Mathematical simulation of a mass transfer in a cylindrical channel

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Abstract. A rarefied gas flow through a long circular tube due to pressure and temperature gradients is studied on the basis of the S-model kinetic equation. The Maxwellian mirror-diffuse reflection model is used as the boundary condition on the channel walls. The mass flow rate is calculated as a function of the small pressure and temperature gradients. Similar results presented in the literature are compared. The thermomolecular pressure effect has been modeled and the coefficient of the thermomolecular pressure difference has been calculated at various values of the accommodation coefficient and in whole range of the Knudsen number.

1. Introduction
The study of mass transfer in a cylindrical channel is essential for many practical applications [1–3]. The description of such a process in a rarefied gas is based on the solution of the Boltzmann kinetic equation or model kinetic equations. Thus, in [4] and [5] the solution of the linearized S-model of the kinetic Boltzmann equation for a cylindrical channel is obtained using the method of discrete ordinates and velocities, in [6] the spectral method using cubic splines is applied, in [7] and [8] – the conservative method of representing an implicit second-order scheme on unstructured grids. The application of these methods requires significant computational costs, and as a consequence, it remains relevant to search for alternative approaches to solving model kinetic equations. It should also be noted that in all the above works the diffuse boundary condition on the channel walls is used. More realistic is its generalization – the Maxwell boundary condition, which leads to an inhomogeneous boundary conditions for a linearized model equation.

The aim of this work is to develop the collocation method [9] for solving the problem of mass transfer in a long cylindrical channel based on the S-model of the kinetic Boltzmann equation [1] using Chebyshev polynomials and Chebyshev rational functions [9, 10]. The Maxwell model of mirror-diffuse reflection is used as a boundary condition on the cylinder surface [11]. The values of the reduced mass flows depending on the value of the rarefaction parameter are obtained and their comparative analysis is carried out.

2. Materials and methods
Let us consider the flow of a rarefied gas in a cylindrical channel of radius \( R' \) in the middle part of the channel. The \( z' \) axis will be directed along the channel axis. We assume that the channel length \( L' \gg R' \) and dimensionless pressure gradients \( G_p \) and temperature \( G_T \) are small.
in absolute value. In the linear approximation for the functions of temperature and gas pressure in the channel we obtain the following expressions

\[ T(z) = T_0(1 + G_T z), \quad G_T = \frac{R'}{T} \frac{dT}{dz}, \quad p(z) = p_0(1 + G_p z), \quad G_p = \frac{R'}{p} \frac{dp}{dz}. \]

The radius \( R' \) of the cylindrical channel is chosen as the length dimension scale. Dimensionless length values we will further denote without a stroke. The state of a rarefied gas at a point, in the channel we obtain the following expressions

\[ \frac{1}{R^2} \rho \frac{d}{dz} \left( \frac{1}{2} \right) \left( \frac{d^2}{dz^2} \right) + \rho \left( \frac{\partial}{\partial z} \right) + \frac{\rho}{2} \frac{d^3}{dz^3} = 0. \]

Following [1] and [2], we introduce a dimensionless mass velocity and a reduced gas mass flow as

\[ u_z = \frac{1}{R^2} \rho \left( \frac{d}{dz} \right) + \frac{\rho}{2} \frac{d^3}{dz^3}, \quad u_z(\mathbf{r}) = \frac{1}{n(z)} \int u_z f(\mathbf{r}, \mathbf{C}) d^3 \mathbf{v}, \]

\[ J_M = \frac{J_M'}{\pi R^2 p(z)} \left( \frac{2k_B T(z)}{m} \right) = G_p J_{M1} + G_T J_{M2}, \quad J_{M,i} = \frac{1}{3} \int U_{z,i}(\rho) d\rho. \]

From (1) and (2) the dimensionless component \( U_{z,i} \) is defined by the function \( h_i \):

\[ U_{z,i}(\rho) = \frac{1}{\pi^{3/2}} \int \exp \left( -C^2 \right) C_z h_i(\rho, \mathbf{C}) d^3 \mathbf{C}, \quad i = 1, 2. \]

To find \( h_1 \) we write the S-model of the kinetic Boltzmann equation in the cylindrical coordinate system [5], [13]

\[ \left( \frac{\partial h_1}{\partial \rho} \cos \psi - \frac{\partial h_1}{\partial \psi} \sin \psi \right) C_z + \delta h_1(\rho, \mathbf{C}) = \delta \frac{1}{\pi^{3/2}} \int K(\mathbf{C}, \mathbf{C}') \exp(-C'^2) h_1(\rho, \mathbf{C}') d^3 \mathbf{C}'. \]

Here \( \delta = \frac{1}{Kn} \) is the rarefaction parameter, \( Kn = l_g / R' \) is the Knudsen number, \( l_g = \eta_0 \beta^{-1/2} / p \) is the mean free path of gas molecules, \( \eta_0 \) is the dynamic viscosity of the gas, \( K(\mathbf{C}, \mathbf{C}') \) is the core of this equation [13]

\[ K(\mathbf{C}, \mathbf{C}') = \frac{4}{15} (C_z'^2 - \frac{5}{2}) (C_z^2 - \frac{5}{2}) + 2 C_z C_z' + \frac{2}{3} \left( C'^2 - \frac{3}{2} \right) (C_z^2 - \frac{3}{2}) + 1. \]

The calculation of \( J_{M,2} \) is carried out according to the Onsager relation \( J_{M,2} = J_{Q,1} \) [1], where \( J_{Q,1} \) is the reduced heat flow at isothermal flow under the pressure gradient:

\[ J_Q = G_p J_{Q,1} = 4G_p \int q_{z,1}(\rho) d\rho, \quad q_{z,1}(\rho) = \frac{1}{\pi^{3/2}} \int \exp \left( -C^2 \right) C_z \left( C_z^2 - \frac{5}{2} \right) h_1(\rho, \mathbf{C}) d^3 \mathbf{C}. \]
Multiply the left and right sides of equation (5) by $C_z^k \exp(-C_z^2)/\sqrt{\pi} \ (k = 1, 3)$ and integrate $C_z$ from $-\infty$ to $+\infty$.

Then, to find the mass velocity $U_{z,1}(\rho)$ and the components of the heat flux vector $q_{z,1}(\rho)$ we come to a system of equations:

$$
\left( \frac{\partial Z_1}{\partial \rho} + \frac{\partial Z_1 (1-\xi^2)}{\rho} \right) C_\perp + \delta Z_1(\rho, C_\perp, \zeta) + \frac{1}{2} = \delta \left( U_{z,1}(\rho) + \frac{2}{15} q_{z,1}(\rho)(C_\perp^2 - 1) \right),
$$

$$
\left( \frac{\partial Z_2}{\partial \rho} + \frac{\partial Z_2 (1-\xi^2)}{\rho} \right) C_\perp + \delta Z_2(\rho, C_\perp, \zeta) + \frac{3}{4} = \delta \left( \frac{3}{2} U_{z,1}(\rho) + \frac{1}{5} q_{z,1}(\rho) C_\perp^2 \right),
$$

where $\zeta = \cos \psi$ and $Z_i(\rho, C_\perp, \zeta) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \exp(-C_z^2)C_z^{2i-1}h_1(\rho, C) dC_z, \quad i = 1, 2$.

Taking into account the Maxwell mirror-diffuse reflection model on the channel walls [11], we obtain the following boundary conditions for the function $Z_i$:

$$
Z_i(1, C_\perp, \zeta) = (1 - \alpha)Z_i(1, C_\perp, -\zeta), \quad \zeta < 0, \quad i = 1, 2,
$$

where $\alpha$ is the accommodation coefficient of the tangential momentum of the gas molecules.

The components $U_{z,1}$ and $q_{z,1}$ are expressed through the introduced functions $Z_i(\rho, C_\perp, \zeta) \ (i = 1, 2)$ as

$$
U_{z,1}(\rho) = \frac{2}{\pi} \int_{0}^{+\infty} \exp(-C_z^2)C_\perp^{1} \int_{-1}^{1} \frac{1}{\sqrt{1-\xi^2}} Z_1(\rho, C_\perp, \zeta) d\xi dC_\perp,
$$

$$
q_{z,1}(\rho) = \frac{2}{\pi} \int_{0}^{+\infty} \exp(-C_z^2)C_\perp^{1} \int_{-1}^{1} \frac{1}{\sqrt{1-\xi^2}} Z_2(\rho, C_\perp, \zeta) d\xi dC_\perp
$$

$$
+ \frac{2}{\pi} \int_{0}^{+\infty} \exp(-C_z^2)C_\perp^{3} \int_{-1}^{1} \frac{1}{\sqrt{1-\xi^2}} Z_1(\rho, C_\perp, \zeta) d\xi dC_\perp - \frac{5}{2} U_{z,1}(\rho) +
$$

To find the solution of the system of equations (6) and (7) with boundary conditions (8), we decompose the unknown functions $Z_i(\rho, C_\perp, \zeta) \ (i = 1, 2)$ in a series of polynomials and Chebyshev rational functions [9, 10]. By limiting in this series members with numbers $j_k \leq n_k$ \ (k = 1, 3), we obtain

$$
Z_i(\rho, C_\perp, \zeta) = T_1(\rho^*)Q(\zeta)W(C_\perp^*)A_1, \quad i = 1, 2.
$$

Here $\rho^* = 2\rho - 1, \ C^*_\perp = (C_\perp - 1)/(C_\perp + 1), \ A_1 = A_{n_1 n_2 n_3 \times 1}$ is unknown column matrix \ (i = 1, 2) (for brevity, we use the notation $n_k = n_1 + 1 (k = 1, 3)$):

$$
A_1 = \begin{pmatrix}
a^{(i)}_{000} & a^{(i)}_{001} & \ldots & a^{(i)}_{00n_3} & a^{(i)}_{n_10} & a^{(i)}_{n_1 n_2} & \ldots & a^{(i)}_{n_1 n_2 n_3}
\end{pmatrix}^T,
$$

$$
T_1(\rho^*) = T_{1 \times n_1'}, \quad T_{1 \times n}(x) = (T_0(x)T_1(x) \ldots T_n(x)), \quad x \in [-1, 1],
$$

and $Q(\zeta)$ and $W(C_\perp)$ are block-diagonal matrices

$$
Q(\zeta) = \Phi_{n_1' \times n_2'}(\zeta), \quad W(C_\perp^*) = \Phi_{n_1' n_2' \times n_3'}(C_\perp^*),
$$

where $\Phi_{n \times n}(\zeta)$ is the Chebyshev rational function.
we multiply the resulting equations by

\[ \Phi_{m \times n}(x) = \text{diag}(T_{1 \times n}(x), T_{1 \times n}(x), \ldots, T_{1 \times n}(x)). \]  

(15)

To determine \( T_i(x) \) in (13) we apply the recompetitive relations [9]

\[ T_0(x) = 1, \quad T_1(x) = x, \quad T_i(x) = 2xT_{i-1}(x) - T_{i-2}(x), \quad i \geq 2. \]

(16)

Derivatives of \( T_1(\rho^*) \) by \( \rho \) and \( T_2(\zeta) \) by \( \zeta \) can be defined as

\[ \frac{dT_1(\rho^*)}{d\rho} = 2T_1(\rho^*)J_1, \quad \frac{dT_2(\zeta)}{d\zeta} = T_2(\zeta)J_2, \]

(17)

where \( J_k = J_n \) is a matrix \((k = 1, 2)\) whose nonzero elements \((J_k)_{i,j+1} \) are calculated by the formulas \((i,j = 1\ldots n) [9]\)

\[ (J_k)_{i,j+1} = \begin{cases} j, & i = 1, j \text{ odd}, \\ 2j & j > i - 1, \text{ even}, j \text{ even}, \\ 2j & j > i - 1, \text{ even}, j \text{ odd, } j \text{ odd}. \end{cases} \]

(18)

By substituting (11) in (9) and (10), for the components \( U_{z,1}(\rho^*) \) and \( q_{z,1}(\rho^*) \), we obtain the following expressions

\[ U_{z,1}(\rho^*) = 4P_1(\rho^*) A_1, \]

(19)

\[ q_{z,1}(\rho^*) = 4 \left( P_3(\rho^*) - \frac{5}{2} P_1(\rho^*) \right) A_1 + 4P_1(\rho^*) A_2. \]

(20)

Here \( P_i \ (i = 1, 3) \) are matrices of size \( 1 \times n_1' n_2' n_3' \), whose nonzero elements are defined as

\[ (P_i)_{1,n_1' n_2' n_3' j_1+1 j_3+1} = I_{i,j_3}(T_1)_{1,j_1+1}(\rho^*), \quad j_1, j_3 = 0, n_1, n_3. \]

(21)

\[ 2I_{i,j_3} = \int_0^{+\infty} \exp(-C^2) C_{1} T_{j_3}(C_{1}) dC_{1}. \]

Integrals \( I_{i,j_3} \ (i = 1, 2, j_3 = 0, n_3) \) are found numerically by the formula Clenshaw-Curtis [14]. To do this, we will Express the variables \( \rho \) and \( C_{1} \) through \( \rho^* \) and \( C_{1}^* \) in (6)–(8). Then we multiply the resulting equations by

\[ w_i(C_{1}^*) = \exp \left( \frac{1}{2} \frac{(1 + C_{1}^*)^2}{(1 - C_{1}^*)^2} \right) \frac{(1 + C_{1}^*)^i}{(1 - C_{1}^*)^{i+2}}, \quad i = 0, n_3, \]

and integrate by the variable \( C_{1}^* \) from \(-1\) to \(1\). From here, taking into account the ratios (11)–(19), we come to the following system of equations

\[ \Delta_{1,1}(\rho^*, \zeta) A_1 + \Delta_{2,1}(\rho^*) A_2 = -\frac{1}{2} I_{i,0}, \quad i = 0, n_3, \]

(22)

\[ \Delta_{1,1}(\rho^*) A_1 + \Delta_{2,1}(\rho^*, \zeta) A_2 = -\frac{3}{4} I_{i,0}, \quad i = 0, n_3, \]

with boundary conditions

\[ \Omega_i(1, \zeta) = 0, \quad \zeta < 0, \ j = 1, 2; \ i = 0, n_3. \]
Here \( \Omega_1(1, \zeta) = T_1(1) (Q(\zeta) - (1 - \alpha)Q(-\zeta)) W_1, \) \( W_{i'j'k'}^{n'i'j'k'} = \text{diag}(I_1, I_1, \ldots, I_1), \) and the matrices \( A_1 \) and \( \Delta_1 \) \((i = 1, 2)\) have the size \( 1 \times n'1n'2n'3 \) and are defined as follows

\[
\begin{align*}
\Lambda_{1,i}(\rho^*, \zeta) &= \Psi_1(\rho^*, \zeta) W_i + \Psi_2(\rho^*, \zeta) W_{i+1} + \frac{4}{3} \delta P_1(\rho^*)(I_{i+2,0} - 4I_{i,0}) + \frac{8}{15} \delta P_3(\rho^*)(I_{i,0} - I_{i+2,0}), \\
\Lambda_{2,i}(\rho^*) &= \frac{8}{15} \delta (I_{i,0} - I_{i+2,0}) P_1(\rho^*), \\
\Delta_{1,i}(\rho^*) &= 2\delta P_1(\rho^*)(I_{i+2,0} - 3I_{i,0}) - \frac{4}{5} \delta P_3(\rho^*) I_{i+2,0}, \\
\Delta_{2,i}(\rho^*, \zeta) &= \Psi_1(\rho^*, \zeta) W_i + \Psi_2(\rho^*, \zeta) W_{i+1} - \frac{4}{5} \delta P_1(\rho^*) I_{i+2,0}, \\
\Psi_1(\rho^*, \zeta) &= \delta T_1(\rho^*) Q(\zeta), \\
\Psi_2(\rho^*, \zeta) &= 2\zeta T_1(\rho^*) J_1 Q(\zeta) + \frac{2(1 - \zeta^2)}{\rho^* + 1} T_1(\rho^*) Q'(\zeta), \\
Q'(\zeta) &= \text{diag}(T_2(\zeta) J_2, T_2(\zeta) J_2, \ldots, T_2(\zeta) J_2).
\end{align*}
\]

As collocation points \( \rho_{i,k} = x_{1,k} \) and \( \zeta_{k_2} = x_{2,k} \) in relations \((20)-(22)\) we will use zeros of polynomials \( T_{n'}(\hat{x}) \) \((i = 1, 2)\) on the segment \([-1; 1]::\)

\[
x_{i,k} = \cos \left( \frac{\pi (2n_i - 2k_i + 1)}{2(n_i + 1)} \right), \quad k_i = 0, n_i, \ i = 1, 2.
\]

By the substituting \((23)\) in \((20)\), we come to a system of linear \( n'1n'2n'3 \)-equations, in which instead of equations with \( \rho^* = \rho_{n_1}^* \) and \( \zeta = \zeta_{k_2} \) we write the equations, arising from the boundary condition \((22)\) for \( Z_1 \) with the values of the variables \( \rho^* = 1 \) and \( \zeta = \zeta_{k_2} \) \((k_2 = 0, k_2')\). Here \( k_2' \) is an index such that \( \zeta_{k_2'} < 0 \) and \( \zeta_{k_2'} \geq 0 \), i.e. \( k_2' = n_2/2 - 1 \) if \( n_2 \) is even, and \( k_2' = (n_2 - 1)/2 \) otherwise. As a result we get

\[
B_1 A_1 + B_2 A_2 = F_1,
\]

where \( B_j \) \((j = 1, 2)\) are matrices of size \( n'1n'2n'3 \times n'1n'2n'3 \), and \( F_1 \) is a column matrix \((n'1n'2n'3 \times 1)\):

\[
B_1 = \begin{pmatrix}
\Lambda_{1,0}(\rho_{n_1}^*, \zeta_0) \\
\Lambda_{1,1}(\rho_{n_1}^*, \zeta_0) \\
\cdots \\
\Lambda_{1,n_3-1}(\rho_{n_3-1}^*, \zeta_{n_3}) \\
\Lambda_{1,n_3}(\rho_{n_3}^*, \zeta_{n_3}) \\
\Omega_{0}(1, \zeta_0) \\
\Omega_{1}(1, \zeta_0) \\
\cdots \\
\Omega_{n_3}(1, \zeta_{n_3}) \\
\Lambda_{1,0}(\rho_{n_1}^*, \zeta_{k_2'+1}) \\
\cdots \\
\Lambda_{1,n_3-1}(\rho_{n_3-1}^*, \zeta_{n_3}) \\
\Lambda_{1,n_3}(\rho_{n_3}^*, \zeta_{n_3})
\end{pmatrix}, \quad B_2 = \begin{pmatrix}
\Lambda_{2,0}(\rho_{n_1}^*, \zeta_0) \\
\Lambda_{2,1}(\rho_{n_1}^*, \zeta_0) \\
\cdots \\
\Lambda_{2,n_3-1}(\rho_{n_3-1}^*, \zeta_{n_3}) \\
\Lambda_{2,n_3}(\rho_{n_3}^*, \zeta_{n_3}) \\
0 \\
0 \\
\cdots \\
0 \\
\Lambda_{2,0}(\rho_{n_1}^*, \zeta_{k_2'+1}) \\
\cdots \\
\Lambda_{2,n_3-1}(\rho_{n_3-1}^*, \zeta_{n_3}) \\
\Lambda_{2,n_3}(\rho_{n_3}^*, \zeta_{n_3})
\end{pmatrix}, \quad F = \begin{pmatrix}
I_{0,0} \\
I_{1,0} \\
\cdots \\
I_{n_3-1,0} \\
I_{n_3,0} \\
0 \\
0 \\
\cdots \\
0 \\
I_{0,0} \\
I_{n_3,0}
\end{pmatrix} \cdot \frac{1}{2}
\]

Similarly, substituting \((23)\) in \((21)\), we come to a system of linear \( n'1n'2n'3 \)-equations, in which instead of equations with \( \rho^* = \rho_{n_1}^* \) and \( \zeta = \zeta_{k_2} \) we entered the equations arising from the boundary condition \((22)\) for \( Z_2 \) with the values of the variables \( \rho^* = 1 \) and \( \zeta = \zeta_{k_2} \) \((k_2 = 0, k_2')\).

As a result we get

\[
D_1 A_1 + D_2 A_2 = F_2,
\]

(25)
where $F_2 = 3/2F_1$, and the matrices $D_1$ and $D_2$ are defined similarly to $B_2$ and $B_1$, in which $\Lambda_{2,1}$ and $\Lambda_{1,1}$ are replaced respectively by $\Delta_{1,1}$ and $\Delta_{2,1}$ ($i = 0, n_3$).

From (24) and (25) we obtain the equation for finding $A_1$

$$\left( B_1 - B_2D_2^{-1}D_1 \right) A_1 = F_1 - B_2D_2^{-1}F_2. \quad (26)$$

The solution of (26) is found by the $LU$-method in the maple computer algebra system. Taking into account the obtained elements of the matrix $A_1$ according to (18), we obtain an expression for $U_{x,1}(\rho^*)$. Substituting (18) in (3), we have

$$J_{M,1} = 4 \int_{-1}^{1} P_1(\rho^*)(T_0(\rho^*) + T_1(\rho^*))d\rho^* A_1 =$$

$$= 8 \sum_{i_3=0}^{n_3} I_{1,i_3} \left( \sum_{i_1=0}^{[n_3/2]} a^{(1)}_{2n_3'\delta i_1 + i_3 + 1, 1} \frac{[n_3'/2] - 1}{1 - 4i_1^2} + \sum_{i_1=0}^{[n_3'/2]} a^{(1)}_{2n_3'\delta (2i_1 + 1) + i_3 + 1, 1} \frac{[n_3'/2] - 1}{4 - (2i_1 + 1)^2} \right). \quad (27)$$

The values $-J_{M,1}$, which are obtained by the formula (27) at $n^* = n_1 = 2n_{2,3}$ for $\delta < 0.5$ and at $n^* = n_1 = 2n_{2,3}$ for $\delta \geq 0.5$ at various values of the accommodation coefficient of the tangential momentum of gas molecules $\alpha$ are given in tables 1 and 2. For comparison, we have included in these tables and the values of $J_{M,1}$, which are represented in [2, 4–7]. Let us note that the the results in [2, 4] and [5] are obtained by solving the linearized S model of the Boltzmann kinetic equation by the method of discrete velocities and ordinates. In [6] has been used a spectral method by using cubic splines ($\delta = 0.1, 0.5$ and 1). In [7] a conservative method representing an implicit second-order scheme on unstructured grids has been used.

We find the matrix $A_2$ from equation (25). On the basis of the obtained matrix elements $A_i$ $(i = 1, 2)$ according to (19) we restore the component $q_{z,1}(\rho^*)$. Next, taking into account the ratio $J_{M,2} = J_{Q,1}$ we get

$$J_{M,2} = 8 \sum_{i_3=0}^{n_3} I_{3,i_3} \left( \sum_{i_1=0}^{[n_3/2]} a^{(2)}_{2n_3'\delta i_1 + i_3 + 1, 1} \frac{[n_3'/2] - 1}{1 - 4i_1^2} + \sum_{i_1=0}^{[n_3'/2]} a^{(2)}_{2n_3'\delta (2i_1 + 1) + i_3 + 1, 1} \frac{[n_3'/2] - 1}{4 - (2i_1 + 1)^2} \right) +$$

$$+ 8 \sum_{i_3=0}^{n_3} I_{1,i_3} \left( \sum_{i_1=0}^{[n_3/2]} a^{(1)}_{2n_3'\delta i_1 + i_3 + 1, 1} \frac{[n_3'/2] - 1}{1 - 4i_1^2} + \sum_{i_1=0}^{[n_3'/2]} a^{(1)}_{2n_3'\delta (2i_1 + 1) + i_3 + 1, 1} \frac{[n_3'/2] - 1}{4 - (2i_1 + 1)^2} \right) - \frac{5}{2} J_{M,1}. \quad (28)$$

The values $J_{M,2}$ depending on $\alpha$ and $\delta$ are given in tables 3 and 4. It can be seen from tables 1–4 that there is rapid convergence on average with an increase of $n_{1,2,3}$.

Thus, in the presented paper, the solution of the linearized mass transfer problem in a cylindrical channel is obtained by the collocation method using polynomials and Chebyshev rational functions within the mirror-diffuse Maxwell boundary condition. The values of the mass flow in the rarefied gas are calculated on the basis of the constructed solution. Note that in the free molecular regime ($\delta = 0$) equations (6) and (7) with the boundary conditions (8) are significantly simplified and can be solved analytically [15]. The values $J_{M,i}$ ($i = 1, 2$) determined by (3) correspond to the values of $J_{M,1} = -2J_{M,2} = (\alpha - 2)8/(3\alpha \sqrt{\pi})$ [1].
Table 1. Values $-J_{M,1}$ for $\alpha = 0.8$ and $\alpha = 0.6$.

| $\delta$ | $\alpha = 0.8$ | $\alpha = 0.6$ |
|----------|----------------|----------------|
| $n^* = 10, (27)$ | $n^* = 20, (27)$ | $n^* = 10, (27)$ | $n^* = 20, (27)$ |
| 0.1  | 1.8433 | 1.8098 | 2.0043 | 2.6023 | 2.5282 | 2.9597 |
| 0.2  | 1.7979 | 1.7676 | 1.9444 | 2.5087 | 2.4402 | 2.8346 |
| 0.5  | 1.7296 | 1.7818 | 1.9033 | 2.3256 | 2.4428 | 2.7184 |
| 1.0  | 1.7961 | 1.8455 | 1.9514 | 2.3716 | 2.4836 | 2.7277 |
| 2.0  | 1.9970 | 2.0447 | 2.1402 | 2.5653 | 2.6748 | 2.8956 |
| 5.0  | 2.6941 | 2.7417 | 2.8283 | 3.2674 | 3.3773 | 3.5677 |
| 10.0 | 3.9140 | 3.9618 | 4.0343 | 4.4936 | 4.6052 | 4.7703 |

Table 2. Values $-J_{M,1}$ for $\alpha = 1.0$.

| $\delta$ | $n^* = 10, (27)$ | $n^* = 20, (27)$ | $n^* = 10, (27)$ | $n^* = 20, (27)$ |
|----------|----------------|----------------|----------------|----------------|
| 0.1  | 1.4097 | 1.4090 | 1.4086 | 1.4101 | 1.4090 | 1.4083 |
| 0.2  | 1.3892 | 1.3899 | 1.3891 | 1.3911 | – | – |
| 0.5  | 1.3986 | 1.4008 | 1.3996 | 1.4011 | 1.4005 | 1.4000 |
| 1.0  | 1.4740 | 1.4768 | 1.4748 | 1.4758 | 1.4764 | 1.4757 |
| 2.0  | 1.6749 | 1.6784 | 1.6772 | 1.6799 | 1.6779 | – |
| 5.0  | 2.3615 | 2.3664 | 2.3646 | 2.3666 | 2.3655 | 2.3642 |
| 10.0 | 3.5726 | 3.5778 | 3.5752 | 3.5749 | 3.5762 | 3.5747 |

Table 3. Values $J_{M,2}$ for $\alpha = 0.8$ and $\alpha = 0.6$.

| $\delta$ | $\alpha = 0.8$ | $\alpha = 0.6$ |
|----------|----------------|----------------|
| $n^* = 10, (28)$ | $n^* = 20, (28)$ | $n^* = 10, (28)$ | $n^* = 20, (28)$ |
| 0.1  | 0.7795 | 0.7681 | 0.8297 | 1.0327 | 1.0100 | 1.1341 |
| 0.2  | 0.6902 | 0.6828 | 0.7244 | 0.8785 | 0.8626 | 0.9435 |
| 0.5  | 0.5450 | 0.5533 | 0.5648 | 0.6412 | 0.6562 | 0.6769 |
| 1.0  | 0.4329 | 0.4365 | 0.4372 | 0.4799 | 0.4858 | 0.4865 |
| 2.0  | 0.3153 | 0.3160 | 0.3118 | 0.3296 | 0.3304 | 0.3230 |
| 5.0  | 0.1744 | 0.1742 | 0.1704 | 0.1725 | 0.1716 | 0.1651 |
| 10.0 | 0.0982 | 0.0986 | 0.0962 | 0.0949 | 0.0949 | 0.0908 |

For the purpose of verifying the results obtained here, we consider the thermomolecular pressure difference (TPD) effect, consisting in the fact that under the action of a temperature difference in the reservoirs, connected a capillary, a pressure differential flow occurs. The TPD effect in the stationary state is characterized by the absence of particle flow through the cross section of the capillary [16]. By setting in equation (3) $J'_M = 0$, we obtain

$$
\frac{1}{p} \frac{dp}{dz} J_{M,1}(\delta) = \frac{1}{T} \frac{dT}{dz} J_{M,2}(\delta).
$$

(29)
Next, the dimensionless temperature and pressure are introduced as
\[ p^* = \frac{p}{p_1}, \quad T^* = \frac{T}{T_1}, \]
the rarefaction parameter \( \delta \) in any cross section may be expressed as \[ \delta = \frac{p^*}{T^*} \delta_1, \quad \delta_1 = \frac{R' p_1}{\eta(T_1)} \sqrt{\frac{m}{2 k_B T_1}}. \]
Then, equation (29) reads
\[ \frac{dp^*}{dT^*} = -\frac{p^* J_{M,2} \left( \frac{p^*}{T^*} \delta_1 \right)}{T^* J_{M,1} \left( \frac{p^*}{T^*} \delta_1 \right)}. \]
The equation (32) is an ordinary differential equation where \( p^* = p^*(T^*) \), with the initial condition \( p^*_1 = p^*(1) = 1 \). The unknown value \( p^*(T^*_2) \) is calculated from the equation (32) by the Runge-Kutta method.

Next, the TPD coefficient \( \gamma \) in the stationary state is defined by \( p^*_2 \) and \( T^*_2 \) as \[ \gamma = \frac{\ln p^*_2}{\ln T^*_2}. \]
In order to calculate this coefficient, we seek to approximate the functions \( J_{M,1}(\delta) = J_{M,1}(\delta^*) \)
\( J_{M,2}(\delta) = J_{M,2}(\delta^*) \) by sums on the interval \( \delta^* \in [-1;1] \). Here, relation between \( \delta \) and \( \delta^* \) written in the following form \( \delta = 5(\delta^* + 1) \). For example, the value \( J_{M,1}(\delta^*) \) is converted to
\[ J_{M,1}(\delta^*) = \sum_{i=0}^{m} a_i \delta^*_i, \]
where \( \sum' \) is the finite summation with first and last terms halved. Unknown coefficients \( a_i \) \( (i = 0, m) \) in (34) are calculated as \[ a_i = \frac{2}{m} \sum_{k=0}^{m} J_{M,1}(\delta^*(k)) \delta^*_i(\delta^*(k)). \]
Here, points \( \delta^*_k \) \( (k = 0, m) \) are the extrema of the polynomial \( T_m(\delta^*) \) on the interval \( \delta^* \in [-1;1] \) defined as \[ \delta^*_i(k) = \cos \left( \frac{\pi (m - k)}{m} \right), \quad k = 0, m. \]
This procedure has been applied, mainly for demonstration purposes, to the circular cross section under investigation for one temperature ratio $T_2^* = 3.8$ and two values of the accommodation coefficient $\alpha = 1$ and $\alpha = 0.8$ and a wide range of $\delta_1$ at $m = 32$. The ratio $T_2^* = 3.8$ corresponds to a situation where one reservoir is maintained at liquid nitrogen temperature, while the other one is maintained at the room temperature [2]. Results for $\gamma$ are presented in table 5, where in the third and fourth columns the TPD coefficient calculated in [2] and [4] for $\alpha = 1$ are presented. Note that in the free molecular regime the equation (32) with the initial condition $p^*(1) = 1$ can be solved analytically ($p^*(T^*) = T^* - \frac{J_{M,2}(0)}{J_{M,1}(0)}$) and the expression (33) is significantly simplified and corresponds to $\gamma = -\frac{J_{M,2}(\delta^{**})}{J_{M,1}(\delta^{**})}$ [1]. The approximate values of the TPD coefficient $\gamma^{**}$ calculated according to $\gamma^{**} = -J_{M,2}(\delta^{**})/J_{M,1}(\delta^{**})$ are presented in table 5. Here, $\delta^{**} = (\delta_1^1 + \delta_1^2)/2$.

| $\delta_1$ | $\alpha = 1$ | $\alpha = 0.8$ |
|------------|---------------|----------------|
|            | $\gamma^{**}$ | $\gamma^{**}$ |
| (33)       | [2]           | [4]            |
| 0.1        | 0.4523        | 0.4531         |
|            | 0.4532        | 0.4506         |
|            | 0.4376        | 0.4312         |
|            | 0.4312        | 0.4353         |
| 0.2        | 0.4276        | 0.4275         |
|            | 0.4273        | 0.4250         |
|            | 0.4108        | 0.3981         |
|            | 0.3981        | 0.4082         |
| 0.5        | 0.3750        | 0.3761         |
|            | 0.3749        | 0.3691         |
|            | 0.3691        | 0.3364         |
|            | 0.3364        | 0.3427         |
| 1.0        | 0.3185        | 0.3186         |
|            | 0.3179        | 0.3082         |
|            | 0.2896        | 0.2761         |
|            | 0.2761        | 0.2744         |
| 2.0        | 0.2462        | 0.2468         |
|            | 0.2454        | 0.2299         |
|            | 0.2176        | 0.2067         |
|            | 0.2067        | 0.1991         |
| 5.0        | 0.1405        | 0.1423         |
|            | 0.1401        | 0.1181         |
|            | 0.1214        | 0.1151         |
|            | 0.1151        | 0.1020         |
| 10.0       | 0.0733        | 0.0743         |
|            | 0.0730        | 0.0538         |
|            | 0.0631        | 0.0600         |
|            | 0.0600        | 0.0464         |

From an analysis of the data given in table 5 it follows that TPD coefficient $\gamma$ depends strongly on the initial rarefaction parameter $\delta_1$ and the accommodation coefficient of the tangential momentum of the gas molecules $\alpha$. As $\delta_1$ is increased and as $\alpha$ is decreased, $\gamma$ is decreased. The first case is explained in [17], the gas becomes more dense the thermal creep flow is decreased and therefore larger temperature drops are needed to maintain the no net flow condition. In contrary, in highly rarefied gases the effect of the thermal creep flow is significant and larger pressure drops are needed to counter balance this flow. The second case can be explained by the properties of the gas-surface interaction. If one compares the values $\gamma^{**}$ with the corresponding values $\gamma$, one will see that the difference between them is small only for the small initial rarefaction parameter $\delta_1$, while for the large initial rarefaction parameter $\delta_1$ the difference is significant. The values of the TPD coefficient $\gamma$ derived from measured values of the temperatures and pressures [1] are presented in figure 1 according to (32) for the gases He, Ar and Kr (curves 2, 3 and 4). The results are plotted by cubic spline interpolation. The TPD coefficient $\gamma$ for two values of the accommodation coefficient $\alpha$ (0.8 and 1.0) are obtained numerically by the proposed procedure for the aspect ratio $T_1^* = 293.3/273.2$ [1] and the results are plotted in figure 1 (curves 1 and 5). From visual comparison of the experimental and the theoretical curves, it is well noticed that the values of the coefficient are less than 1.0, and are in the range 0.8–1.0 for all gases.

3. Conclusion
In the transition regime, the expression for mass flow in an cylindrical channel under a constant pressure and temperature gradients directed along the symmetry axis of the channel has been derived in the framework of the Maxwell specular-diffuse reflection model. The expression
obtained is numerically analyzed. The values of the mass flow through the cross section of the channel were obtained in a wide range of Knudsen numbers. The thermomolecular pressure difference is calculated and its dependence on the rarefaction parameter and on the accommodation coefficient of the tangential momentum of the gas molecules is shown.

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