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CHOICE OF THE INTERMOLECULAR COLLISION FREQUENCY FOR MODEL KINETIC EQUATIONS IN THE THEORY OF MOTION OF A RAREFIED GAS

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The effect of the intermolecular collision frequency on the nonisothermal motion of a rarefied gas is considered.

1. The motion of a one-component rarefied gas in a channel has been theoretically treated using various methods based on the Boltzmann equation or models derivable from it. A fairly complete review of this approach can be found in [1-4]. The problem has been solved using the BGK equations [1-3], the ellipsoidal statistical model (EL model) of [5, 6], and the S model of [7, 8]. The advantage of third-order models, such as the EL and S models, compared to the BGK model is that in the approach to a continuous medium, the former give correct expressions for the stress tensor and heat-flux density [9].

The general form of the linearized kinetic equation for the third-order models is given in [10]. In the solution of the equation, one must choose the intermolecular collision frequency γ. The choice for γ is fairly arbitrary [9, 10], but at the same time it should be done such that the solution obtained from the model equation correspond to that of the Boltzmann equation.

In [11, 12] the effect of the choice for the intermolecular collision frequency on the solutions for Couette flow and the structure of shock waves was studied using a method based on the model equations proposed by Gross and Jackson [13].

In the present paper, we study the heat and mass transport of a rarefied gas moving in a plane channel under temperature and pressure gradients using the third-order model kinetic equation [10] for different values of the frequency γ. We then study the effect of the value γ on the solution over the whole range of Knudsen numbers.

2. We consider motion of a monoatomic one-component rarefied gas in a channel formed by two infinite parallel plates ($x = \pm d/2$) and induced by pressure and temperature gradients along the channel, where the z axis is taken along the channel. We consider the state of the gas to be weakly perturbed and therefore the distribution function can be written in the form

$$f(\vec{r}, \vec{v}) = f_0(z, \vec{v})[1 + h(x, \vec{v})], \ \|h(x, \vec{v})\| \ll 1, \tag{1}$$

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

where $n(z)$, $T(z)$, and m are, respectively, the number density, temperature of the gas, and mass of the molecule. The function $h(x, \vec{v})$ is the perturbation.

We write the third-order linearized model kinetic equation in the form [7, 10]

$$v_x \frac{\partial h}{\partial x} + v_z\left[\nu + \tau\left(c^2 - \frac{5}{2}\right)\right] = -\gamma h + 2\gamma u_z c_z + 4P_{xz}(\gamma - \nu^{(3)} + \nu^{(4)}) c_x c_z + \frac{8}{5} q_z (\gamma - \nu^{(5)} + \nu^{(6)})\left(c^2 - \frac{5}{2}\right) c_z, \tag{2}$$

where the macroscopic quantities, in correspondence with their kinetic definitions, can be written in the form

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$$\begin{bmatrix} u_z \\ P_{xz} \\ q_z \end{bmatrix} = \pi^{-3/2} \int \begin{bmatrix} c_z \\ c_x c_z \\ \frac{1}{2}\left(c^2 - \frac{5}{2}\right) c_z \end{bmatrix} h e^{-c^2} \vec{dc}, \tag{3}$$

$$\vec{c} = \beta \vec{v}, \quad \beta = \left(\frac{m}{2kT_0}\right)^{1/2}, \quad \nu = \left(\frac{d}{P}\right)\frac{dP}{dz},$$

$$\tau = \left(\frac{d}{T}\right)\frac{dT}{dz}, \quad T_0 = T(z = 0).$$

Explicit forms for $\nu^{(3)}$, $\nu^{(4)}$, $\nu^{(5)}$, $\nu^{(6)}$ are given in [10]:

$$\nu^{(4)} - \nu^{(3)} = -\frac{8}{5} n\Omega^{(22)}, \tag{4}$$

$$\nu^{(6)} - \nu^{(5)} = -\frac{16}{15} n\Omega^{(22)}.$$

Because of the linearity of the problem and the smallness of the perturbation h, one can write

$$h = h^P \nu + h^T \tau. \tag{5}$$

Following [7], we transform the kinetic equation (2) into a system of three linear integral equations for the heat flux density q_z, stress tensor P_{xz}, and macroscopic gas velocity u_z

$$\vec{\psi} = A\vec{\psi} + \vec{B}. \tag{6}$$

Where the following notation is used in (6):

$$A\vec{\psi} = \frac{\delta}{\sqrt{\pi}} \int_{-1/2}^{+1/2} D\vec{\psi}\, ds, \quad \vec{B} = -\frac{1}{2\sqrt{\pi}} \int_{-1/2}^{+1/2} \vec{E}\, ds,$$

$$D = \begin{bmatrix} J_{-1} & 2(1 - s_0) J_0 \operatorname{sign}(x - s) & \frac{4}{5}\left(1 - \frac{2}{3} s_0\right)\left(J_1 - \frac{1}{2} J_{-1}\right) \\ J_0 \operatorname{sign}(x - s) & 2(1 - s_0) J_1 & \frac{4}{5}\left(1 - \frac{2}{3} s_0\right)\left(J_2 - \frac{1}{2} J_0\right) \operatorname{sign}(x - s) \\ \frac{1}{2}\left(J_1 - \frac{1}{2} J_{-1}\right) & (1 - s_0)\left(J_2 - \frac{1}{2} J_0\right) \operatorname{sign}(x - s) & \frac{2}{5}\left(1 - \frac{2}{3} s_0\right)\left(J_3 - J_1 + \frac{9}{4} J_{-1}\right) \end{bmatrix}, \tag{7}$$

$$\vec{\psi} = \begin{bmatrix} u_z \\ P_{xz} \\ q_z \end{bmatrix}, \quad \vec{E} = \begin{bmatrix} J_{-1}\nu + \left(J_1 - \frac{1}{2} J_{-1}\right)\tau \\ J_0 \operatorname{sign}(x - s)\nu + \left(J_2 - \frac{1}{2} J_0\right) \operatorname{sign}(x - s)\tau \\ \frac{1}{2}\left(J_1 - \frac{1}{2} J_{-1}\right)\nu + \frac{1}{2}\left(J_3 - J_1 + \frac{9}{4} J_{-1}\right)\tau \end{bmatrix},$$

$$\delta = \beta d \gamma, \quad s_0 = \frac{\gamma_{BGK}}{\gamma} = \frac{8n\Omega^{(22)}}{5\gamma},$$

$$J_n(t) = \int_0^\infty c^n \exp\left(-c^2 - \frac{t}{c}\right) dc.$$

The argument of the functions J_n, which have been studied in detail in [14], is $(\delta|x - s|)$. Information on these functions can be found in [15].

The system of equations (6) determine the local values of the macroscopic gas velocity, stress tensor, and heat flux density. With the help of (5), they divide into two sets of integral equations, one of which describes the motion of the gas under a temperature gradient and the other under a pressure gradient. In practice we are interested in the number flux I_N and heat flux I_q averaged over the channel cross section:

$$I_q = \frac{2P_0}{\beta}\int\limits_{-1/2}^{+1/2} q_z(x)\,dx = L_{qq}X_q + L_{qN}X_N, \tag{8}$$

$$I_N = \frac{n_0}{\beta}\int\limits_{-1/2}^{+1/2} u_z(x)\,dx = L_{Nq}X_q + L_{NN}X_N.$$

Then the macroscopic fluxes corresponding to the thermodynamic forces are taken in the following form [16-18]:

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

In (8) the off-diagonal coefficients satisfy the symmetry relation

$$L_{qN} = L_{Nq}. \tag{10}$$

Equations (8) are next written in the convenient form

$$I_q = \frac{P_0T_0}{\beta}\ l_{qq}X_q + \frac{n_0T_0}{\beta}l_{qN}X_N, \tag{11}$$

$$I_N = \frac{n_0T_0}{\beta}l_{Nq}X_q + \frac{n_0}{\beta k}l_{NN}X_N.$$

From the equality of the coefficients (10) it follows that

$$l_{qN} = l_{Nq}. \tag{12}$$

In (11), P_0 and T_0 are the pressure and temperature of the gas in the center of the channel ($z = 0$).

Equations (6) were solved using the method of Galerkin [19] with the following approximation for $\overset{\rightrightarrows}{\psi}$:

$$\overset{\rightrightarrows}{\psi} = \begin{bmatrix} \tilde{A} + \tilde{B}x^2 \\ \tilde{C}x \\ \tilde{D} \end{bmatrix}. \tag{13}$$

This form for $\overset{\rightrightarrows}{\psi}$ is correct in the continuum limit.

After solving (6) it is convenient to transform to dimensionless quantities, related to the kinetic coefficients as follows [7, 18]:

$$G_P = \frac{2\beta k}{n_0}L_{NN} = 2l_{NN},\quad G_T = -\frac{2\beta}{n_0T_0}L_{Nq} = -2l_{Nq},$$

$$Q_P = -\frac{\beta}{2n_0T_0}L_{qN} = -\frac{1}{2}l_{qN},\ Q_T = \frac{\beta}{2P_0T_0}L_{qq} = \frac{1}{2}l_{qq}. \tag{14}$$

These quantities are convenient to use in comparisons with those of other authors. From the Onsager reciprocity relations for the off-diagonal coefficients (10) it follows that

$$G_T = 4Q_P. \tag{15}$$

In calculations for a specific case, the intermolecular collision frequency γ must be chosen. We considered three forms for γ:

$$\gamma = \frac{8}{5}n\Omega^{(22)}. \tag{16}$$

In this case we obtain from (2) the linearized S model equation of Shakhov [9, 20]. If we ignore the heat flux density q_z on the right-hand side of (2), we obtain the well-known BGK model equation [21]

$$\gamma = \frac{16}{15}n\Omega^{(22)}. \tag{17}$$

Here we obtain the linearized EL model of Holway [22].

TABLE 1. Values of the Parameter s_0

γ	s_0
S model [9, 20]	1
EL model [22, 10]	1.5
	0.7742 for the hard sphere potential [24]
	0.8613 for the (6-12) Lennard - Jones potential for Ar at T = 300°K [25]
	0.8740 for the (6-12) Lennard - Jones potential for He, at T = 300°K [25]

$$\gamma = \frac{8}{15} n \left(\Omega^{(22)} + \Omega^{(13)} - 5\Omega^{(12)} + \frac{35}{4} \Omega^{(11)} \right). \tag{18}$$

This form for γ was suggested in [10] and was used in the study of the motion of a mixture of rarefied gases [18]. Here $\Omega^{(lr)}$ are the Chapman–Cowling integrals [23] which depend on the form of the molecular interaction potential.

In the solution of the system of integral equations (6), the quantity s_0, determined by (7), appears explicitly. Values of s_0 used in the present paper are given in Table 1. The data on the $\Omega^{(lr)}$ was taken from [23-25].

3. We now discuss the results for different values of γ. In doing this, it is convenient to compare the fluxes (14) taken as functions of the product δs_0, rather than as functions of the rarefaction parameter δ alone. It can easily be shown that δs_0 is inversely proportional to the Knudsen number [6, 21]. The dependence of the fluxes G_P, G_T, Q_P, and Q_T on δs_0 are shown in Table 2.

It follows from comparison of the results in Tables 1 and 2 that (15) is correct for different values of s_0. Consequently, for any choice of δ, the Onsager reciprocity relations are satisfied for all Knudsen numbers. Also the G_P are identical to within less than 1% as a function of s_0 if $\delta s_0 > 10$. G_P increases with increasing s_0 for all δs_0. G_T values are identical for different values of s_0 (to less than 1%) if $\delta s_0 \geqslant 50$. However if $\delta s_0 < 0.5$, G_T increases with increasing s_0 and if $\delta s_0 > 0.5$, it decreases with increasing s_0. A similar dependence is observed for Q_P, as suggested by (15), and also for Q_T. Thus for $\delta s_0 < 1$, Q_T increases with increasing s_0, and for $\delta s_0 > 1$ it decreases with increasing s_0.

From the values of G_P and Q_T in the viscous case ($\delta s_0 \to \infty$), the viscosity η and thermal conductivity λ can be calculated as follows:

$$\eta = \frac{1}{12} (\delta s_0) \alpha_0 \frac{1}{l_{NN} (\delta s_0 \to \infty)}, \tag{19}$$

$$\lambda = 2 (\delta s_0) \alpha_0 \beta_0 l_{qq} (\delta s_0 \to \infty), \tag{20}$$

$$\alpha_0 = 0.266949 \cdot 10^{-5} \frac{\sqrt{MT}}{\sigma^2} \frac{1}{\Omega^{(22)*}}, \quad \beta_0 = 8314.36 \frac{1}{M}. \tag{21}$$

Where M is the mass of a gas molecule in a.e., σ is the scattering cross section of the molecule in Å, and $\Omega^{(lr)*}$ are the reduced Ω integrals [23-25].

The fact that the fluxes $G_P(Q_T)$ are constant with respect to s_0 for large δs_0 shows that η and λ do not depend on the intermolecular collision frequency γ.

In Table 3 we show the results for the viscosities of the inert gases using (19) for the (6-12) Lennard–Jones potential as compared to values obtained in the first Chapman–Enskog approximation [25], as well as to values obtained by experiment [26] and to values recommended in [27]. The results for the thermal conductivity of the inert gases according to (20) and the (6-12) Lennard–Jones potential are compared to those obtained in the first approximation in the Chapman–Enskog method [25], and to the handbook values recommended in [27, 28] and given for comparison in Table 4.

Comparison of the values of the transport coefficients given in Tables 3 and 4 shows that our approach for calculating the kinetic coefficients for the viscous flow of a gas is correct.

TABLE 2. Fluxes G_P, G_T, Q_P, Q_T as functions of δs_0

δs_0	s_0				
	0,7742	0,8613	0,8740	1	1,5
			G_P		
0,01	2,925	2,978	2,985	3,052	3,257
0,05	2,206	2,242	2,249	2,306	2,479
0,1	1,951	1,987	1,992	2,040	2,193
0,5	1,564	1,584	1,587	1,614	1,706
1	1,518	1,532	1,534	1,553	1,620
5	1,984	1,991	1,992	2,001	2,031
10	2,760	2,765	2,765	2,772	2,800
50	9,360	9,362	9,362	9,364	9,372
100	$1{,}768\cdot 10^{1}$	$1{,}769\cdot 10^{1}$	$1{,}769\cdot 10^{1}$	$1{,}769\cdot 10^{1}$	$1{,}769\cdot 10^{1}$
500	8,434	8,434	8,434	8,434	8,434
1000	$1{,}677\cdot 10^{2}$	$1\cdot 677\cdot 10^{2}$	$1{,}677\cdot 10^{2}$	$1{,}677\cdot 10^{2}$	$1{,}677\cdot 10^{2}$
			G_T		
0,01	1,189	1,213	1,216	1,247	1,341
0,05	$8{,}350\cdot 10^{-1}$	$8{,}475\cdot 10^{-1}$	$8{,}503\cdot 10^{-1}$	$8{,}720\cdot 10^{-1}$	$9{,}386\cdot 10^{-1}$
0,1	7,052	7,162	7,178	7,325	7,820
0,5	4,634	4,624	4,623	4,619	4,659
1	3,732	3,689	3,683	3,636	3,537
5	1,658	1,636	1,633	1,603	1,508
10	$9{,}679\cdot 10^{-2}$	$9{,}613\cdot 10^{-2}$	$9{,}603\cdot 10^{-2}$	$9{,}508\cdot 10^{-2}$	$9{,}145\cdot 10^{-2}$
50	2,185	2,182	2,182	2,179	2,165
100	1,109	1,108	1,108	1,108	1,104
500	$2{,}243\cdot 10^{-3}$	$2{,}243\cdot 10^{-3}$	$2{,}243\cdot 10^{-3}$	$2{,}243\cdot 10^{-3}$	$2{,}241\cdot 10^{-3}$
1000	1,123	1,123	1,123	1,123	1,123
			Q_P		
0,01	0,2974	0,3034	0,3041	0,3116	0,3353
0,05	0,2087	0,2119	0,2126	0,2181	0,2346
0,1	0,1763	0,1791	0,1795	0,1831	0,1956
0,5	0,1158	0,1156	0,1156	0,1155	0,1165
1	$0{,}9332\cdot 10^{-1}$	$0{,}9221\cdot 10^{-1}$	$0{,}9208\cdot 10^{-1}$	$0{,}9088\cdot 10^{-1}$	$0{,}8843\cdot 10^{-1}$
5	0,4144	0,4089	0,4082	0,4007	0,3771
10	0,2419	0,2404	0,2400	0,2378	0,2286
50	$0\ 5462\cdot 10^{-2}$	$0{,}5456\cdot 10^{-2}$	$0{,}5454\cdot 10^{-2}$	$0{,}5447\cdot 10^{-2}$	$0{,}5413\cdot 10^{-2}$
100	0,2771	0,2769	0,2769	0,2768	0,2760
500	$0{,}5608\cdot 10^{-3}$	$0{,}5608\cdot 10^{-3}$	$0{,}5608\cdot 10^{-3}$	$0{,}5606\cdot 10^{-3}$	$0{,}5604\cdot 10^{-3}$
1000	0,2809	0,2809	0,2809	0,2809	0,2807
			Q_T		
0,01	1,614	1,643	1,647	1,684	1,796
0,05	1,156	1,177	1,180	1,208	1,294
0,1	0,9724	0,9893	0,9915	1,013	1,083
0,5	0,5852	0,5899	0,5906	0,5972	0,6201
1	0,4341	0,4352	0,4354	0,4373	0,4453
5	0,1537	0,1535	0,1534	0,1532	0,1525
10	$0{,}8479\cdot 10^{-1}$	$0{,}8475\cdot 10^{-1}$	$0{,}8473\cdot 10^{-1}$	$0{,}8468\cdot 10^{-1}$	$0{,}8447\cdot 10^{-1}$
50	0,1838	0,1837	0,1837	0,1837	0,1837
100	$0{,}9281\cdot 10^{-2}$	$0{,}9281\cdot 10^{-2}$	$0{,}9281\cdot 10^{-2}$	$0{,}9281\cdot 10^{-2}$	$0{,}9279\cdot 10^{-2}$
500	0,1871	0,1871	0,1871	0,1871	0,1871
1000	$0{,}9366\cdot 10^{-3}$	$0{,}9366\cdot 10^{-3}$	$0{,}9366\cdot 10^{-3}$	$0{,}9366\cdot 10^{-3}$	$0{,}9366\cdot 10^{-3}$

TABLE 3. Dynamic Viscosity for the Inert Gases, $\eta\cdot 10^{8}$ Pa-sec, $T = 300°K$, $P = 1.013\cdot 10^{5}$ Pa

Literature source	He	Ne	Ar	Kr	Xe
Eq. (19)	1986	3173	2266	2578	2354
Chapman – Enskog meth. [25]	1998	3192	2282	2594	2369
[26]	1972	3203	2272	2530	2308
[27]	—	3175	2275	2554	2350

When δs_0 is large, the following asymptotic formulas for G_P and G_T are valid:

$$G_P = \frac{\delta s_0}{6} + \frac{\sqrt{\pi}}{2}\,\sigma_P, \tag{22}$$

where

$$\sigma_P = \frac{1}{2} + \frac{2}{\pi}, \tag{23}$$

TABLE 4. Thermal Conductivities of the Inert Gases, $\lambda \cdot 10^5$ W(m-deg), T = 300°K, P = $1.013 \cdot 10^5$ Pa

Literature source	He	Ne	Ar	Kr	Xe
Eq. (20)	15544	4926	1780	964	562
Chapman – Enskog meth. [25]	15560	4931	1782	964	563
[28]	15200	4900	1770	958	569
[27]	—	4908	1777	951	558

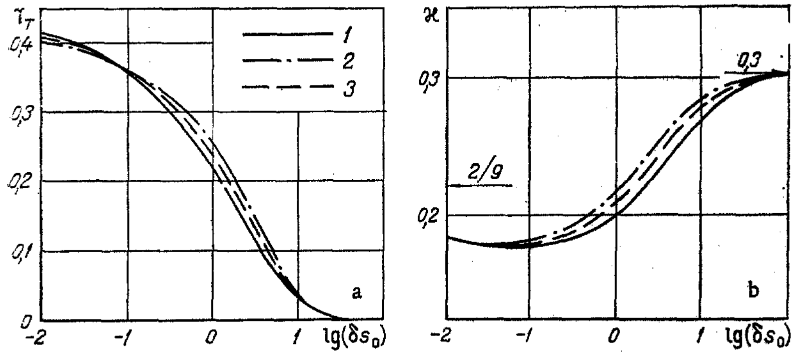

Fig. 1. Indices for the TPD effect (a) and thermoeffect (b) as a function of log (δs_0): Curve 1) $s_0 = 1.5$ (EL model); curve 2) $s_0 = 0.7742$; curve 3) $s_0 = 1$ (S model).

$$G_T = \frac{A_T}{\delta s_0}, \quad A_T = \frac{9}{8}. \tag{24}$$

Here σ_P is the Poiseuille slip constant [1] and A_T is the thermal slip constant [2]. Equation (22) agrees completely with earlier results using the BGK and EL models [1] and the S model [29, 30] for diffusive scattering of gas molecules at the walls of the channel. We note that in the numerical results for σ_P in [31] there is an error; in place of $\frac{\sqrt{\pi}}{2}\sigma_P = 1.0073$ the value 1.0161 is given.

The thermal slip constant A_T is obtained as in the S model [8, 30], but differs from the value $A_T = 0.75$ obtained in the BGK model [32, 33]. This is due to the inability of the BGK model to describe both heat and mass transport in a gas simultaneously [9].

We consider first-order cross-over effects in a rarefied gas: the thermomolecular pressure difference effect (TPD) and the thermoeffect due to a pressure gradient. According to a theorem of Prigogine on stationary states of order k [16], the following condition is satisfied for the TPD effect:

$$I_N = 0. \tag{25}$$

For thermoeffect, the analogous condition is

$$I_q = 0. \tag{26}$$

On the other hand, the TPD effect is described by the relations [3, 8, 34]

$$\frac{P_1}{P_2} = \left(\frac{T_1}{T_2}\right)^{\gamma_T}, \quad \gamma_T = \frac{G_T}{G_P}, \tag{27}$$

where γ_T is usually called the TPD effect index.

The dependence of γ_T on δs_0 for different values of s_0 is shown in Fig. 1a. The maximum dispersion is observed for $\delta s_0 \sim 1$ and is about 13%. For the thermoeffect, the analogous formula to (27) is

$$\frac{T_1}{T_2} = \left(\frac{P_1}{P_2}\right)^{\varkappa}, \quad \varkappa = \frac{Q_P}{Q_T}, \tag{28}$$

where $\varkappa$ is the thermoeffect index. In Fig. 1b, the dependence of $\varkappa$ on δs_0 is shown for different values of s_0. The maximum dispersion is observed for $\delta s_0 \sim 5$ and is about 9%.

In the free molecule case ($\delta s_0 \to 0$) $\gamma_T = 0.5$ and $\varkappa = 2/9$. In the viscous flow regime ($\delta s_0 \to \infty$) $\gamma_T \to 0$ and $\varkappa = 0.3$ and is independent of s_0.

NOTATION

d, distance between the plates; f_0, Maxwell distribution function; $\vec{v}$, velocity of gas molecules; k, Boltzmann constant; ν, logarithmic pressure gradient; τ, logarithmic temperature gradient; δ, rarefaction parameter; G_P, Poiseuille flow; G_T thermal creep flow; Q_T, Q_P, heat fluxes under temperature and pressure gradients, respectively.

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STRESSES, VISCOSITY, AND SCALES IN MOLAR TRANSFER

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The article presents unified relations describing the profiles of molar stresses and viscosity.

For the calculation of heat and mass transfer in engineering devices it is indispensable to know the distribution of molar stresses and viscosity in the turbulent boundary layer. However, to this day there is no unified relations describing the molar stress and viscosity profiles for complex flow conditions, e.g., in case of a rough surface, the entrance section of a channel, etc. [1].

It is known [1] that in the turbulent core of a two-dimensional steady turbulent boundary layer the terms of the stress tensor satisfy the inequality

$$\sigma_u^{+2} > \sigma_w^{+2} > \sigma_v^{+2} > \tau^+. \tag{1}$$

For flow in the boundary layer on a plate, taking (1) into account, we represent σ_V^{+2} in the form

$$\tau^+ = \sigma_v^{+2} - \xi_v \sigma_v^{+2}. \tag{2}$$

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