basis of the hydrodynamic equations. The Maxwell approach to deriving the equations of motion of a viscous fluid from the kinetic theory of gases, in contrast with the method of deriving the hydrodynamic equations from the Boltzmann equations, as developed in the work of Enskog and Chapman [9], does not require knowledge of the distribution function and is based on the following assumption.

The transport velocities of the two colliding molecules are equal; this means that a continuum in motion has a filamentary structure, i.e., the minimum dimensions of the jets correspond to the mean distance between molecules. The first to give attention to the possibility of generalizing this hypothesis was Predvoditelev [1], who stressed that the physical situation corresponding to Maxwell's hypothesis will not hold for motion of a continuum at large enough speed near a wall or when vortices are generated. In addition, the breakdown of the Maxwell hypothesis that the molecular transport speeds are equal will be evident in motion of a rarefied gas, when the flow dimensions are comparable with the average distance between molecules. The Predvoditelev hypothesis was further developed in regard to generalization of the equations of hydrodynamics in the work of Bubnov [10, 11].

In the present paper the concept of work [1] is used to derive a generalized heat-conduction equation for a rarefied gas, when the gradients of the transport speeds vary appreciably over a molecular mean free path.

### 1. Derivation of the Basic Equation

To derive a generalized heat-conduction equation we begin from the energy equation, obtained from microscopic theory [12]:

$$3\rho \frac{Dq}{Dt} = - \frac{\partial}{\partial x} \rho (\bar{\xi}^3 + \bar{\xi}\bar{\eta}^2 + \bar{\xi}\bar{\zeta}^2) - \frac{\partial}{\partial y} \rho (\bar{\eta}^3 + \bar{\xi}\bar{\eta}^2 + \bar{\eta}\bar{\zeta}^2)$$

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$$\begin{aligned}
& -\frac{\partial}{\partial z} \rho (\bar{\xi}^3 + \bar{\xi}\bar{\xi}^2 + \bar{\xi}\eta^2) - 2\rho \left[ \left( \bar{\xi}^2 \frac{\partial u}{\partial x} + \bar{\xi}\eta \frac{\partial u}{\partial y} + \bar{\xi}\zeta \frac{\partial u}{\partial z} \right) \right. \\
& \left. + \left( \bar{\xi}\eta \frac{\partial v}{\partial x} + \bar{\eta}^2 \frac{\partial v}{\partial y} + \bar{\eta}\zeta \frac{\partial v}{\partial z} \right) + \left( \bar{\xi}\zeta \frac{\partial w}{\partial x} + \bar{\xi}\eta \frac{\partial w}{\partial y} + \bar{\xi}^2 \frac{\partial w}{\partial z} \right) \right] + \Delta (u_0^2 + v_0^2 + w_0^2), \quad (1)
\end{aligned}$$

where  $u$ ,  $v$ , and  $w$  are the molecular velocity components, describing an ordered motion;  $\xi$ ,  $\eta$ ,  $\zeta$  are the molecular velocity components describing a random motion, such that the total speed of a molecule is

$$V_x = u + \xi, \quad V_y = v + \eta, \quad V_z = w + \zeta; \quad (2)$$

the quantities  $u_0$ ,  $v_0$ ,  $w_0$  are velocity components for an element of hydrodynamic volume;  $\Delta f$  is the variation in the quantity  $f$ , due to molecular collisions; and the quantity  $q$  equals

$$q = \frac{1}{3} (\bar{\xi}^2 + \bar{\eta}^2 + \bar{\zeta}^2). \quad (3)$$

Here and below the bar signifies a statistical average. To calculate the mean value of  $\xi^3$ , following [13], we shall find the quantity

$$B_3(\xi^3) = 2 \int_0^\infty \int_0^{2\pi} (V'_{1x}{}^3 - V_{1x}^3) g b d b d \epsilon, \quad (4)$$

where the velocity after the collision, according to [13], is

$$V'_{1x} = V_{1x} + (V_{2x} - V_{1x}) \cos^2 \theta + \frac{g^2 - (V_{2x} - V_{1x})^2}{g^2} \sin \theta \cos \theta \cos \epsilon. \quad (5)$$

Here

$$g^2 = (V_{2x} - V_{1x})^2 + (V_{2y} - V_{1y})^2 + (V_{2z} - V_{1z})^2. \quad (6)$$

Then from Eq. (4) it is easy to obtain

$$\begin{aligned}
\int_0^\infty \int_0^{2\pi} (V'_{1x}{}^3 - V_{1x}^3) g b d b d \epsilon &= \sqrt{\frac{k}{2m}} \left\{ \frac{1}{2} (A_1 - A_2 - A_3) (V_{2x} - V_{1x})^3 \right. \\
&+ \frac{3}{2} V_{1x} (V_{2x} - V_{1x})^2 (A_1 - A_2) + \frac{3}{4} A_3 [g^2 - (V_{2x} - V_{1x})^2] \\
&\left. + \frac{3}{4} A_2 V_{1x} [g^2 - (V_{2x} - V_{1x})^2] + \frac{3}{2} A_1 V_{1x}^2 (V_{2x} - V_{1x}) \right\}, \quad (7)
\end{aligned}$$

where  $m$  is the particle mass, and  $k$  is some constant; the following notation is used [13]:

$$A_1 = 4\pi \int_0^\infty \alpha \cos^2 \theta d\alpha, \quad (8)$$

$$A_2 = \pi \int_0^\infty \alpha \sin^2 2\theta d\alpha, \quad (9)$$

$$A_3 = \pi \int_0^\infty \alpha \sin^2 2\theta \cos^2 \theta d\alpha. \quad (10)$$

Using Eqs. (4) and (7), we easily find the expression

$$\begin{aligned}
B_3(\xi^3) &= 2 \sqrt{\frac{k}{2m^3}} \rho^2 \left\{ \frac{1}{2} (A_1 - A_2 - A_3) [(u_2 - u_1)^3 + 6\bar{\xi}^2 (u_2 - u_1)] \right. \\
&+ \frac{3}{2} (A_1 - A_2) [u_1 (u_2 - u_1)^2 + 2u_1 \bar{\xi}^2 - 2\bar{\xi}^2 (u_2 - u_1) + \bar{\xi}^3] \\
&+ \frac{3}{4} A_3 [(u_2 - u_1) (v_2 - v_1) + 2\bar{\eta}^2 (u_2 - u_1) + (u_2 - u_1) (w_2 - w_1)^2 \\
&\quad + 2\bar{\zeta}^2 (u_2 - u_1) + 4\bar{\xi}\bar{\eta} (v_2 - v_1) + 4\bar{\xi}\bar{\zeta} (w_2 - w_1)] \\
&\left. + \frac{3}{4} A_2 [u_1 (v_2 - v_1)^2 + 2u_1 \bar{\eta}^2 + u_1 (w_2 - w_1)^2 + 2\bar{\zeta}^2 u_1 \right]
\end{aligned}$$

$$\begin{aligned}
& -2\bar{\xi}\bar{\eta}(v_2 - v_1) - 2\bar{\xi}\bar{\zeta}(w_2 - w_1) + \bar{\xi}\eta^2 + \bar{\xi}\zeta^2] \\
& + \frac{3}{2} A_1 [u_1^2(u_2 - u_1) - 2\bar{\xi}^2 u_1 + \bar{\xi}^2(u_2 - u_1) - \bar{\xi}^3] \}. \quad (11)
\end{aligned}$$

In Eq. (11) we now drop terms of higher order of smallness and also the terms  $(u_2 - u_1)^2$ ,  $(u_2 - u_1)^3$  and so on; in addition, we shall assume that

$$\bar{\xi}^2 = \bar{\eta}^2 = \bar{\zeta}^2 = \frac{p}{\rho}, \quad \bar{\xi}\bar{\eta} = \bar{\xi}\bar{\zeta} = \bar{\zeta}\bar{\eta} = 0. \quad (12)$$

Then, taking account of Eq. (11), we can simplify appreciably to obtain

$$\begin{aligned}
B_5(\bar{\xi}^3) &= 2 \sqrt{\frac{k}{2m^5}} \rho^2 \left\{ -\frac{3}{2} A_2 \bar{\xi}^3 + \frac{3}{4} A_2 \bar{\xi}\eta^2 \right. \\
& \left. + \frac{3}{4} A_2 \bar{\xi}\zeta^2 + \frac{3}{2} A_1 (u_2 - u_1) \frac{p}{\rho} + \frac{3}{2} A_1 u_1^2 (u_2 - u_1) \right\}. \quad (13)
\end{aligned}$$

In a similar way we can derive an expression for

$$\begin{aligned}
B_5(\bar{\xi}\eta^2) &= 2 \sqrt{\frac{k}{2m^5}} \rho^2 \left\{ \frac{1}{4} A_2 \bar{\xi}^3 - 2A_2 \bar{\xi}\eta^2 + \frac{1}{4} A_2 \bar{\xi}\zeta^2 \right. \\
& \left. + \left( \frac{1}{2} A_1 + A_3 \right) (u_2 - u_1) \frac{p}{\rho} + \frac{1}{2} A_1 v_1^2 (u_2 - u_1) + A_1 u_1 v_1 (v_2 - v_1) \right\} \quad (14)
\end{aligned}$$

and, correspondingly, for

$$\begin{aligned}
B_5(\bar{\xi}\zeta^2) &= 2 \sqrt{\frac{k}{2m^5}} \rho^2 \left\{ \frac{1}{4} A_2 \bar{\xi}^3 + \frac{1}{4} A_2 \bar{\xi}\eta^2 - 2A_2 \bar{\xi}\zeta^2 \right. \\
& \left. + \frac{1}{2} (A_1 + A_3) (u_2 - u_1) \frac{p}{\rho} + \frac{1}{2} A_1 w_1^2 (u_2 - u_1) + A_1 u_1 w_1 (w_2 - w_1) \right\}. \quad (15)
\end{aligned}$$

Taking into account Eqs. (13), (14), and (15), we find directly that

$$\begin{aligned}
B_5(\bar{\xi}^3 + \bar{\xi}\eta^2 + \bar{\xi}\zeta^2) &= -2A_2 \sqrt{\frac{k}{2m^5}} \rho^2 \left\{ \bar{\xi}^3 + \bar{\xi}\eta^2 + \bar{\xi}\zeta^2 - \frac{1}{A_2} \left[ \left( \frac{5}{2} A_1 + 2A_3 \right) (u_2 - u_1) \frac{p}{\rho} + \frac{3}{2} A_1 u_1^2 (u_2 - u_1) \right. \right. \\
& \left. \left. + \frac{1}{2} A_1 v_1^2 (u_2 - u_1) + A_1 u_1 v_1 (v_2 - v_1) + \frac{1}{2} A_1 w_1^2 (u_2 - u_1) + A_1 u_1 w_1 (w_2 - w_1) \right] \right\}. \quad (16)
\end{aligned}$$

From Eq. (16), taking the transport velocities of the colliding molecules as being equal, we easily obtain the classical value for the quantity  $B_5(\bar{\xi}^3 + \bar{\xi}\eta^2 + \bar{\xi}\zeta^2)$ , evaluated by Boltzmann [13].

On the other hand, from the transport equations, following [13], we can also obtain an expression for  $B_5(\bar{\xi}^3 + \bar{\xi}\eta^2 + \bar{\xi}\zeta^2)$

$$mB_5(\bar{\xi}^3 + \bar{\xi}\eta^2 + \bar{\xi}\zeta^2) = 5\rho \frac{\partial \left( \frac{p}{\rho} \right)}{\partial x}. \quad (17)$$

From Eqs. (16) and (17) we find the expression

$$\begin{aligned}
\rho(\bar{\xi}^3 + \bar{\xi}\eta^2 + \bar{\xi}\zeta^2) &= -\frac{15}{2} R \frac{\partial \left( \frac{p}{\rho} \right)}{\partial x} + \rho \frac{1}{A_2} \left[ \left( \frac{5}{2} A_1 + 2A_3 \right) \right. \\
& \times (u_2 - u_1) \frac{p}{\rho} + \frac{3}{2} A_1 u_1^2 (u_2 - u_1) + \frac{1}{2} A_1 v_1^2 (u_2 - u_1) \\
& \left. + A_1 u_1 v_1 (v_2 - v_1) + \frac{1}{2} A_1 w_1^2 (u_2 - u_1) + A_1 u_1 w_1 (w_2 - w_1) \right], \quad (18)
\end{aligned}$$

where R is some constant.

Similarly, we obtain

$$\begin{aligned} \rho (\bar{\eta}^3 + \bar{\eta}_x^2 + \bar{\eta}_y^2) = & -\frac{15}{2} R \frac{\partial \left( \frac{p}{\rho} \right)}{\partial y} + p \frac{1}{A_2} \left[ \left( \frac{5}{2} A_1 + 2A_3 \right) (v_2 - v_1) \right. \\ & \times \frac{p}{\rho} + \frac{3}{2} A_1 v_1^2 (v_2 - v_1) + \frac{1}{2} A_1 u_1^2 (v_2 - v_1) + A_1 u_1 v_1 (u_2 - u_1) \\ & \left. + \frac{1}{2} A_1 w_1^2 (v_2 - u_1) + A_1 v_1 w_1 (w_2 - w_1) \right], \end{aligned} \quad (19)$$

$$\begin{aligned} \rho (\bar{\xi}^3 - \bar{\xi}_x^2 + \bar{\xi}_y^2) = & -\frac{15}{2} R \frac{\partial \left( \frac{p}{\rho} \right)}{\partial z} + p \frac{1}{A_2} \left[ \left( \frac{5}{2} A_1 + 2A_3 \right) \right. \\ & \times (w_2 - w_1) \frac{p}{\rho} + \frac{3}{2} A_1 w_1^2 (w_2 - w_1) + \frac{1}{2} A_1 v_1^2 (w_2 - w_1) \\ & \left. + A_1 w_1 v_1 (v_2 - v_1) + \frac{1}{2} A_1 u_1^2 (w_2 - w_1) + A_1 w_1 u_1 (u_2 - u_1) \right]. \end{aligned} \quad (20)$$

According to the Predvoditelev hypothesis, we have

$$\begin{aligned} u_1 = u_0 + A \left[ (x - x_0) \frac{\partial u_0}{\partial x} - (y - y_0) \frac{\partial u_0}{\partial y} + (z - z_0) \frac{\partial u_0}{\partial z} \right], \\ u_2 = u_0 - A \left[ (x - x_0) \frac{\partial u_0}{\partial x} - (y - y_0) \frac{\partial u_0}{\partial y} + (z - z_0) \frac{\partial u_0}{\partial z} \right]. \end{aligned} \quad (21)$$

Now substituting Eqs. (18)-(20) into Eq. (1), taking account of Eq. (21), and using the notation

$$\frac{A_1 A}{A_2} = \beta, \quad (22)$$

$$\frac{A_3 A}{A_2} = \gamma, \quad (23)$$

we obtain a generalized heat-conduction equation:

$$\begin{aligned} \frac{\partial T}{\partial t} + \mathbf{V}_0 \nabla T = & \frac{5}{2} \cdot \frac{R}{\rho} \Delta T - \frac{2}{3} T \operatorname{div} \mathbf{V}_0 \\ & + \frac{2R}{3R_1 \rho} \left\{ \frac{2}{3} \left[ \left( 2 \frac{\partial u_0}{\partial x} - \frac{\partial v_0}{\partial y} - \frac{\partial w_0}{\partial z} \right) \frac{\partial u_0}{\partial x} + \left( 2 \frac{\partial v_0}{\partial y} - \frac{\partial u_0}{\partial x} \right. \right. \right. \\ & \left. \left. - \frac{\partial w_0}{\partial z} \right) \frac{\partial v_0}{\partial y} + \left( 2 \frac{\partial w_0}{\partial z} - \frac{\partial u_0}{\partial x} - \frac{\partial v_0}{\partial y} \right) \frac{\partial w_0}{\partial z} \right] + \\ & + \left( \frac{\partial v_0}{\partial x} - \frac{\partial u_0}{\partial y} \right) \frac{\partial u_0}{\partial y} + \left( \frac{\partial w_0}{\partial x} + \frac{\partial u_0}{\partial z} \right) \frac{\partial u_0}{\partial z} + \left( \frac{\partial v_0}{\partial x} + \frac{\partial u_0}{\partial y} \right) \frac{\partial v_0}{\partial x} \\ & + \left( \frac{\partial v_0}{\partial z} + \frac{\partial w_0}{\partial y} \right) \frac{\partial v_0}{\partial z} + \left( \frac{\partial w_0}{\partial x} + \frac{\partial u_0}{\partial z} \right) \frac{\partial w_0}{\partial x} \\ & \left. + \left( \frac{\partial v_0}{\partial z} + \frac{\partial w_0}{\partial y} \right) \frac{\partial w_0}{\partial y} \right\} - \frac{1}{5} (5\beta + 4\gamma) T \operatorname{div} \mathbf{V}_0 \\ & + \frac{\beta}{R_1} \left\{ \left( u_0^2 \frac{\partial u_0}{\partial x} + v_0^2 \frac{\partial v_0}{\partial y} + w_0^2 \frac{\partial w_0}{\partial z} \right) + \frac{1}{3} \left[ (v_0^2 + w_0^2) \frac{\partial u_0}{\partial x} \right. \right. \\ & \left. \left. + (u_0^2 + w_0^2) \frac{\partial v_0}{\partial y} + (u_0^2 + v_0^2) \frac{\partial w_0}{\partial z} \right] - \frac{2}{3} \left( w_0 u_0 \frac{\partial u_0}{\partial z} + v_0 u_0 \frac{\partial u_0}{\partial y} \right. \right. \\ & \left. \left. + u_0 v_0 \frac{\partial v_0}{\partial x} + w_0 v_0 \frac{\partial v_0}{\partial z} + u_0 w_0 \frac{\partial w_0}{\partial x} + v_0 w_0 \frac{\partial w_0}{\partial z} \right) \right\}, \end{aligned} \quad (24)$$

where  $R_1$  is the gas constant.

## 2. Discussion of Results

The heat-conduction equation (24) describes the process of heat transport in a rarefied gas and is similar in form to the classical expression, except for the dissipation function.

We see that allowing for the effect of gradients of transport velocities in a rarefied gas has led to the appearance of additional terms in the dissipation function, each coinciding in structure with the term  $T \operatorname{div} \mathbf{V}_0$ , while the remainder have a more specific form. When there are considerable gradients of transport velocities over the volume elements, the contribution of the terms with coefficients  $\beta$  and  $\gamma$  will be appreciable. Even in the case of an incompressible gas the dissipation energy due to the specific terms can be appreciable. Clearly, one must take account of this kind of variation of the dissipation function, due to volume elements, in the case of gases and liquids which have a complex microstructure.

#### NOTATION

$\mathbf{V}$ , total molecular velocity vector;  $u, v, w$ , components of the molecular velocity describing an ordered motion;  $\xi, \eta, \zeta$ , components of the molecular velocity describing a random motion;  $p$ , pressure;  $\rho$ , density;  $u_0, v_0, w_0$ , components of the hydrodynamic volume element;  $T$ , temperature;  $\beta, \gamma, R$ , constants.

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#### EXERGY REPRESENTATION IN THE THERMODYNAMICS OF IRREVERSIBLE PROCESSES

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UDC 536.70

It is proposed to use the exergy of a system as the thermodynamic Lagrangian. The corresponding variational principle is formulated and its relationship to other variational principles of non-equilibrium thermodynamics is demonstrated.

For constant parameters of the surrounding medium the exergy is a function of the thermodynamic state [1, 2] and in general depends on the generalized coordinates and velocities  $x_1, \dot{x}_1$ . For the case of flux the exergy may be expressed in the form of two alternative forms (Euler and Lagrange) [3]:

$$\delta E = \delta E^{(L)} + \delta K, \quad (1)$$

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