THEORY OF THERMOMOLECULAR PRESSURE AND OF THE

MECHANOCALORIC EFFECT IN A CYLINDRICAL CHANNEL

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The effect of thermomolecular pressure in a cylindrical channel is analyzed, at any values of the Knudsen number, on the basis of the S-model kinetic equation.

The theory of thermomolecular pressure in a cylindrical channel at any values of the Knudsen number has been outlined earlier [1-3]. While in [1,2] the problem was solved on the basis of the Bubnov-Galerkin-Knudsen model equation, in [3] a special "Maxwell spheres" model was used and calculations were performed by the Monte Carlo method. A completely diffuse scattering of gas molecules by the channel surface was assumed in [1,3], but a specular-diffuse model of boundary conditions was used in [2] on the erroneous premise of thermal creep being independent of the specularity coefficient.

The main deficiency of the Bubnov-Galerkin-Knudsen model is that it does not describe processes which accompany simultaneous heat and mass transfer. The results obtained on its basis must, therefore, be further refined. This can be done with the aid of the S-model equation [4], which represents a higher-order approximation.

It has been shown in an earlier study [5] that the effect of thermomolecular pressure at any values of the Knudsen number can be described by the expression

$$\frac{P_1}{P_2} = \left(\frac{T_1}{T_2}\right)^{\gamma},\tag{1}$$

where P_i , T_i are the pressure and the temperature in the respective volumes, and exponent γ can depend on various parameters such as, foremost, the Knudsen number.

Well-known is the Knudsen relation with $\gamma = 1/2$ for the free-molecular mode of flow [6].

Available experimental data [7-9] indicate that γ has different values for different gases. An analysis has further revealed that these differences are due to different modes of interaction of molecules with a capillary wall, and that these differences increase as the gases become rarefied (i.e., with a higher Knudsen number). This must be accounted for in the theory, in defining the boundary conditions.

It can be demonstrated that the specular-diffuse model does not explain the experimental results. Specifically, according to this model, $\gamma = 1/2$ for all gases when $N_{Kn} \rightarrow \infty$ [10]. According to the experiments, meanwhile, the value of γ depends most on the kind of gas exactly in the free-molecular mode of flow [7,8]. Consequently, the specular-diffuse model of boundary conditions must be abandoned.

The object of this study is, first of all, to obtain a solution to the problem of thermomolecular pressure over the entire range of Knudsen number values on the basis of a correct kinetic equation and, secondly, to explain the dependence of exponent γ on the kind of gas with a special model of boundary conditions.

We consider the motion of a monoatomic one-component gas in a cylindrical capillary tube of radius R_0 , due to longitudinal pressure and temperature gradients. The axis of this capillary coincides with the z axis of coordinates. The state of the gas is assumed to be one of small perturbation and is described by a distribution function insignificantly little different from the Maxwell distribution function

$$f = f_0 (1 + h), \ |h| \ll 1,$$
 (2)

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$$f_0 = n(z) \left(\frac{m}{2\pi kT(z)}\right)^{3/2} \exp\left(-\frac{mv^2}{2kT(z)}\right),$$

where n, T are the gas concentration and temperature; m, the mass of a gas molecule; and k, the Boltzmann constant.

Then the linearized kinetic equation with the S-model collision integral [4] can be written as

$$\mathbf{c}_{\mathbf{p}} \; \frac{\partial h}{\partial \mathbf{x}} + c_{z} \left[\mathbf{v} + \left(c^{2} - \frac{5}{2} \right) \mathbf{\tau} \right] = R \left[2c_{z}u + Qc_{z} \left(c^{2} - \frac{5}{2} \right) - h \right], \tag{3}$$

$$\mathbf{v} = \frac{1}{P} - \frac{dP}{dz}, \ \tau = \frac{1}{T} - \frac{dT}{dz}, \ R = \frac{\sqrt{\pi}}{2} - \frac{R_0}{l} = \frac{\sqrt{\pi}}{2} \ N_{\rm Kn} - \mathbf{i}, \ c_i = \left(\frac{m}{2kT_0}\right)^{1/2} v_i,$$
$$T_0 = T \ (z = 0), \ u = \left(\frac{m}{2kT_0}\right)^{1/2} U = \pi^{-3/2} \int hc_z \exp\left(-c^2\right) dc,$$
$$Q = \frac{4}{15} \left(\frac{m}{2kT_0}\right)^{1/2} \frac{1}{P_0} \ q = \frac{4}{15} \ \pi^{-3/2} \int hc_z \left(c^2 - \frac{5}{2}\right) \exp\left(-c^2\right) dc,$$
(4)

where U is the macroscopic velocity of the gas, q is the thermal flux density along the capillary tube, x and c_{ρ} are two-dimensional vectors in a plane normal to the z axis, and the x,z coordinates are referred to the tube radius R_{o} .

As the boundary conditions we stipulate a completely diffuse scattering of gas molecules by the capillary wall (later the results will be extended to the case of an arbitrary tangential-momentum accommodation level)

$$h(\mathbf{x}, \mathbf{c}) = 0|_{|\mathbf{x}|=1}, \ \mathbf{n} \cdot \mathbf{c}_{\rho} > 0, \tag{5}$$

where **n** is the normal to the channel surface toward the center. With condition (5), Eq. (3) can be formally integrated along the characteristic curves [2]. Using the definitions (4), we easily obtain a system of integral equations for the macroscopic velocity of a gas and for the density of the thermal flux

$$\begin{pmatrix} \psi_{1} \\ \psi_{2} \end{pmatrix} = -\begin{pmatrix} \gamma \\ 1 \end{pmatrix} + \frac{R}{\pi} \int \frac{d\mathbf{x}'}{|\mathbf{x} - \mathbf{x}'|} \begin{pmatrix} J_{0} & (J_{2} - J_{0}) \\ \frac{2}{15} (J_{2} - J_{0}) & \frac{2}{15} (J_{4} - 2J_{2} + \frac{5}{2} J_{0}) \end{pmatrix} \begin{pmatrix} \psi_{1} \\ \psi_{2} \end{pmatrix},$$
(6)

where

$$\psi_{1} = 2R \frac{u}{\tau} - \gamma; \quad \psi_{2} = R \frac{Q}{\tau} - 1; \quad \gamma = \frac{v}{\tau};$$

$$J_{n}(t) = \int_{0}^{\infty} c^{n} \exp\left(-c^{2} - \frac{t}{c}\right) dc; \quad (7)$$

 $(\mathbf{R}|\mathbf{x} - \mathbf{x}'|)$ is the argument of function J_n , parameter γ appears also in Eq. (1) and is called the thermomolecular pressure exponent.

Equations (6) yield the local values of macroscopic parameters. Of practical interest, however, are the mean-over-the-section numerical gas flux I_N and thermal flux I_q in the capillary

$$I_{N} = 2\pi n_{0} \left(\frac{2kT_{0}}{m}\right)^{1/2} \int_{0}^{1} ux dx = L_{NN}X_{N} + L_{Nq}X_{q},$$

$$I_{q} = 2\pi \frac{15}{4} \left(\frac{2kT_{0}}{m}\right)^{1/2} P_{0} \int_{0}^{1} Qx dx = L_{qN}X_{N} + L_{qq}X_{q},$$
(8)

with the thermodynamic forces stipulated in the form [11]

$$X_N = -kv, \ X_q = -\tau/T_0. \tag{9}$$

The reciprocity relation applies to the cross coefficients

$$L_{Na} = L_{aN} \,. \tag{10}$$

(10)

Numerical calculations are more conveniently done with dimensionless quantities which are related to the kinetic coefficients as follows:

$$G_{P} = \left(\frac{m}{2kT_{0}}\right)^{1/2} \frac{2k}{n_{0}} L_{NN}, \ G_{T} = -\left(\frac{m}{2kT_{0}}\right)^{1/2} \frac{2k}{P_{0}} L_{Nq},$$

$$Q_{P} = -\frac{4}{15} \left(\frac{m}{2kT_{0}}\right)^{1/2} \frac{k}{P_{0}} L_{qN}, \ Q_{T} = \frac{4}{15} \left(\frac{m}{2kT_{0}}\right)^{1/2} \frac{1}{P_{0}T_{0}} L_{qq},$$
(11)

and, according to relation (10),

$$Q_P = -\frac{2}{15} \ G_{\rm T} \,. \tag{12}$$

There are also the obvious relations between fluxes $I_N,\ I_q$ and functions $\psi_1\,,\,\psi_2\, respectively$

$$I_{N} = \frac{n_{0}\tau}{2R} \left(\frac{2kT_{0}}{m}\right)^{1/2} \left(\gamma + 2\pi \int_{0}^{1} \psi_{1}xdx\right),$$

$$I_{q} = \frac{15}{4} \frac{P_{0}\tau}{R} \left(\frac{2kT_{0}}{m}\right)^{1/2} \left(1 + 2\pi \int_{0}^{1} \psi_{2}xdx\right).$$
(13)

Important special cases are the thermomolecular pressure and the mechanocaloric effect. The former represents a steady state of the first order, with the temperature gradient main-tained constant and a corresponding pressure gradient established in the system. This state is characterized by a zero numerical mean-over-the-section gas flux, i.e., $I_N = 0$. Expressions (8), (7), (9), (11), and (13) yield here

$$\gamma = \frac{G_{\mathbf{r}}}{G_P} = -2\pi \int_0^1 \psi_{\mathbf{i}} x dx. \tag{14}$$

The mechanocaloric effect represents a steady state of the second order and characterizes a heat transfer along the channel at a constant pressure gradient but without a temperature gradient ($\tau = 0$). Expressions (8), (9), (10), (11), and (14) yield here

$$I_q = \frac{L_{Nq}}{L_{NN}} I_N = -\gamma k T_0 I_N.$$
⁽¹⁵⁾

Thus the universal exponent of thermomolecular pressure γ also determines the magnitude of the mechanocaloric effect.

For determining the fluxes (13) and the thermomolecular pressure exponent (14), one must solve the system of integral equations (6). It is easy to show that these equations are of the Fredholm kind. Therefore, they can be solved by the Bubnov-Galerkin method [12]. For this we select trial functions of the form

$$\tilde{\psi}_1 = a + bx^2, \quad \tilde{\psi}_2 = c. \tag{16}$$

Such a selection is justified by the trend of macroscopic parameters in a continuum ($N_{Kn} \rightarrow 0$) and corresponds to the solution of Navier-Stokes equations or of the equation of heat conduction.

For determining the constants a, b, c the trial functions (16) must be inserted into the system of Eqs. (6), with the requirement of a left-hand orthogonality of the resulting expressions to the basis functions (1 0), (x^2 0), (0, 1), and with the scalar product being

$$(\mathbf{f}, \mathbf{g}) = \int_{0}^{1} \mathbf{f} \cdot \mathbf{g} x dx.$$

Thus the constants a, b, c (and, therefore, also $\tilde{\psi}_1$, $\tilde{\psi}_2$) are found from the solution to a system of three linear algebraic equations. Upon inserting expressions (16) into expressions (13) and (14), we can easily determine the fluxes I_N and I_q as well as the thermomolecular pressure exponent γ . The final expressions are rather unwieldy and will not be shown here. It is worthwhile, however, to show their asymptotic expansions:

1. $R \ll 1$



Fig. 1. Poiseuille flux Gp as a function of the rarefaction index R and of the tangential-momentum accommodation coefficient α : 1) $\alpha = 1.0$; 2) 0.97; 3) 0.90 (I -Ne; II - Ar) [14].

Fig. 2. Thermal creep G_T as a function of the rarefaction index R: 1) S-model, 2) Bubnov-Galerkin-Knudsen model [1,2].

$$G_{P} = 1.5045 + R \ln R - 0.3842R - 0.8024R^{2},$$

$$G_{T} = 0.7523 + R \ln R + 0.1158R - 1.2036R^{2},$$

$$Q_{T} = 0.4514 + \frac{R}{3} \ln R - 0.06139R - 0.3477R^{2}.$$
(17)

2. $R \gg 1$

$$G_{P} = \frac{R}{4} + 1.0073 + \frac{1}{R} \quad 0.6712 - \frac{1}{R^{2}} \quad 0.8657,$$

$$G_{r} = \frac{1}{R} \quad 1.125 - \frac{1}{R^{2}} \quad 1.4687 + \frac{1}{R^{3}} \quad 0.6704 - \frac{1}{R^{4}} \quad 2.3424,$$

$$Q_{r} = \frac{1}{R} \quad 0.5 - \frac{1}{R^{2}} \quad 0.5078 + \frac{1}{R^{3}} \quad 0.2469 - \frac{1}{R^{4}} \quad 0.3146.$$
(18)

The solution must be extended to the case of an arbitrary accommodation of gas molecules at the channel surface. Following the procedure in [13], we rewrite the boundary condition (5) as

$$h(\mathbf{x}, \mathbf{c}) = Ac_{\mathbf{z}|_{\mathbf{r}=1}}, \ \mathbf{n} \cdot \mathbf{c}_{\rho} > 0.$$
⁽¹⁹⁾

The constant A is determined in terms of the tangential-momentum accommodation coefficient α from the expression

$$\alpha = \frac{|P_{xz}| - |P_{xz}|}{|P_{xz}|}, \qquad (20)$$

where P_{xz}^{\pm} denote the fluxes of molecules impinging on and reflected from the capillary wall respectively.

Faithfully repeating the procedure proposed in [13], we can easily establish the following relation between fluxes at complete and at an arbitrary tangential-momentum accommodation level respectively:

$$G_P(R; \alpha) = G_P(R; 1) + \sqrt{\pi} \frac{1-\alpha}{\alpha},$$

$$G_T(R; \alpha) = G_T(R; 1), \ Q_T(R; \alpha) = Q_T(R; 1).$$
(21)

We have thus found that thermal creep $G_{\rm T}$ and thermal flux $Q_{\rm T}$ do not depend on $\alpha.$

According to relations (14) and (21),

$$\gamma(R; \alpha) = \frac{G_{\tau}(R; 1)}{G_{P}(R; 1) + \sqrt{\pi} \frac{1 - \alpha}{\alpha}}.$$
(22)



Fig. 3. Universal exponent of thermomolecular pressure γ as a function of the rarefaction index R and of the tangential-momentum accommodation coefficient α : 1) S-model, $\alpha = 1.0, 2$) S-model, $\alpha = 0.97, 3$) S-model, $\alpha = 0.85, 4$) Bubnov-Galerkin-Knudsen model, $\alpha = 1.0$ [1, 2]; (I - neon, II - argon) [8].

Fig. 4. Universal exponent of thermomolecular pressure γ as a function of the rarefaction index R in the slip mode: 1) S-model, 2) Bubnov-Galerkin-Knudsen model [2]; (I - neon, II - argon) [9].

For the free-molecular mode, moreover, the Knudsen relation [6] extends to arbitrary values of coefficient α , namely

$$\lim_{R \to 0} \gamma = \frac{1}{2 + \frac{3}{4} \pi \frac{1 - \alpha}{\alpha}}.$$
 (23)

Numerical calculations of fluxes Gp, $G_{\rm T}$, and $Q_{\rm T}$ for various values of the gas rarefaction index R were performed on a BESM-6 high-speed computer with a precision not worse than 0.1%.

The theoretical results for a Poiseuille flux Gp are compared in Fig. 1 with the experimental data in [14]. The experiments had been performed in long glass capillaries with fused walls, by the method of relaxation of a small pressure drop. The theoretical curves, corresponding to $\alpha = 0.97$ (curve 2) and $\alpha = 0.90$ (curve 3), accurately describe the data for argon and neon over the entire range of radii R, the discrepancy not exceeding the measurement error.

The data on thermal creep G_T obtained in this study and on the basis of the Bubnov-Galerkin-Knudsen model [1,2] are shown in Fig. 2, curves 1 and 2 respectively. The discrepancy reaches 31% at R \approx 10, and is due to an inadequate approximation of the total intermolecular-collision operator in the Bubnov-Galerkin-Knudsen model. The results according to this model can be improved by a special matching of the gas rarefaction index [1], but even then their deviation from the S-model will amount to $\sqrt{5\%}$ at R \approx 3. These authors could not make comparisons with the data in [3], unfortunately, because the latter had been presented in an inconvenient form.

Theoretical values of the thermomolecular pressure exponent γ are compared in Fig. 3 with the experimental values in [8]. That experiment was performed in long glass capillaries at the temperature ratio $T_1/T_2 = 77/299$. The theoretical curves, corresponding to $\alpha = 0.97$ and $\alpha = 0.85$, describe the experimental data for argon and neon with satisfactory accuracy. Interestingly, the same value of α was obtained also for an isothermal Poiseuille flow of argon, a somewhat different accommodation coefficient in the case of neon.

Theoretical values and experimental values obtained in [9] under conditions with slip $(R \gg 1)$ are compared in Fig. 4. This mode is described by expressions (18). The accommodation coefficient selected on the basis of closest agreement between theory and experiment is for neon $\alpha \approx 0.5$. Such a decrease of α can be explained by the formation, with rising pressure, of a layer of adsorbed molecules on the capillary wall and by the surface thus becoming molecularly smooth. There is also another possible cause: the effect of thermomolecular pressure in the slip mode can depend not only on the tangential-momentum accommodation coefficient but also on the accommodation coefficients relative to other macroscopic parameters (e.g., of the tangential energy flux). Even if such a dependence exists, however, it weakens

to an intermediate one and disappears entirely in the free-molecular mode. This is confirmed by a comparative analysis of experimental data on isothermal Poiseuille flow and thermomolecular pressure.

NOTATION

Here N_{Kn} is the Knudsen number; γ , the universal exponent of thermomolecular pressure; R_o, the radius of a cylindrical capillary; P, the pressure; T, the temperature, ν , the logarithmic pressure gradient; τ , the logarithmic temperature gradient; U, the macroscopic gas velocity; q, the thermal flux density; R, the gas rarefaction index; l, the length of the mean free path; I_N , the numerical mean-over-the-section gas flux; I_q , the mean-over-thesection thermal flux; and α , the tangential-momentum accommodation coefficient.

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MEASUREMENT OF NONSTATIONARY HEAT FLUXES BY

"AUXILIARY WALL" SENSORS

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Computational dependences are obtained to determine the nonstationary heat flux by using sensors executing the method of an auxiliary wall. The dependences are valid for an arbitrary relationship between the thermophysical properties of the sensor and the object on which it is located.

The peculiarities of measuring nonstationary heat fluxes by heat meters executing the method of an auxiliary wall are considered in [1]. A number of dependences is presented to determine the flux $q(\tau)$ of heat meters located on the surface of a semi-infinite body for particular values of the thermophysical properties of the heat meter and the base, defined by the magnitude of the criterion $\kappa = (\lambda_2/\lambda_1)\sqrt{(\alpha_1/\alpha_2)} = 0$; 1.0; ∞ . A solution of the problem is presented below for any values of κ . As in [1], the model of the heat meter is represented in the form of a plate located on a half-space (sketch). The temperature fields of the heat meter $t_1(x, \tau)$ and the base $t_2(x, \tau)$ are described by the equations

$$\frac{\partial t_i}{\partial \tau} = a_i \left(\frac{\partial^2 t_i}{\partial x^2} \right), \ i = 1; 2.$$
⁽¹⁾

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