NONISOTHERMAL FLOW OF A RAREFIED MULTIATOMIC GAS IN A CHANNEL

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Previous studies of nonisothermal flow of rarefied gases in channels have mainly been dedicated to monoatomic gases. There are only a few studies in which methods based on use of the kinetic equations are employed to describe the flow of a polyatomic gas [1, 2]. Interest in nonisothermal flow in channels and the thermomolecular pressure difference produced by such a flow is due to the possibility of determining the translational component of thermal conductivity (the Aiken translation factor), which given experimental data on the total thermal conductivity of the gas provides an independent source of data on internal energy relaxation times, which are usually determined by experiments on ultrasound absorption or other methods. In [1] the problem of nonisothermal flow of a polyatomic gas in a planar channel was solved using the linearized kinetic equation of Wang-Chang and Uhlenbeck with a third-order model collision operation in the Hanson-Morze form. To calculate the dimensionless Poisseuille flow, thermocreep flux, and thermal flux in the function for the reciprocal Knudsen number a numerical procedure was used to solve the integral equations obtained from the original kinetic equation. The results of numerical calculations for certain special cases indicate a quite strongly expressed dependence of the thermomolecular pressure difference effect on the translational Aiken factor f^t and a weak dependence on total Aiken factor f. In the present study we will use the method proposed in [3] and employed previously in [3-5] for study of the flow of monoatomic gases and gas mixtures to analyze the flow of a polyatomic gas. Although its use must be limited to a range of Knudsen numbers not exceeding 0.25, this method has the advantage of permitting use of an exact (not model) collision operator in the kinetic equation. Analytical expressions will be obtained for the Poiseuille flow, thermocreep flux, and heat flux of a polyatomic gas in a plane channel, valid for the indicated Knudsen number range, and results will be compared with the numerical calculations of [1].

We will consider the slow flow of a polyatomic gas in a plane channel, bounded at $x = \pm d/2$ by two infinite parallel planes. In the z-direction there exist small relative pressure ($k = p_0^{-1}dp/dz$) and temperature ($\tau = T_0^{-1}dT/dz$) gradients. A solution for the molecular distribution function can then be sought in the form

$$f_i(\mathbf{v}, x, z, \varepsilon_i) = f_{i0}\left[1 + kz + \tau z\left(\beta v^2 - \frac{5}{2} + \varepsilon_i - \bar{\varepsilon}\right) + \Phi_i(\mathbf{v}, x, \varepsilon_i)\right],$$
$$f_{i0} = n_0\left(\frac{m}{2\pi k_B T_0}\right)^{3/2} Q_0^{-1}\exp(-\beta v^2 - \varepsilon_i), \quad \beta = m/2k_B T_0. \tag{1}$$

Here the subscript 0 corresponds to parameters of an absolute Maxwell-Boltzmann distribution $\varepsilon_i = E_i/k_B T_0$; E_i is the internal energy of molecules located in the i-th quantum state; $\bar{\varepsilon} = Q_0^{-1}\sum_i \varepsilon_i \exp(-\varepsilon_i)$; $Q_0 = \sum_i \exp(-\varepsilon_i)$. The nonequilibrium addition to the distribution function $\Phi_i(V, x, \varepsilon_i)$ is determined from the linearized kinetic equation of Wang-Chang and Unlenbeck [6]

$$v_x\frac{\partial\Phi_i}{\partial x} + v_z k + v_z\tau\left(\beta v^2 - \frac{5}{2} + \varepsilon_i - \bar{\varepsilon}\right) = \sum_{jkl}\int f_{j0}\left(\Phi_k' + \Phi_{1l}' - \Phi_i - \Phi_{1j}\right) g\sigma(ij/kl, g, \chi)\, d\Omega d\mathbf{v}_1. \tag{2}$$

Multiplying Eq. (2) successively by $\Psi(c, \varepsilon_i)\exp(-c^2 - \varepsilon_i)$, where $\Psi(c, \varepsilon_i) = c_r$, $c_r c_s - (1/3)c^2\delta_{rs}$, $c_r(c^2 - 5/2)$, $c_r c_s c_t - (1/5)c^2(c_r\delta_{st} + c_s\delta_{rt} + c_t\delta_{rs})$, $c_r(\varepsilon_i - \bar{\varepsilon})$, $c = \beta^{1/2}v$, integrating over velocities and summing over the i-th quantum states, given the planar geometry of the problem we arrive at moment equations of the form

$$p_0 k + \frac{\partial}{\partial x}\pi_{xz} = 0; \tag{3}$$

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$$\frac{\partial}{\partial x}\left(ms_{zxx}+\frac{2}{5}q_z^{\mathrm{t}}+p_0u_z\right)=-\frac{8n_0\Omega_\eta}{5}\pi_{xz}; \tag{4}$$

$$\frac{\partial}{\partial x}(M_{zxxx}+M_{zxyy}+M_{zxzz})+5\frac{p_0^2}{\rho_0 m}(k+\tau)=-\frac{32}{15}\frac{n_0}{m}\left(\Omega_\eta+\frac{25}{24}\Omega_E\right)q_z^{\mathrm{t}}+\frac{10k_{\mathrm{B}}n_0}{3c^{\mathrm{in}}m}\Omega_E q_z^{\mathrm{in}}; \tag{5}$$

$$\frac{\partial}{\partial x}M_{xz}^{\varepsilon}+\frac{p_0c^{\mathrm{in}}}{k_{\mathrm{B}}m}\tau=\frac{2}{3}n_0^2\Omega_E\frac{1}{p_0}q_z^{\mathrm{t}}-\frac{8}{3}n_0^2\left(\Omega_D+\frac{3k_{\mathrm{B}}}{8c^{\mathrm{in}}}\Omega_E\right)\frac{1}{p_0}q_z^{\mathrm{in}}; \tag{6}$$

$$\frac{\partial}{\partial x}(4M_{zxxx}-M_{zxyy}-M_{zxzz})=-12n_0\Omega_\eta s_{zxx}; \tag{7}$$

$$\frac{\partial}{\partial x}(4M_{zxyy}-M_{zxxx}-M_{zxzz})=-12n_0\Omega_\eta s_{zyy}; \tag{8}$$

$$s_{zxx}+s_{zyy}+s_{zzz}=0. \tag{9}$$

The right sides of Eqs. (4)-(6) coincide with the expressions obtained in the 17-moment approximation in [7]. The additional moments of the collision integrals appearing in Eqs. (7), (8) are obtained upon consideration of yet another polynomial of the form $c_rc_sc_t - (1/5)c^2(c_r\delta_{st} + c_s\delta_{rt} + c_t\delta_{rs})$, the use of which corresponds to a 20-moment approximation, the case of single component gases. In Eqs. (3)-(9) u_z is the hydrodynamic velocity; π_{xz} is the viscous stress tensor; q_z^{t} is the thermal flux produced by translational motion of molecules; q_z^{in} is the thermal flux produced by internal degrees of molecular freedom. The expressions for these moments and for the higher-order moments s_{rst}, M_{rs}^{ε}, and M_{rstk} can be written in the form

$$\begin{bmatrix} u_r \\ \pi_{rs} \\ q_r^{\mathrm{t}} \\ q_r^{\mathrm{in}} \\ ms_{rst} \\ \\ mM_{rs}^{\varepsilon} \\ mM_{rstk} \end{bmatrix}=2p_0\beta^{-1/2}\pi^{-3/2}Q_0^{-1}\sum_i\int\begin{bmatrix} (2p_0)^{-1}c_r \\ \beta^{1/2}\left(c_rc_s-\frac{1}{3}c^2\delta_{rs}\right) \\ \frac{1}{2}c_r\left(c^2-\frac{5}{2}\right) \\ \frac{1}{2}c_r(\varepsilon_i-\bar{\varepsilon}) \\ c_rc_sc_t-\frac{1}{5}c^2(c_r\delta_{st}+ \\ +c_s\delta_{rt}+c_t\delta_{rs}) \\ \beta^{1/2}c_rc_s(\varepsilon_i-\bar{\varepsilon}) \\ \beta^{-1/2}c_rc_sc_tc_k \end{bmatrix}\Phi_i\exp(-c^2-\varepsilon_i)\,d\mathbf{c}. \tag{10}$$

The heat capacity c^{in}, corresponding to the internal degrees of freedom, and the integral quantities Ω_E, Ω_η, Ω_D were defined in [7].

Far from the walls the system of equations must correspond to the approximation obtained within the framework of the conventional Grade model, generalized to the case of a polyatomic gas in [7, 8]. After linearization with consideration of the smallness of the quantities u_z, π_{xz}, q_z^{t}, q_z^{in}, s_{rst} the distribution function in this region can be written in the form

$$\begin{aligned}\Phi_i^{\mathrm{as}}(\mathbf{c},x,\varepsilon_i)&=2\beta^{1/2}u_z^{\mathrm{as}}c_z+2p_0^{-1}\pi_{xz}^{\mathrm{as}}c_xc_z+\frac{4}{5}p_0^{-1}\beta^{1/2}q_z^{\mathrm{t.as}}c_z\left(c^2-\frac{5}{2}\right)+\\&+2k_{\mathrm{B}}\beta^{1/2}(p_0c^{\mathrm{in}})^{-1}q_z^{\mathrm{in.as}}c_z(\varepsilon_i-\bar{\varepsilon})+2\beta^{1/2}p_0^{-1}mc_z\left(s_{zxx}^{\mathrm{as}}c_x^2+\right.\\&\left.+s_{zyy}^{\mathrm{as}}c_y^2+\frac{1}{3}s_{zzz}^{\mathrm{as}}c_z^2\right),\end{aligned} \tag{11}$$

where the superscript "as" indicates asymptotic values of the corresponding quantities, i.e., values outside the Knudsen layer.

Substituting Eq. (11) in M_{rs}^{ε} and M_{rstk}, integrating over velocities, and summing over the i-th quantum states, we have

$$M_{zxxx}^{as}=\frac{3\pi_{xz}^{as}}{2m\beta},\ M_{zxyy}^{as}=\frac{\pi_{xz}^{as}}{2m\beta},\ M_{zxzz}^{as}=\frac{3\pi_{xz}^{as}}{2m\beta},\ M_{xz}^{\varepsilon\,as}=0. \tag{12}$$

Solution of the system (3)-(9) with consideration of Eq. (12) and the symmetry of the problem relative to the longitudinal channel axis ($\Phi_i(x, c_x, c_y, c_z, \varepsilon_i) = \Phi_i(-x - c_x, c_y, c_z, \varepsilon_i)$) allows us to obtain explicit expressions for u_z^{as}, π_{xz}^{as}, $q_z^{t.as}$, $q_z^{in.as}$, s_{rst}^{as}:

$$\begin{gathered}
u_z^{as}(x)=u_z^{as}\left(\frac{d}{2}\right)+\frac{1}{2\eta}\left(x^2-\frac{d^2}{4}\right)\frac{dp}{dz},\ \pi_{xz}^{as}(x)=-x\frac{dp}{dz},\\
q_z^{t.as}=-\lambda^{t}\frac{dT}{dz}+\chi^{t}\frac{dp}{dz},\ q_z^{in.as}=-\lambda^{in}\frac{dT}{dz}+\chi^{in}\frac{dp}{dz},\\
s_{zxx}^{as}=\frac{16}{15}\frac{\eta}{m\rho_0}\frac{dp}{dz},\ s_{zyy}^{as}=-\frac{1}{4}s_{zxx}^{as},\ s_{zzz}^{as}=-\frac{3}{4}s_{zxx}^{as},
\end{gathered} \tag{13}$$

where

$$\lambda^{t}=\frac{15k_B}{4m}\eta\left\{1-\frac{4c^{in}}{3\pi k_B Z\Delta}\left[\frac{5}{2}-\left(\frac{\rho_0 D^{in}}{\eta}\right)\right]\right\}; \tag{14}$$

$$\begin{gathered}
\lambda^{in}=\left(\frac{\rho_0 D^{in}}{\eta}\right)\frac{c^{in}}{m}\eta\left\{1+\frac{2}{\pi Z\Delta}\left[\frac{5}{2}-\left(\frac{\rho_0 D^{in}}{\eta}\right)\right]\right\},\\
\chi^{t}=\frac{3\eta}{2\rho_0}\left(1-\frac{10\,c^{in}}{3\pi k_B Z\Delta}\right),\quad \chi^{in}=\frac{2c^{in}}{\pi k_B\rho_0 Z\Delta}\eta\left(\frac{\rho_0 D^{in}}{\eta}\right),\\
\Delta=1+\frac{2}{\pi Z}\left[\left(\frac{\rho_0 D^{in}}{\eta}\right)+\frac{5c^{in}}{3k_B}\right].
\end{gathered} \tag{15}$$

We then have $Z=\frac{4}{\pi}\frac{\tau_E}{\tau_\eta}$, $\rho_0 D^{in}=p_0\tau_D$, $\eta=\rho_0\tau_\eta$, $\tau_E^{-1}=(2k_B/c^{in})n_0\Omega_E$, $\tau_\eta^{-1}=8n_0\Omega_\eta/5$, $\tau_D^{-1}=8n_0\Omega_D/3$. Here Z corresponds to some mean number of collisions, necessary for relaxation of the energy deviations of the internal degrees of freedom from the translational energy; D^{in} is the internal energy diffusion coefficient.

Following the method of [3-5], we find expressions averaged over the channel area for the thermal flux and hydrodynamic velocity. It follows from solution of Eq. (3) that in the entire flow region

$$\pi_{xz}(x) = -x dp/dz. \tag{16}$$

Substituting this value in Eq. (4), integrating the relationship obtained over x, the averaging over channel section, we have

$$m\langle s_{zxx}\rangle+\frac{2}{5}\langle q_z^{t}\rangle+p_0\langle u_z\rangle=L_1, \tag{17}$$

where

$$L_1=ms_{zxx}\left(\frac{d}{2}\right)+\frac{2}{5}q_z^{t}\left(\frac{d}{2}\right)+p_0u_z\left(\frac{d}{2}\right)-\frac{p_0 d^2}{12\eta}\frac{dp}{dz},\ \langle Q\rangle=d^{-1}\int_{-d/2}^{d/2}Q(x)\,dx.$$

Also averaging Eqs. (5)-(7) over the channel section, we obtain

$$\begin{gathered}
-\frac{4p_0}{3m\eta}\left(1+\frac{10c^{in}}{3\pi k_B Z}\right)\langle q_z^{t}\rangle+\frac{20p_0}{3\pi m\eta Z}\langle q_z^{in}\rangle=L_2,\\
\frac{4n_0c^{in}}{3\pi k_B\eta Z}\langle q_z^{t}\rangle-\frac{n_0}{\eta}\left(\frac{\rho_0 D^{in}}{\eta}\right)^{-1}\left[1+\frac{2}{\pi Z}\left(\frac{\rho_0 D^{in}}{\eta}\right)\right]\langle q_z^{in}\rangle=L_3,\\
-\frac{15p_0}{2\eta}\langle s_{zxx}\rangle=L_4,
\end{gathered} \tag{18}$$

where

$$L_2=\frac{2}{d}\left[M_{zxxx}\left(\frac{d}{2}\right)+M_{zxyy}\left(\frac{d}{2}\right)+M_{zxzz}\left(\frac{d}{2}\right)\right]+\frac{5p_0^2}{m\rho_0}(k+\tau);\quad L_3=$$
$$=\frac{2}{d}M_{xz}^{\varepsilon}\left(\frac{d}{2}\right)+\frac{p_0c^{in}}{k_Bm}\tau;\quad L_4=\frac{2}{d}\left[4M_{zxxx}\left(\frac{d}{2}\right)-M_{zxyy}\left(\frac{d}{2}\right)-M_{zxzz}\left(\frac{d}{2}\right)\right].$$

Solution of Eqs. (17), (18) leads to the results

$$\langle u_z\rangle = \frac{1}{p_0} L_1 + \frac{m\rho_0}{5p_0^2}\chi^{t} L_2 + \frac{mk_B}{p_0 c^{in}}\chi^{in} L_3 + \frac{2m\eta}{15p_0^2} L_4,$$
$$\langle q_z\rangle = \langle q_z^{t}\rangle + \langle q_z^{in}\rangle = -\frac{m^2\lambda^{t}}{5k_B p_0} L_2 - \frac{m\lambda^{in}}{n_0 c^{in}} L_3. \tag{19}$$

To determine the unknown quantities on the channel wall we use the approximate method of [9]. We introduce distribution functions for incident and reflected molecules such that $\Phi_i = \Phi_i^+$ for $c_x > 0$ and $\Phi_i = \Phi_i^-$ for $c_x < 0$. For the kinetic boundary condition we assume that a portion of the incident molecules are reflected specularly (with no change in the distribution over internal states of the molecules), while the other portion is initially adsorbed on the wall, and then emitted with a Maxwell–Boltzmann distribution at temperature T. According to Eq. (11), for the function $\Phi_i^{\pm}$ at $x = d/2$ we have

$$\Phi_i^+(\mathbf{c}, \varepsilon_i, d/2) = 2\beta^{1/2}c_z a + 2p_0^{-1}\pi_{xz}^{as}\left(\frac{d}{2}\right)c_x c_z + \frac{4}{5}p_0^{-1}\beta^{1/2}q_z^{t.as}c_z\Big(c^2 -$$
$$-\frac{5}{2}\Big) + 2k_B\beta^{1/2}\left(p_0 c^{in}\right)^{-1}q_z^{in.as}c_z(\varepsilon_i - \bar{\varepsilon}) + 2\beta^{1/2}p_0^{-1}mc_z\left(s_{zxx}^{as}c_x^2 + s_{zyy}^{as}c_y^2 + \frac{1}{3}s_{zzz}^{as}c_z^2\right), \quad c_x > 0, \tag{20}$$
$$\Phi_i^-(\mathbf{c}, \varepsilon_i, d/2) = (1-\varkappa)\Phi_i^+(-c_x, c_y, c_z, \varepsilon_i, d/2), \quad c_x < 0,$$

where $\varkappa$ is the fraction of molecules experiencing diffuse reflection on the wall, and in place of $u_z^{as}(d/2)$ we introduce the arbitrary constant a.

Using Eq. (16) and the definition of π_{xz}, Eq. (10), on the channel wall, after calculating the corresponding integrals with consideration of Eq. (20) we find

$$a = -\beta^{-1/2}\frac{\sqrt{\pi}}{4}d\frac{(2-\varkappa)}{\varkappa p_0}\frac{dp}{dz} - \frac{1}{5p_0}q_z^{t.as} - \frac{m}{2p_0}s_{zxx}^{as}. \tag{21}$$

Substituting Eq.(21) in Eq. (20), we obtain the unknown quantities on the channel wall appearing in L_i.

According to the thermodynamics of irreversible processes for continuous systems [10], the relationship between the fluxes and gradients can be represented as

$$\langle q_z\rangle = -\Lambda_{qq}T^{-2}\frac{dT}{dz} - \Lambda_{qm}T^{-1}\frac{dp}{dz},$$
$$\langle \bar{u}_z\rangle = -\Lambda_{mq}T^{-2}\frac{dT}{dz} - \Lambda_{mm}T^{-1}\frac{dp}{dz}. \tag{22}$$

We introduce the dimensionless quantities

$$J_m^* = J_m/mJ_0 = 2\beta^{1/2}\langle u_z\rangle,\; J_q^* = J_q/k_B T_0 J_0 = 2\beta^{1/2}p_0^{-1}\langle q_z\rangle,$$

where J_m and J_q are the corresponding averaged mass and heat fluxes per unit cross-sectional area of the channel; $J_0 = n_0/2\beta^{1/2}$. Then $J_m^* = -L_{mm}kd - L_{mq}\tau d$, $J_q^* = -L_{qm}kd - L_{qq}\tau d$.

The expressions for the dimensionless kinetic coefficients L_{ik}, obtained by comparison of Eqs. (22) and (19), have the form

$$L_{mm} = \frac{\delta}{6} + (2-\varkappa)\left[\frac{(2-\varkappa)}{\varkappa}\frac{\sqrt{\pi}}{4} + \frac{1}{\sqrt{\pi}}\right] + \frac{\varkappa\rho_0}{5\eta}\left(\chi^{t} + \frac{8}{3}\frac{\eta}{\rho_0}\right)\frac{1}{\delta} -$$
$$\frac{32\varkappa}{25\sqrt{\pi}}\left\{\frac{\rho_0}{3\eta}\left(\chi^{t} + \frac{3\eta}{\rho_0}\right) + \frac{3\rho_0^2}{8\eta^2}\left[(\chi^{t})^2 + \frac{25}{12}\frac{k_B}{c^{in}}(\chi^{in})^2\right]\right\}\frac{1}{\delta^2}; \tag{23}$$

$$L_{mq} = L_{qm} = -\frac{(2+\varkappa)m}{10k_B\eta}\lambda^{t}\frac{1}{\delta} + \frac{12\varkappa m\rho_0}{25\sqrt{\pi}k_B\eta^2}\left[\lambda^{t}\left(\chi^{t} + \frac{4}{9}\frac{\eta}{\rho_0}\right) + \frac{25}{12}\frac{k_B}{c^{in}}\lambda^{in}\chi^{in}\right]\frac{1}{\delta^2}; \tag{24}$$

$$L_{qq} = \frac{m\lambda}{k_B\eta}\frac{1}{\delta} - \frac{12\varkappa m^2}{25\sqrt{\pi}k_B^2\eta^2}\left[(\lambda^{t})^2 + \frac{25}{12}\frac{k_B}{c^{in}}(\lambda^{in})^2\right]\frac{1}{\delta^2}, \tag{25}$$

where $\delta = \mathrm{Kn}^{-1} = p_0\beta^{1/2}d/\eta$ is the reciprocal Knudsen number; $\lambda = \lambda^{t} + \lambda^{in}$.

The results of a numerical calculation of the coefficients L_{mm}, L_{mq}, and L_{qq} were presented in [1] for a planar channel and the case of totally diffuse reflection ($\varkappa = 1$) in the reciprocal Knudsen number function δ. An analysis was performed of the dependence of these coefficients on the total and translational Aiken factors, defined as

TABLE 1

δ	$f^t=2,24$ L_{mm} 1	L_{mm} 2	$f=1,96$ $-L_{mq}$ 1	$-L_{mq}$ 2	L_{qq} 1	L_{qq} 2
3	1,6085	1,7154	0,1560	0,2054	1,1450	1,2230
5	1,9384	1,9952	0,1368	0,1491	0,8042	0,8218
7	2,2551	2,2988	0,1109	0,1170	0,6103	0,6178
10	2,7367	2,7717	0,0846	0,0883	0,4460	0,4494
20	4,3755	4,4003	0,0463	0,0481	0,2340	0,2348
30	6,0313	6,0580	0,0318	0,0330	0,1584	0,1588
40	7,6923	7,7326	0,0242	0,0251	0,1198	0,1199

TABLE 2

δ	$-L_{mq}/L_{mm}$ $f=1,96$; $f^t=2,31$ 1	2	$f=1,96$; $f^t=2,24$ 1	2	$f=1,96$; $f^t=2,17$ 1	2
3	0,0980	0,1225	0,0970	0,1197	0,0952	0,1167
5	0,0721	0,0767	0,0706	0,0747	0,0688	0,0727
7	0,0504	0,0523	0,0492	0,0509	0,0479	0,0494
10	0,0318	0,0328	0,0309	0,0318	0,0300	0,0309
20	0,0109	0,0112	0,0106	0,0109	0,0103	0,0106
30	0,0054	0,0056	0,0053	0,0054	0,0051	0,0052
40	0,0032	0,0033	0,0031	0,0032	0,0030	0,0031

$$f = f^t \frac{c^t}{c_V} + f^{in} \frac{c^{in}}{c_V}, \quad f^t = \frac{\lambda^t m}{\eta c^t}, \quad f^{in} = \frac{\lambda^{in} m}{\eta c^{in}}.$$

The calculations assumed that $c^t = 3k_B/2$, $c^{in} = k_B$.

For comparison with the results of [1], we can express the quantities λ^t, λ^{in}, χ^t, χ^{in} appearing in Eqs. (23)-(25) in terms of f_t and f with consideration of relationships following from Eqs. (14), (15).

Table 1 presents a comparison of results of calculating the kinetic coefficients for $f = 1.96$ and $f^t = 2.24$ on the basis of Eqs. (23)-(25) of the present study for the case of totally diffuse reflection ($\varkappa = 1$) (first column) with the data of [1] (second column) for values $\delta \geqslant 3$.

The comparison shows that the coefficient values calculated with Eqs. (23)-(25) prove to be somewhat lower, with the difference from the results of [1] not exceeding 3% for L_{mm} and L_{qq}, and from 4 to 10% for L_{mq} at $\delta \geq 5$ (Kn $\leqslant$ 0.2). In the limit of small Knudsen numbers our results coincide completely with the data using values of the viscous and thermal slip coefficients obtained with the aid of the variation method of [11]. Calculation of coefficients for f = 1.92, 1.96, and 2.0 for fixed $f^t = 2.24$ confirm the conclusion of [1] as to the weak dependence of these coefficients on total Aiken factor. In addition, as was observed in [1], there is a clearly expressed dependence of the coefficient L_{mq} on translational Aiken factor f^t for f = const. As is well known, the thermomolecular pressure difference effect (appearance of a pressure difference Δp between volumes joined by a thin capillary or slit at fixed temperature difference ΔT) is defined by the expression

$$\frac{\Delta p/p_0}{\Delta T/T_0} = -\frac{L_{mq}}{L_{mm}}.$$

Table 2 presents a comparison of values of the ratio $-L_{mq}/L_{mm}$, calculated with the expressions of the present study (first column) and in [1] (second column) at f = 1.96 for f^t = 2.17, 2.24, 2.31. The observed dependence on f^t confirms the possibility of using the thermomolecular pressure difference effect to determine internal energy relaxation times (or the factor Z).

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VIBRATIONAL AND CHEMICAL KINETICS EQUATIONS IN A COMPLEX GAS MIXTURE

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As a result of the development of computer engineering, as well as the achievements of experimental and theoretical science on the kinetics of elementary processes in gas systems, as a research instrument supplementing, or even replacing completely, the tedium of experiment in the last two decades, computation of complex mixtures in composition and gasdynamics are widespread. In particular, a broad class of problems exists for the analysis of multicomponent gas mixture flow which requires taking account jointly of the chemical reaction kinetics and the vibrational energy exchange processes. On the basis of utilizing simplifying assumptions in the majority of problems of this kind, the kinetic equations are formulated in the form of macroscopic equations for the concentration and the mean vibrational energies of the components or separate vibrational degrees of freedom (modes) (see [1, 2], e.g.). However, knowledge of the population of the vibrational levels of the separate molecular components of the mixture that changes as a result of chemical and vibrational interaction with a large number of other components can have value, in principle, in solving a number of problems (for instance, in modeling working media flows in chemical lasers [3]). Sequential formulation of the kinetic equations in the form of population balance equations for the vibrational states of a large number of complex mixture components, without already speaking about the extreme tedium of solving them in conjunction with the gasdynamics equations, evidently simply have no practical meaning because of the absence of detailed information about the quantitative characteristics of a very large number of elementary processes required in this case.

Such a formulation of the kinetic equations, in which one group of chemical components and vibrational states is considered microscopically (i.e., in the form of population balance equations) and the other macroscopically (i.e., in the form of equations for the mean vibrational energies and concentrations), results in a significant reduction in the vibrational states taken into account and in their associated elementary processes as compared with the sequential microscopic approach. An example is given in this paper of such a combined formulation of the kinetic equations. Here the subsystem considered microscopically is a mixture of diatomic gases, anharmonic oscillators, chemically and vibrationally interacting mutually and with other polyatomic components comprising the subsystem considered macroscopically, in the general case.

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