POISEUILLE'S FLOW AND THERMAL CREEP FOR DIFFERENT SCATTERING KERNELS

FOR A GAS SCATTERED BY A CHANNEL SURFACE

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The well-known Maxwellian diffuse-specular model of boundary conditions cannot completely describe the presently available experimental results on the flow of a rarefied gas in long channels. Within the scope of this model, it is not possible to explain Hobson's accommodation pumping effects [1] and the temperature dependence of the free-molecular reduced gas flow rate in capillaries [2, 3]. For this reason, it is necessary to develop and examine new, more suitable, models of boundary conditions that can describe the interaction of a gas with the surface. In [4], a quite simple two-parameter scattering kernel is proposed, which follows both from a physical and from a purely mathematical analysis of the problem. However, this kernel does not take into account the possibility of capture of molecules on the surface followed by their diffusive evaporation. In this paper, we propose to take into account this mechanism of the interaction of molecules with the surface by superposing the kernel proposed in [4] with the diffusion scattering function. The combined model proposed for the boundary conditions and the Cercignani-Lampis scattering kernel are then applied to the problem of isothermal and nonisothermal gas flow in the free molecular regime in a long channel in order to check their effectiveness in describing the corresponding experimental data.

<u>1.</u> Formulation of the Problem. We are examining an isothermal flow of a monatomic gas in the free molecular regime in an infinitely long cylindrical channel in the presence of a pressure gradient along the channel. The geometry of the problem is illustrated in Fig. 1. It is convenient to represent the velocity vector of a molecule in terms of the components v_n , v_{ϕ} , and v_z , which depend on the coordinates of the point of observation (v_n is the radial component). The gas has the temperature of the wall T.

In calculating the macroscopic properties of the gas flow, we used the relations obtained in [5] in which for the Poiseuille's flow the following expression is obtained:

$$I_{p} = I_{p0}(1 + 3\langle h + h_{0} \rangle), \qquad (1.1)$$

$$\langle f(\mathbf{v}) \rangle = \frac{2\beta^{2}}{\pi} \int_{-1}^{1} v_{n} \exp(-\beta v^{2}) f(\mathbf{v}) d\mathbf{v},$$

where $I_{p0} = -\frac{4}{3} \left(\frac{\pi}{\beta}\right)^{1/2} R^3 n'$ is the Poiseuille's flow through the channel with a completely

accommodating surface; n' is the gradient of the number density of molecules; R is the radius of the channel; $\beta = m/2kT$; m is the mass of a molecule; k is Boltzmann's constant; $h_o = v_n v_z/(v_n^2 + v_\phi^2)$ follows from the geometry of the problem; h⁺ is the solution of the integral equation

$$h^{+} = \widehat{P}h_{0} + \widehat{P}h^{+}, \qquad (1.2)$$

$$\widehat{P}f(\mathbf{v}) = \int_{+} P(\mathbf{v}_{R} \rightarrow \mathbf{v}')f(\mathbf{v}') d\mathbf{v}', \quad \mathbf{v}_{R} = (-v_{n}, v_{\phi}, v_{z}),$$

 $P(\mathbf{v}' \rightarrow \mathbf{v})$ is the scattering kernel for molecules of a rarefied gas scattered by the surface [4]. The sign "+" in the integrand indicates integration over the upper velocity half-space.

The molecular flow under the action of the pressure gradient is accompanied by a flow of kinetic energy (mechanocaloric effect):

$$Q = Q_0 \left(1 + \frac{3}{2} \beta \langle v^2 h^+ h_0 \rangle \right), \tag{1.3}$$

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where

$$Q_0 = -\frac{8}{3} \left(\frac{\pi}{\beta}\right)^{1/2} R^3 n' kT.$$

The mechanocaloric effect is the cross effect with respect to thermal creep (flux of molecules I_T in the presence of a temperature gradient on the channel wall). Following [5], it is possible to obtain the relation

$$\gamma = 5/2 - Q/I_p kT, \tag{1.4}$$

where $\gamma = (I_T/I_{To})I_{Po}/I_p$ is the characteristic of the thermal molecular pressure difference (TPD), arising in the system of two columns with gas connected by a capillary and kept at

different temperatures; $I_{\tau 0} = \frac{2}{3} \left(\frac{\pi}{\beta}\right)^{1/2} R^3 \frac{n}{T} \frac{dT}{dz}$ is the flux of thermal creep under complete

diffuse reflection.

Knowledge of the expressions for the Poiseuille's flow (1.1) and for the TPD index γ (1.4) permits calculating the nonisothermal molecular flux I_T.

2. Calculation of the Isothermal and Nonisothermal Flows of Gas for a Scattering Kernel of General Form. In order to carry out the calculations using Eqs. (1.1) and (1.3), it is necessary to solve the integral equation (1.2). An approximation solution of this equation can be obtained by a variational method without the restrictions of any specific model for the scattering kernel. For Eq. (1.1), we form the variational functional [5]

$$J\{h^+\} = \langle h^+(2\hat{P}h_0 + \hat{P}h^+ - h^+)\rangle$$

$$(2.1)$$

and assume that

$$h^+ = A \widehat{P} h_0. \tag{2.2}$$

For A = 1, this function is the first approximation of the solution of Eq. (1.2) by the iteration method. Expression (2.2) minimizes the functional with

$$A = S_2 / (S_2 - S_3), \ S_h = \langle h_0 \hat{P}^h h_0 \rangle.$$
(2.3)

Now, knowing $h^+(\mathbf{v})$, it is possible to write an expression for the flows and TPD index γ for an arbitrary scattering kernel

$$I_{\rm p} = I_{\rm p0}(1 + 3AS_{\rm l}); \tag{2.4}$$

$$Q = Q_0 (1 + (3/2)\beta A \langle v^2 h_0 \hat{P} h_0 \rangle);$$
(2.5)

$$\gamma = \frac{5}{2} - \frac{2\left(1 + \frac{1}{2}\beta A \langle v^{*}h_{0}Ph_{0} \rangle\right)}{(1 + 3AS_{1})}.$$
(2.6)

The solution of Eq. (1.2) can also be represented in the form of a Neumann series

$$h^{+} = \hat{P}h_{0} + \hat{P}^{2}h_{0} + \hat{P}^{3}h_{0} + \dots$$
(2.7)

If the Neumann series (2.7) converges, then the fluxes have the form

$$I_{p} = I_{p0} \left(1 + 3 \sum_{h=1}^{\infty} S_{h} \right);$$
 (2.8)

$$Q = Q_0 \left(1 + \frac{3}{2} \beta \sum_{k=1}^{\infty} V_k \right),$$
 (2.9)

$$V_{\mu} = \langle v^2 h_0 \widehat{P}^{\mu} h_0 \rangle.$$

It is convenient to use the expression obtained in analyzing the effect of different scattering kernels, describing the interaction of a gas with a surface, on the macroscopic characteristics of the flow of a rarefied gas.

3. Calculation of the Macroscopic Characteristic of Gas Flow for Some Scattering Kernels. For a Maxwellian model of the boundary conditions, Eq. (1.2) has an exact solution. After a number of simple transformations, we can obtain

$$I_p = I_{p_0}\left(\frac{2-\alpha}{\alpha}\right), \quad Q = Q_0\left(\frac{2-\alpha}{\alpha}\right), \quad \gamma = \frac{1}{2}, \tag{3.1}$$

where α is the fraction of diffusely reflected molecules.

Cercignani and Lampis propose the following two parameter scattering kernel [4]:

$$P_{c}(\mathbf{v}' \to \mathbf{v}) = \frac{2\beta^{2}}{\pi} \frac{v_{n}}{\alpha_{n}\alpha_{t}(2-\alpha_{t})} \exp\left\{-\beta\left(\frac{v_{n}^{2} + (1-\alpha_{n})v_{n}'^{2}}{\alpha_{n}} + \frac{|\mathbf{v}_{t} - (1-\alpha_{t})\mathbf{v}_{t}'|^{2}}{\alpha_{t}(2-\alpha_{t})}\right)\right\} I_{0}\left(\frac{\sqrt{1-\alpha_{n}}}{\alpha_{n}}2\beta v_{n}v_{n}'\right), \quad (3.2)$$

$$v_{n} < 0, \quad v_{n} > 0, \quad 0 \leq \alpha_{t} \leq 2, \quad 0 \leq \alpha_{n} \leq 1,$$

where I_o is the zeroth-order Bessel function of the first kind with imaginary argument.

The parameters α_n and α_t coincide with the Knudsen coefficients of accommodation of normal energy and tangential momentum [6].

Due to the complexity of the form of the kernel, it is not possible to obtain an analytic variational solution of Eq. (1.2) for this kernel. Only if α_n and α_t are close to 1, is it possible to arrive at the following simple expressions for the flows and the index γ :

$$I_{p} = I_{p_{0}} \left\{ 1 + \frac{3\pi (1 - \alpha_{t})}{8\alpha_{t}} \left[1 + \frac{1 - \alpha_{n}}{16} \right] \right\};$$
(3.3)

$$Q' = Q_0 \left\{ 1 \pm \frac{3\pi (1 - \alpha_t)}{32\alpha_t} \left[5 - \frac{1 - \alpha_n}{46} \right] \right\};$$
(3.4)

$$\gamma = \frac{1}{2} - \frac{3\pi (1 - \alpha_l)}{16} \left[1 - \frac{5}{16} (1 - \alpha_n) - \frac{3\pi - 8}{8} (1 - \alpha_l) \right].$$
(3.5)

As is evident from expressions (3.3)-(3.5), the dependence of the macroscopic characteristics of the gas flow on the parameter α_n is weaker than on α_t . This makes it possible to examine the Cercignani-Lampis kernel (3.2) with a single parameter α_t , when $\alpha_n = 1$. In this case, it is possible to carry out all the mathematical calculations in solving the integral equation (1.2) by the variational method and to calculate the expressions S_k and V_k in the parentheses, necessary for calculating the macroscopic characteristics of the gas flow, without any simplifications for arbitrary values of α_t :

$$S_{k} = \frac{\pi}{2(1-\alpha_{l})^{k}} \left\{ \ln \left| \frac{1+\sqrt{1-(1-\alpha_{l})^{2k}}}{2} \right| + 1 - \sqrt{1-(1-\alpha_{l})^{2k}} \right\};$$
(3.6)

$$V_{k} = \frac{3}{2\beta} S_{k} + \frac{\pi}{8\beta} (1 - \alpha_{l})^{k}.$$
(3.7)

It should be noted that if the accommodation is nearly total, then the expressions for the macroscopic characteristics, obtained for a single-parameter Cercignani-Lampis kernel, coincide with expressions (3.3)-(3.5), if in the latter the terms of order $(1 - \alpha_{n,t})^2$ are neglected.

Substituting for S_k and V_k in Eqs. (2.8) and (2.9) permits calculating the values of I_p , Q, γ , and I_T when $h^+(v)$ can be represented in the form of a Neumann series.

In order to obtain the temperature dependence $I_p(T)$, we shall examine the physical derivation of the Cercignani-Lampis scattering kernel [4]. In this paper, the interaction of the gas molecules with a solid body is viewed as a random wandering of molecules in a surface layer of thickness d with characteristic diffusion length l in velocity space in a direction tangential to the surface. The parameter α_t in the kernel (3.2) is determined in terms of the properties of the gas-solid-body interaction l, d as follows [4]:

$$\alpha_l = 1 - \exp\{-2d/l\}.$$
 (3.8)

TABLE 1

Param- eter	Т, К	He	Ne	Ar	Kr	Xe
α _t [1] α _t [2]	$77-295 \\ 77 \\ 295$	0,79 0,75 0,91	0,80 0,84 0,89	0,91 0,89 0,97	0,94 0,99	0,94 1,00



We will assume that the finiteness of the diffusion length stems from the thermal fluctuations of the solid body and the nonideal nature of the structure of the surface (e.g., the presence of roughness). Then, the probability of collisions of molecules in the surface layer 2d/l will be the sum of the probabilities of collisions with surface defects p and with phonons of thermal oscillations. Assuming that the probability of collisions with phonons is proportional to their number, which, in its turn, is proportional to temperature, expression (3.8) can be rewritten in the form

$$\alpha_t = 1 - \exp\{-(p + qT)\},\tag{3.9}$$

where q is some constant that characterizes the cross section of the interaction of gas atoms with the phonons of the solid body.

The physical derivation of the scattering function (3.2) does not take into account the possibility for gas molecules to be captured by the surface followed by their evaporation according to a diffusion law. For this reason, it is completely logical to combine the Cercignani-Lampis kernel (3.2) with the diffusion kernel $P_0(\mathbf{v}' \rightarrow \mathbf{v})$ by introducing the condensation coefficient (or attachment coefficient) s in the form

$$P_{h}(\mathbf{v}' \to \mathbf{v}) = sP_{0}(\mathbf{v}' \to \mathbf{v}) + (1 - s)P_{c}(\mathbf{v}' \to \mathbf{v}).$$
(3.10)

The simplest approach to condensation and accommodation phenomena was proposed in [7]. Following [7], the expression for the attachment coefficient s can be represented in the form

$$s = 1 - \exp\{-T_s/T\},\tag{3.11}$$

where T_s is the temperature, corresponding to the critical energy for capture of a molecule by the surface.

The calculation of the isothermal flow, according to Eq. (2.4), using the kernel (3.10) and expressions (3.9) and (3.11), leads to the following temperature dependence of the reduced flow rate ω :

$$\omega = \frac{I_p}{I_{p_0}} - 1 + \frac{3\pi}{8} e^{-\frac{T_s}{T}} (e^{p+qT} - 1)^{-1}.$$
(3.12)

4. Comparison with Experiment. In [1], it was shown experimentally that the TPD index γ in the free-molecular regime differs from the value $\gamma = 1/2$, which follows not only for complete diffuse reflection, but also for the specular-diffuse scheme with arbitrary fraction of diffuse reflection (3.1). Application of the Cercignani-Lampis boundary conditions yields Eq. (3.5), which explains the deviation of γ from 1/2.

According to the experimental data in [1, 2], using relations (3.3) and (3.5) with $\alpha_n = 1$, it is possible to calculate the parameter α_t for the Cercignani-Lampis kernel.

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Parameter	He	Ne	Ar	H₂	D ₂
T_s , K	33,1	33,9	122,0	45,1	66,0
$\pm \Delta T_s \cdot 10^1$	3	14	23	48	66
$p \pm \Delta p \cdot 10^3$	0,741	1,271	0,280	0,920	0,666
	3	16	23	60	74
$q \cdot 10^2, \mathrm{K}^{-1} \pm \Lambda q \cdot 10^5$	0,451 1	0,232 4	0,919 6	0,640 16	$\begin{array}{c} 0,716\\ 20\end{array}$

Table 1 shows the values of α_t for a number of inert gases on fused glass, calculated from data on the investigation of the accommodation pumping effect [1] and isothermal flow of rarefied gases [2]. The values of the parameter α_t , corresponding to isothermal gas flow, are presented for two temperatures, at which the ends of the channels in Hobson's experiments were maintained.

The satisfactory agreement between the values of α_t obtained in different types of experiments confirms the effectiveness of using the Cercignani-Lampis boundary conditions in describing the isothermal and nonisothermal motion of rarefied gases.

The experimental data on the temperature dependence of the reduced free molecular isothermal flows ω , obtained in [2-3] for long capillaries made of fused glass, are summarized in Table 2. The deviation of ω from unity is a result of incomplete accommodation of gas molecules on the surface of the solid body. For each of the gases presented in Table 2, the values of the parameters p, q, and T_s, which are presented in Table 3, were obtained by a nonlinear least-squares method from the condition that the deviation of the experimental set of values $\omega(T_i)$ from the theoretical dependence (3.12) is a minimum.

Expression (3.12) with the values of p, q, and T_s from Table 3 describes the experimental temperature dependence $\omega(T)$ to within 3%, which confirms the usefulness of the combined scattering kernel (3.10) with the temperature dependences (3.9) and (3.11) for its parameters as boundary conditions for the molecular distribution function of a rarefied gas.

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