PHYSICAL REVIEW E **69**, 061201 (2004)

Heat transfer in the Knudsen layer

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(Received 4 September 2003; published 1 June 2004)

A concept of the surface heat conductivity determining a heat transfer in the Knudsen layer was introduced. It has the same order with respect to the Knudsen number as the bulk heat transfer and must be taken into account in practical calculations. Using the Onsager principle the coefficient of the surface heat conductivity was related to the thermal slip coefficient.

DOI: 10.1103/PhysRevE.69.061201 PACS number(s): 44.15.+a, 44.20.+b, 47.45.Gx

I. INTRODUCTION

As is known, a heat flux in any medium is determined by the Fourier law, i.e., the heat flux vector is proportional to a temperature gradient. However, the heat transfer in a gaseous medium has two features. First, besides a temperature gradient the heat flow vector is proportional to a pressure gradient too. Such a phenomenon is called viscous heat flow and was discussed in many works, see, e.g., Refs. [1–3]. Second, in the Knudsen layer there is one more type of heat flux, which is determined by a stress tensor on a boundary between a gas and solid surface. Note that the Knudsen layer has the thickness of the order of the molecular mean free path. The existence of this flux is confirmed in several papers, see, e.g., Refs. [4–9], where the viscous slip coefficient was calculated. All these phenomena have the same order with respect to the Knudsen number defined as a ratio of the molecular mean free path to a characteristic size of the gas flow. So, in practical calculations, all three types of heat flow must be taken into account even if the Knudsen number is small.

It is quite clear how to calculate the ordinary heat flux applying the Fourier law. It is not difficult to take into account the viscous heat flow determined by a pressure gradient. However, a consideration of the heat flux in the Knudsen layer represents some difficulties in practical calculations. The aim of the present paper is threefold. First, a concept of the surface heat conductivity coefficient is introduced as a proportionality constant between the surface heat flux and stress tensor on a solid surface. Second, this coefficient is calculated using numerical data published previously. Third, applying the Onsager reciprocity principle [10,11] the coefficient is related to the thermal slip coefficient, which is calculated in many papers, see, e.g., Refs. [12–16]. Such a relation allows us to know the surface heat conductivity immediately from the data on the thermal slip coefficient.

II. STATEMENT OF THE PROBLEM

A kinetic description of gas flows is based on the velocity distribution function, which obeys the Boltzmann equation [17,18]. The Chapman-Enskog solution of this equation implies an expansion of the distribution function f with respect to the Knudsen number (Kn) as

$$f = f^{(0)} + \mathrm{Kn}\, f^{(1)} + \mathrm{Kn}^2 f^{(2)} + \cdots . \tag{1}$$

In the case of monoatomic gas the distribution function $f = f(t, \mathbf{r}, \mathbf{v})$ depends on time t, position $\mathbf{r}$, and molecular velocity $\mathbf{v}$. So, the expansion (1) is valid in the hydrodynamic limit ($\mathrm{Kn} \to 0$) when the mean free path is sufficiently small compared with the flow scale.

As a result of the expansion (1) some moments of the distribution function are presented as an expansion too. For instance, the heat flux vector defined as

$$\mathbf{q}(t,\mathbf{r}) = \frac{m}{2}\int f(t,\mathbf{r},\mathbf{v}) V^2 \mathbf{V}\, d\mathbf{v}, \quad \mathbf{V} = \mathbf{v} - \mathbf{u} \tag{2}$$

reads

$$\mathbf{q} = \mathbf{q}^{(0)} + \mathbf{q}^{(1)} + \mathbf{q}^{(2)} + \cdots , \tag{3}$$

where

$$\mathbf{q}^{(i)} = (\mathrm{Kn})^i \frac{m}{2}\int f^{(i)} V^2 \mathbf{V}\, d\mathbf{v}, \quad i = 0,1,2, \ldots . \tag{4}$$

m is the molecular mass of the gas and $\mathbf{u}$ is the bulk velocity of the gas.

The zero order term $f^{(0)}$ of the expansion (1) corresponds to the local Maxwellian

$$f^{(0)}(t,\mathbf{r},\mathbf{v}) = n\,(t,\mathbf{r})\left[\frac{m}{2\pi k T(t,\mathbf{r})}\right]^{3/2} \exp\left[-\frac{m[\mathbf{v}-\mathbf{u}(t,\mathbf{r})]^2}{2kT(t,\mathbf{r})}\right], \tag{5}$$

where $n(t,\mathbf{r})$ is the local number density, $T(t,\mathbf{r})$ is the local temperature, and k is the Boltzmann constant. Substituting Eq. (5) into Eq. (4) we obtain $\mathbf{q}^{(0)} = 0$, i.e., there is no heat flux for the zero order approximation.

Solving the Boltzmann equation with the first order term $f^{(1)}$ and substituting it into Eq. (4) one obtains the Fourier law

$$\mathbf{q}^{(1)} = -\kappa \nabla T, \tag{6}$$

where κ is the heat conductivity obtained from the Boltzmann equation as [17]

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$$\kappa = \frac{k}{3}\int (\mathbf{A}\cdot\mathbf{V})\left(\frac{mV^2}{2kT} - \frac{5}{2}\right) f^{(0)}\mathrm{d}\mathbf{v}. \tag{7}$$

The vector function $\mathbf{A}=\mathbf{A}(\mathbf{V})$ satisfies the integral equation

$$nI(\mathbf{A}) = f^{(0)}\left(\frac{mV^2}{2kT} - \frac{5}{2}\right)\mathbf{V}, \tag{8}$$

where the function I is defined as

$$I(F) = \frac{1}{n^2}\int\int\int f^{(0)}(\mathbf{v}_1) f^{(0)}(\mathbf{v})[F(\mathbf{v}) + F(\mathbf{v}_1) - F(\mathbf{v}') - F(\mathbf{v}_1')]g\, b\mathrm{d}b\, \mathrm{d}\varepsilon\, \mathrm{d}\mathbf{v}_1, \tag{9}$$

F is any function of the molecular velocity, $\mathbf{v}$ and $\mathbf{v}_1$ are pre-collision molecular velocities, while $\mathbf{v}'$ and $\mathbf{v}_1'$ are the corresponding post-collision velocities, $g=|\mathbf{v}-\mathbf{v}_1|$ is the relative velocity, b is the impact parameter, and ε is the azimuthal angle of the molecular collision plane.

The second approximation term $\mathbf{q}^{(2)}$ has a complicated expression given by Eq. (5.8-32) of Ref. [17]. Since this term is calculated via $f^{(2)}$ by Eq. (4) it should be of the order of Kn^2, but paradoxically it can be of the same order as $\mathbf{q}^{(1)}$ with respect to the Knudsen number. For instance, if one considers a gas flow caused by a pressure gradient, then one obtains

$$\mathbf{q}^{(2)} = \frac{\theta_4}{2}\frac{\mu}{\varrho}\nabla P, \tag{10}$$

where μ is the stress viscosity, ρ is the mass density of the gas. Equation (10) follows from the fourth term of Eq. (5.8-32) of Ref. [17]. The coefficient θ_4 can be obtained with the help of Eqs. (5.8-22) and (5.8-32) of Ref. [17] as

$$\theta_4 = \frac{2m^2}{15P\mu}\int (\mathbf{A}\cdot\mathbf{V})\; V^2 f^{(0)}\, \mathrm{d}\mathbf{v}. \tag{11}$$

The coefficient θ_4 depends on the intermolecular potential, for instance, for the Maxwellian molecules we have [17]

$$\mathbf{A}(\mathbf{V}) = \frac{3\mu}{2kT}\left(\frac{mV^2}{2kT} - \frac{5}{2}\right)\mathbf{V}, \quad \theta_4 = 3. \tag{12}$$

For other molecular models it is expected it to be not far from this value.

Since both κ and μ are proportional to the molecular mean free path, the term corresponding to the heat flux due to a pressure gradient $\mathbf{q}^{(2)}$, i.e., viscous heat transfer, cannot be neglected in the hydrodynamic limit ($\mathrm{Kn}\to 0$) in comparison with the Fourier term, i.e., $\mathbf{q}^{(1)}$, as was pointed out previously; see, e.g., Refs. [1–3].

As has been noted above, the total heat flux contains one more component of the same order as those presented by Eqs. (6) and (10), namely, the heat flux in the Knudsen layer. To define it let us introduce the Cartesian coordinates with the origin fixed at the surface, the x axis directed normally to the surface into the gas, and the y axis being tangential to the surface. If a gas flows over a solid surface in the y direction, then a heat flux $q_y(x)$ appears near the surface, i.e., in the Knudsen layer. The numerical data on this flux can be found in Refs. [4–6].

In practice we need to know just the total heat flux through the Knudsen layer defined as

$$Q_s = \int_0^\infty q_y(x)\; \mathrm{d}x. \tag{13}$$

In accordance with Refs. [4–9] the heat flow $q_y(x)$ tends to zero far from the surface so that the integral (13) converges. Moreover, the heat flow $q_y(x)$ is proportional to the stress tensor Π_{xy} on the surface. Thus the total heat flux is also proportional to Π_{xy}, i.e.,

$$Q_s = -\kappa_s \prod_{xy} = \kappa_s\, \mu \frac{\partial u_y}{\partial x}, \quad \text{at} \quad x = 0. \tag{14}$$

Here, the relation $\Pi_{xy} = -\mu(\partial u_y/\partial x)$ has been used, where u_y is the tangential velocity of the gas.

Since the Knudsen layer has the mean free path order then in the hydrodynamic limit ($\mathrm{Kn}\ll 1$) the layer thickness is negligible compared with characteristics sizes of the gas flow. One of the characteristic sizes is the surface curvature radius. Thus to calculate the heat flux vector $q_y(x)$ the Knudsen layer is assumed to be plane, i.e., the surface curvature can be neglected on the Knudsen layer level. So, Eq. (14) is a local relation of the surface heat flux Q_s to the stress tensor Π_{xy}, which is valid even for a curved surface.

Below, we are going to calculate the surface heat conductivity κ_s and to relate it to the thermal slip coefficient.

III. METHOD OF CALCULATION

The heat flow vector $q_y(x)$ is calculated together with the viscous slip coefficient [4–9,16]. We consider a gas flow over a semi-infinite space $x \geq 0$. The gas is maintained at an equilibrium pressure P_0 and at an equilibrium temperature T_0. At the infinity $x\to\infty$ the velocity gradient tends to a constant value. Under this condition a local heat flux $q_y(x)$ is established over the space, which has only the y component and vanishes far from the surface.

Further, the following dimensionless quantities will be used:

$$\tilde{q} = \frac{q_y}{P_0 \upsilon_0 \xi_u}, \quad \upsilon_0 = \left(\frac{2kT_0}{m}\right)^{1/2}, \tag{15}$$

where υ_0 is the most probable molecular velocity and ξ_u is the velocity gradient at the infinity, i.e.,

$$\xi_u = \frac{\ell_0}{\upsilon_0}\lim_{x\to\infty}\frac{\mathrm{d}u_y}{\mathrm{d}x}, \quad \ell_0 = \frac{\mu\, \upsilon_0}{P_0}. \tag{16}$$

Note that ℓ_0 has the order of the mean free path corresponding to the pressure P_0 and temperature T_0. If we introduce the reduced integral heat flux as

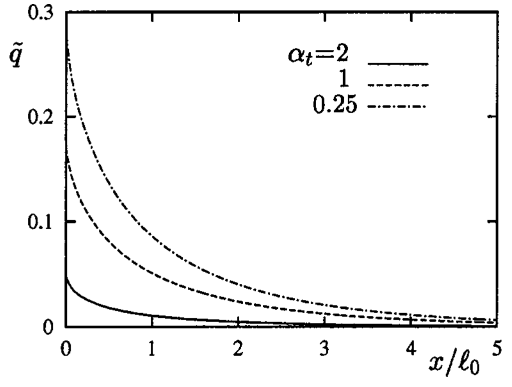

FIG. 1. Local heat flux in the Knudsen layer caused by the velocity gradient.

$$\tilde{Q}_s = \frac{1}{\ell_0}\int_0^\infty \tilde{q}(x)\ \mathrm{d}x, \tag{17}$$

then the surface heat conductivity coefficient reads

$$\kappa_s = \frac{\mu_0 v_0^2}{P_0}\tilde{Q}_s. \tag{18}$$

To calculate the quantity $\tilde{Q}_s$ the numerical data given in Table II of Ref. [4] can be used. However, to show the dependence of this quantity on the gas-surface interaction law we will use the solution obtained in Ref. [9] based on the S kinetic equation and on the Cercignani-Lampis [19] model of the gas-surface interaction. This model contains the momentum accommodation coefficient α_t and the energy accommodation coefficient α_n.

Since the numerical values of the quantity $\tilde{q}$ were not reported in Ref. [9] we present these data on Fig. 1 for three values of the momentum accommodation coefficient α_t: 0.25, 1, and 2 assuming that the energy accommodation coefficient α_n is fixed and equal to 0.25. The first value of α_t corresponds to a reflection close to the specular law, the second value provides the diffuse scattering, and the third value represents the almost back reflection. One can see that far from the surface, i.e., $x \gg \ell_0$, the local heat flux $\tilde{q}$ tends to zero independently on the accommodation coefficient α_t, while near the surface the behavior of $\tilde{q}$ depends significantly on α_t. The numerical values of the integral heat flux $\tilde{Q}_s$ calculated by integrating of $\tilde{q}$ obtained in Ref. [9] are given in Table I. It can be seen that the surface heat flux $\tilde{Q}_s$ increases by decreasing the accommodation coefficient α_t.

TABLE I. Reduced heat flux $\tilde{Q}_s$ and thermal slip coefficient vs α_t at $\alpha_n=0.25$.

α_t	$\tilde{Q}_s$	σ_{T}
0.25	0.2731	0.9536
0.5	0.2327	1.034
1.	0.1626	1.175
1.5	0.0973	1.305
2.	0.03497	1.430

So, the total heat flux through a gas is given by the three terms. The first one $\mathbf{q}^{(1)}$ given by Eq. (6) depends on the temperature distribution in the gas bulk. The second term given by Eq. (10) is determined by the pressure distribution in the gas. And the third term is calculated only on the solid surface by Eq. (14). This heat flow vector is tangential to the surface and directed along the tangential velocity of the gas. The surface heat conductivity κ_s is given by Eq. (18) with the values of $\tilde{Q}_s$ given in Table I. It is important that all these terms have the same order with respect to the Knudsen number and all of them must be taken into account at any small Knudsen number.

IV. RELATION TO THE THERMAL SLIP COEFFICEINT

The surface heat conductivity coefficient κ_s introduced above can be related to the thermal slip coefficient σ_{T}, which determines a tangential velocity of gas near a solid surface due to a longitudinal temperature gradient, i.e.,

$$u_y = \sigma_{\mathrm{T}}\frac{\mu}{\varrho}\frac{\mathrm{d}\ln T}{\mathrm{d}y}. \tag{19}$$

A critical review of numerical data on the coefficient σ_{T} and its recommended data can be found in Ref. [16].

To relate κ_s to the thermal slip coefficient we consider the classical problem of gas flow between two parallel plates fixed at $x=\pm a/2$, which was solved by many authors, see, e.g., Refs. [12–16]. The gas flows along the plates due to a longitudinal pressure gradient, while the temperature is maintained constant. In the hydrodynamic regime $(\mathrm{Kn} \ll 1)$ the total heat flux through a cross section of the channel is given as

$$Q = \int_{-a/2}^{a/2} q_y \mathrm{d}x = a q_y^{(2)} + 2Q_s, \tag{20}$$

where $q_y^{(2)}$ is given by Eq. (10), while Q_s is determined by Eq. (14). The factor 2 appeared because of the two surfaces. In this case the velocity profile due the pressure gradient reads

$$u_y(x) = -\frac{P\nu}{2\mu a}\left[\left(\frac{a}{2}\right)^2 - x^2\right], \quad \nu = \frac{a}{P}\frac{\mathrm{d}P}{\mathrm{d}y}. \tag{21}$$

Using this profile the stress tensor on the plates is calculated as

$$\prod_{xy} = \frac{1}{2}P\nu \quad \text{at} \quad x=-a/2. \tag{22}$$

Then with the help of Eqs. (10), (14), and (18) we obtain

$$Q = \left(\frac{\theta_4}{4} - \tilde{Q}_s\right)\mu v_0^2 \nu. \tag{23}$$

Usually, see, e.g., Refs. [15,16], the reduced heat flux is used

$$Q_{\mathrm{P}} = \frac{2Q}{aP_0 v_0 \nu} = \frac{2}{\delta}\left(\frac{\theta_4}{4} - \tilde{Q}_s\right), \quad \delta = \frac{aP}{\mu v_0}. \tag{24}$$

If we consider the gas flow between the parallel plates caused by a longitudinal temperature gradient, then using Eq. (19) we obtain the mass flow rate in the hydrodynamic regime

$$\dot{M} = \int_{a/2}^{a/2} \varrho u_y \mathrm{d}x = \sigma_{\mathrm{T}} \mu \tau, \qquad \tau = \frac{a}{T}\frac{\mathrm{d}T}{\mathrm{d}y}. \tag{25}$$

The reduced mass flow rate is defined as

$$G_{\mathrm{T}} = \frac{\dot{M} v_0}{a P_0 \tau} = \frac{\sigma_{\mathrm{T}}}{\delta}. \tag{26}$$

The quantities G_{T} and Q_{P} are equal to each other according to the Onsager relation [10,11], i.e.,

$$Q_{\mathrm{P}} = G_{\mathrm{T}}, \tag{27}$$

which is valid for any Knudsen number. Combining Eqs. (24), (26), and (27) we obtain

$$\tilde{Q}_s = \frac{1}{2}\left(\frac{\theta_4}{2} - \sigma_{\mathrm{T}}\right). \tag{28}$$

Some numerical data on the thermal slip coefficient σ_{T} based on the S model and reported in Ref. [8] are presented in Table I. Taking into account that $\theta_4 = 3$ for the S model one can verify that the equality (28) is fulfilled within the numerical accuracy. Note that the quantities $\tilde{Q}_s$ and σ_{T} were obtained from two different equations, i.e. Q_s corresponds to the isothermal gas flow over a solid surface, while σ_{T} determines a gas flow caused by a longitudinal temperature gradient over a solid surface.

According to Refs. [9,16] the thermal slip coefficient σ_{T} varies from 0.75 up to 1.5, where the first value corresponds to the specular reflection of molecules on surface, while the second value corresponds to the opposite situation, i.e., back reflection. Thus the quantity $\tilde{Q}_s$ varies in the range $0 \leqslant \tilde{Q}_s \leqslant 0.375$. Note that if the gas-surface interaction is given by the back reflection the surface heat flux vanishes.

Substituting the expression (28) into Eq. (18) the surface thermal conductivity can be related to the thermal slip coefficient as

$$\kappa_s = \frac{\mu v_0^2}{2P}\left(\frac{\theta_4}{2} - \sigma_{\mathrm{T}}\right). \tag{29}$$

V. CONCLUSIONS

The concept of the surface heat conductivity determining the heat flux in the Knudsen layer was introduced. Since the bulk heat flux and the surface heat flux have the same order with respect to the Knudsen number, both of them must be taken into account in practical calculations, i.e., the surface heat flux cannot be neglected for small Knudsen numbers.

Using the Onsager principle a relation between the surface heat conductivity and the thermal slip coefficient was obtained. Since there are many reliable results on the thermal slip coefficient reported in the open literature, see, e.g., Refs. [9,16], then the surface heat conductivity is automatically known. Such a relation once again shows that the slip coefficients are so important in the theory of transport phenomena as the viscosity and the thermal conductivity.

On the other hand, Eq. (28) can reduce significantly the computational efforts to calculate the slip coefficients. Usually, the viscous and thermal slip coefficients are calculated separately solving two different kinetic equations, see, e.g., the works [4–6,8,9,16]. However, solving one kinetic equation to calculate the viscous slip coefficient one calculates also the heat flux $\tilde{q}$. Integrating it over the Knudsen layer and using Eq. (28) one immediately calculates the thermal slip coefficient without solving the other kinetic equation.

ACKNOWLEDGMENTS

The author takes this opportunity to thank C. E. Siewert for very helpful discussions about this (and other) paper. Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq, Brazil) is acknowledged for the support of this research.

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