FLUID MODELING FOR THE KNUDSEN COMPRESSOR: CASE OF POLYATOMIC GASES

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Abstract. A fluid-dynamic system describing the behavior of a polyatomic gas in a Knudsen compressor, based on a periodic arrangement of narrower and wider two-dimensional channels and on a periodic saw-tooth temperature distribution, is derived, using the polyatomic version of the ellipsoidal statistical (ES) model of the Boltzmann equation, under the assumption that the channel width is much smaller than the length of a unit of the compressor (narrow channel approximation). The difference from the corresponding fluid-dynamic system for a monatomic gas is shown to be confined in the transport coefficients occurring in the fluid-dynamic equation. It is also shown that these coefficients in the present polyatomic-gas case are readily obtained by a simple conversion from the corresponding coefficients for the BGK model for a monatomic gas. Some numerical simulations based on the fluid-dynamic model are carried out, the results of which show that the properties of the Knudsen pump are little affected by the internal structure of a molecule.

1. Introduction. The Knudsen pump (or compressor) is a non-mechanical thermal pump for gases, the prototype of which is the device made by Knudsen in 1910 [24, 25]. The driving mechanism is the thermal transpiration, a gas flow caused by a temperature gradient along the wall of a pipe, which is peculiar to rarefied gases (gases in low-density circumstances or in micro scales). Since the pump does not contain any moving parts, it has a potential applicability for specific purposes in vacuum and micro technologies. Therefore, the properties of the pump have been investigated in detail numerically and experimentally [30, 41, 43, 23, 39, 4, 37, 40, 20, 19].

A typical configuration of the Knudsen pump is a long tube, consisting of alternately arranged thin and thick pipes, with an imposed periodic temperature distribution along the pipe wall (say, saw-tooth distribution increasing in the thin pipes and decreasing in the thick pipes). Because of the opposite temperature gradients, the flows induced in the thick pipes are in the opposite direction to the flows induced in the thin pipes. However, these flows in the opposite directions do not cancel out completely because of the different thickness of the pipes. As a result, the flows in the thin pipes become dominant and cause a global one way flow, which
has a pumping effect. As is seen from this mechanism, the performance of the pump can be improved by a cascade system using many thick and thin pipes (i.e., many units).

Since the thermal transpiration is an effect of a rarefied gas, one has to use kinetic theory to analyze the behavior of the gas in the Knudsen pump. The most widely used tool for simulations of rarefied gas flows is the direct simulation Monte Carlo (DSMC) method [8]. However, for the pump consisting of large number of units, the computational cost required for the DSMC method makes it impossible to perform practical computations. The same is true for other numerical methods, such as finite-difference methods based on the model Boltzmann equations. In contrast, a simple and convenient macroscopic system, composed of an equation of convection-diffusion type and a connection condition at the junctions of the thick and thin pipes, was proposed recently for the purpose of overcoming the computational difficulty [2, 42, 3]. The system, which is valid for any Knudsen number (the mean free path of the gas molecules divided by the characteristic length of the system), was derived systematically from the Boltzmann equation under the assumption that the pipes are sufficiently thin compared with their length. The convection-diffusion-type equation contains variable coefficients (say, transport coefficients), which correspond to the mass-flow rate of the thermal transpiration and that of the Poiseuille flow (the flow caused by the pressure gradient along the pipe axis) in an infinitely long single pipe as the functions of the Knudsen number. Applying the macroscopic system with the transport coefficients based on the model Boltzmann equations, some quantitative results for two-dimensional Knudsen pumps composed of wider and narrower channels between two plates have been obtained [42, 3]. For instance, the fact that the Knudsen pump is applicable to gas separation was pointed out in [42].

The previous results are formally based on the Boltzmann equation for a single gas or a mixture of gases of monatomic molecules, and the quantitative results are based on the transport coefficients obtained by using the model Boltzmann equations for monatomic molecules [the Bhatnagar–Gross–Krook (BGK) model [7, 44] for a single gas in [3], the ellipsoidal statistical (ES) model [21, 22] for a single gas in [5], and the McCormack model [26] for a gaseous mixture in [42]]. The aim of the present paper is to extend the macroscopic system to a single polyatomic gas and clarify the effect of the polyatomic molecules on the properties of the Knudsen pump. We employ the ES model for a polyatomic gas [1] as the basic equation and derive the macroscopic system following the procedure in [2, 42, 3]. As in the examples in [42, 3], we restrict ourselves to the case of a two-dimensional Knudsen pump consisting of wider and narrower channels between two plates.

The paper is organized as follows. In Sec. 2, we first formulate the flow of a rarefied polyatomic gas between two parallel infinite plates using the ES model and then derive a convection-diffusion-type equation by a formal asymptotic analysis, under the assumption that the channel width is much smaller than the length scale of variation of the wall temperature along the channel. In Sec. 3, we derive the connection condition at the junctions of wider and narrower channels for the convection-diffusion-type equation when it is applied to each channels. In Sec. 4, we show that the transport coefficients in the convection-diffusion-type equation can be obtained readily from the corresponding quantities for the BGK model for
2. Fluid-dynamic model for a single channel. In this section, we consider a rarefied gas in a single channel between two parallel plates, and following the analysis in [42], [3], we derive a macroscopic equation of convection-diffusion type in the case where the channel width is much smaller than the length scale of variation along the channel.

2.1. Problem and assumptions. Let us consider a rarefied gas in a channel between two infinite parallel plates. We take the $X_1$ axis (of a rectangular coordinate system $X_i$) perpendicular to the plates and $X_2$ axis along them and let the plates be located at $X_1 = \pm D/2$. The temperature of the plates, which is common to both plates and depends only on $X_2$, is denoted by $T_w(X_2)$.

We investigate the motion of the gas in the channel under the following assumptions:

(i) The behavior of the gas is described by the ES model [1] of the Boltzmann equation for a polyatomic gas.

(ii) The gas molecules undergo diffuse reflection on the plates.

(iii) The problem is two dimensional, i.e., the physical quantities do not depend on $X_3$.

(iv) The scale of variation $L_*$ of the plate temperature is much longer than the width of the channel $D$, i.e., $L_* \gg D$.

2.2. Basic equation and boundary conditions. Let us consider a polyatomic gas consisting of molecules with internal degree of freedom $\delta$. The number of the molecules with position in $dX$ around $X$, velocity in $d\xi$ around $\xi$, and energy related to the internal degree of freedom in $dE$ around $E$ at time $t$ is written as

$$\frac{1}{m} f(t, X, \xi, E)dXd\xi dE,$$

where $f$ is the velocity and energy distribution function of the gas molecules, and $m$ is the mass of a molecule. The equation for $f$, the ES model for a polyatomic gas, can be written in the following form [1] (see the last paragraph of this subsection for the difference in notations between [1] and the present paper):

$$\frac{\partial f}{\partial t} + \xi_1 \frac{\partial f}{\partial X_1} + \xi_2 \frac{\partial f}{\partial X_2} = A_c(T)\rho (G - f),$$

$$G = \frac{\rho \Lambda_\delta \delta^{\delta-1}}{(2\pi)^{\delta/2} T^{1/2}(RT_{rel})^{\delta/2}} \exp\left(-\frac{1}{2}(\xi - \nu) \cdot T^{-1} \cdot (\xi - \nu) - \frac{E}{RT_{rel}}\right),$$

$$T = (1 - \eta) \left\{ (1 - \nu) RT_{tr} l d + \nu \Theta \right\} + \eta RT l d,$$

$$\Theta = \frac{1}{\rho} \int_0^\infty (\xi - \nu) \cdot ' (\xi - \nu) f dE d\xi,$$

$$\rho = \int_0^\infty f dE d\xi,$$

$$v_i = \frac{1}{\rho} \int_0^\infty \xi_i f dE d\xi,$$
\[ T_{tr} = \frac{1}{3 \rho R} \int_{0}^{\infty} (\xi_i - v_i)^2 f dE d\xi, \]  
\[ T_{int} = \frac{2}{\delta \rho R} \int_{0}^{\infty} \mathcal{E} f dE d\xi, \]  
\[ T = \frac{3T_{tr} + \delta T_{int}}{3 + \delta}, \]  
\[ T_{rel} = \eta T + (1 - \eta) T_{int}. \]

Here, \( \rho \) is the mass density of the gas, \( v_i \) is the flow velocity, \( T \) is the temperature, \( T_{tr} \) is the temperature related to the translational energy, \( T_{int} \) is the temperature related to the energy of the internal degree of freedom, and \( R \) is the specific gas constant (the Boltzmann constant divided by the mass of a molecule); \( \nu \in [-1/2, 1] \) and \( \eta \in (0, 1) \) are the parameters to adjust the Prandtl number and the bulk viscosity to the gas under consideration [see Eqs. (6c) and (6d)]; \( A_c(T) \) is a function of \( T \) such that \( A_c(T) \rho \) is the collision frequency of the gas molecules, and \( \Lambda_\delta \) is a dimensionless constant defined by

\[ \Lambda_\delta^{-1} = \int_{0}^{\infty} s^{\delta/2-1} e^{-s} ds. \]  

In addition, \( \mathbf{T} \) and \( \Theta \) are \( 3 \times 3 \) symmetric matrices, \( \mathbf{I}d \) is the \( 3 \times 3 \) identity matrix, \( \det \mathbf{T} \) and \( \mathbf{T}^{-1} \) are the determinant and the inverse matrix of \( \mathbf{T} \), respectively, and the symbol \( ^t \) indicates the transpose operation. In what follows, for an arbitrary matrix \( \mathbf{A} \), its \((i, j)\) component, determinant, inverse matrix, and transposed matrix are denoted by \( A_{ij} \), \( |\mathbf{A}| \), \( \mathbf{A}^{-1} \), and \( ^t \mathbf{A} \), respectively. In the above equations, \( d\xi = d\xi_1 d\xi_2 d\xi_3 \), and the domain of integration with respect to \( \xi_i \) is the whole space of \( \xi_i \). It should be noted that the pressure \( p \) and the stress tensor \( p_{ij} \) are given by

\[ p = \rho RT, \]  
\[ p_{ij} = \rho \Theta_{ij} = \int_{0}^{\infty} (\xi_i - v_i)(\xi_j - v_j) f dE d\xi. \]

The vanishing right-hand side of Eq. (2a) is equivalent to the fact that \( f \) is a local equilibrium distribution \( \text{f}_{eq} \) [1]:

\[ f_{eq} = \frac{\rho \Lambda_\delta}{(2\pi RT)^{3/2}} \mathcal{E}^{\delta/2-1} \exp \left( -\frac{(\xi_i - v_i)^2}{2RT} - \frac{\mathcal{E}}{RT} \right). \]

It is also known [1] that Eq. (2) leads to the viscosity \( \mu \), the thermal conductivity \( \kappa \), the Prandtl number \( \text{Pr} \), and the bulk viscosity \( \mu_b \) in the following form:

\[ \mu = \frac{1}{1 - \nu + \eta \nu} A_c(T), \]  
\[ \kappa = \frac{\gamma}{\gamma - 1} \frac{RT}{A_c(T)}, \]  
\[ \text{Pr} = \frac{\gamma}{\gamma - 1} \frac{R \mu}{\kappa} = \frac{1}{1 - \nu + \eta \nu}, \]  
\[ \mu_b = \frac{1}{\eta} \left( \frac{5}{3} - \gamma \right) \frac{\mu}{\text{Pr}}, \]

with \( \gamma \) the ratio of the specific heats given by

\[ \gamma = \frac{\delta + 5}{\delta + 3}. \]
Equation (2a) contains the set of parameters \((\nu, \eta, \delta)\) characterizing the gas under consideration. In place of this set, we may use another set \((Pr, \mu_b/\mu, \delta)\) because of relations (6c), (6d), and (7) (cf. Secs. 2.4 and 4 and Appendix A).

The diffuse-reflection condition [10, 11, 35, 36], adapted to the present polyatomic case, on the channel walls are expressed as

\[
f = \frac{\rho_w \Lambda_\delta}{(2\pi RT_w)^{3/2}(RT_w)^{3/2}} \exp\left(-\frac{\xi^2}{2RT_w} - \frac{E}{RT_w}\right),
\]

\[(X_1 = \pm D/2, \ \xi_1 \not\equiv 0), \quad (8a)\]

\[
\rho_w = \pm \left(\frac{2\pi}{RT_w}\right)^{1/2} \int_{\xi_1 \geq 0} \int_0^\infty \xi_1 f d\xi d\xi, \quad (X_1 = \pm D/2), \quad (8b)\]

where the upper (or lower) signs go together. The initial condition is given by

\[
f(0, X_1, X_2, \xi, E) = f^0(X_1, X_2, \xi, E). \quad (9)\]

The mass-flow rate \(M\) in the \(X_2\) direction (per unit time and per unit length in \(X_3\)) is expressed as

\[
M = \int_{-D/2}^{D/2} p_w v_2 dX_1. \quad (10)\]

In [1], the energy \(E\), which is denoted by \(\varepsilon\) there, is assumed to be expressed as \(E = I^{2/3}\) in terms of a variable \(I\), and \(I\) is used as an independent variable. More specifically, the distribution function in [1], which we denote by \(\overline{f}(t, X, \xi, I)\) here, is defined in such a way that

\[
\frac{1}{m} \overline{f}(t, X, \xi, I) dX d\xi dI,
\]

indicates the number of the molecules with position in \(dX\) around \(X\), velocity in \(d\xi\) around \(\xi\), and the variable \(I\) in \(dI\) around \(I\) at time \(t\). Therefore, the relation between \(\overline{f}\) and the present \(f\) is as follows:

\[
f(t, X, \xi, E) = (\delta/2)E^{5/2-1}\overline{f}(t, X, \xi, E^{5/2}). \quad (12)\]

In addition, \(\Lambda_\delta\) in [1], which we denote \(\overline{\Lambda}_\delta\) here, is related to \(\Lambda_\delta\) in Eq. (3) as

\[
\overline{\Lambda}_\delta^{-1} = (2/\delta)(\overline{\Lambda}_\delta)^{-1}. \quad (13)\]

2.3. Dimensionless form. Let us introduce the following dimensionless quantities:

\[
\hat{t} = t/t_*, \quad x_1 = X_1/D_*, \quad x_2 = X_2/L_*,
\]

\[
\zeta_i = \xi_i/(2RT_*)^{1/2}, \quad \hat{\xi} = \xi/RT_*,
\]

\[
(f, \hat{f}) = (f, \frac{2\rho(2RT_*)^{-5/2}}{2}\hat{f}),
\]

\[
\hat{\rho} = \rho/\rho_*, \quad \hat{v}_i = v_i/(2RT_*)^{1/2},
\]

\[
(\hat{T}_{tr}, \hat{T}_{int}, \hat{T}, \hat{T}_{rel}) = (T_{tr}, T_{int}, T, T_{rel})/T_*,
\]

\[
\hat{p} = p/p_*, \quad \hat{p}_{ij} = p_{ij}/p_*, \quad \hat{M} = M/\rho_*(2RT_*)^{1/2}D_*,
\]

\[
\hat{\rho}_w = \rho_w/\rho_*, \quad \hat{T}_w = T_w/T_*, \quad a = D/D_*,
\]

\[
\hat{A}_c(\hat{T}) = A_c(T)/A_c(T_*), \quad (\hat{\xi}, \hat{\xi}) = (\xi, \xi)/RT_*,
\]

where \(t_*\) is the reference time, \(D_* (\ll L_*)\) is the reference width of the channel, \(\rho_*\) is the reference density, \(T_*\) is the reference temperature, \(p_* = R\rho_*T_*\) is the reference
pressure. The mean free path \( l_* \) of the gas molecules in the equilibrium state at rest is given as \( l_* = (2/\sqrt{\pi})(2RT_*)^{1/2}/A_0(T_*)\rho_* \).

Then, Eq. (2) is transformed to the following dimensionless form:

\[
\begin{align}
\text{Sh} \frac{\partial \hat{f}}{\partial t} + \zeta_0 \frac{\partial \hat{f}}{\partial x_1} + \zeta_2 \frac{\partial \hat{f}}{\partial x_2} = \frac{2}{\sqrt{\pi}K_*} \hat{A}_0 \hat{\rho}(\hat{G} - \hat{f}), \quad (15a) \\
\hat{G} = \frac{\hat{\rho} \Lambda_0}{\pi^{3/2}T_*^{1/2}T_{\text{rel}}^{3/2}} \hat{\nu}^{3/2-1} \exp\left(-\frac{t}{(\zeta - \hat{v}) \cdot \hat{T}^{-1} \cdot (\zeta - \hat{v}) - \frac{E}{T_{\text{rel}}}}\right), \quad (15b) \\
\hat{T} = (1 - \eta)(1 - \nu)T_{\text{tr}} \hat{I}_d + \eta T_{\text{tr}} \hat{I}_d, \quad (15c) \\
\hat{\Theta} = \frac{2}{\rho} \int_0^\infty (\zeta - \hat{v}) \cdot \hat{f} d\hat{\zeta}, \quad (15d) \\
\hat{\rho} = \int_0^\infty \hat{f} d\hat{\zeta}, \quad (15e) \\
\hat{v}_i = \frac{1}{\hat{\rho}} \int_0^\infty \zeta_i \hat{f} d\hat{\zeta}, \quad (15f) \\
\hat{T}_{\text{tr}} = \frac{2}{3} \frac{1}{\rho} \int_0^\infty (\zeta_i - \hat{v}_i)^2 \hat{f} d\hat{\zeta}, \quad (15g) \\
\hat{T}_{\text{int}} = \frac{2}{3} \frac{1}{\rho} \int_0^\infty \hat{f} d\hat{\zeta}, \quad (15h) \\
\hat{T} = 3\hat{T}_{\text{tr}} + \delta \hat{T}_{\text{int}}, \quad (15i) \\
\hat{T}_{\text{rel}} = \eta \hat{T} + (1 - \eta)\hat{T}_{\text{int}}, \quad (15j)
\end{align}
\]

where \( d\zeta = d\zeta_1 d\zeta_2 d\zeta_3 \), and the domain of integration with respect to \( \zeta_i \) is the whole space of \( \zeta_i \). The \( \text{Sh}, \), \( \epsilon \), and \( K_* \) in Eq. (15) are the dimensionless parameters defined by

\[
\text{Sh} = \frac{D_*}{l_*(2RT_*)^{1/2}}, \quad \epsilon = \frac{D_*}{L_*}, \quad K_* = \frac{l_*}{D_*}, \quad (16)
\]

where \( \text{Sh} \) is the reference Strouhal number, and \( K_* \) is the reference Knudsen number. Corresponding to Eqs. (4a) and (4b), we have

\[
\begin{align}
\hat{\rho} &= \hat{\rho} \hat{T}, \quad (17a) \\
\hat{\rho}_{ij} &= \hat{\rho} \hat{\Theta}_{ij} = \int_0^\infty 2(\zeta_i - \hat{v}_i)(\zeta_j - \hat{v}_j) \hat{f} d\hat{\zeta}, \quad (17b)
\end{align}
\]

The dimensionless form of the boundary condition (8) is given by

\[
\hat{f} = \frac{\hat{\rho}_w \Lambda_0}{(\pi T_w)^{3/2}T_{\text{rel}}^{1/2}} \hat{\nu}^{3/2-1} \exp\left(-\frac{\zeta_0^2}{T_w} - \frac{E}{T_w}\right) \quad (x_1 = \pm a/2, \quad \zeta_1 \leq 0), \quad (18a)
\]

\[
\hat{\rho}_w = \pm 2 \sqrt{\frac{\pi}{T_w}} \int_{1 \geq 0}^\infty \int_0^\infty \zeta_1 \hat{f} d\hat{\zeta}, \quad (18b)
\]

and that of the initial condition (9) is given by

\[
\hat{f}(0, x_1, x_2, \zeta_0, \hat{\zeta}) = \hat{f}^0(x_1, x_2, \zeta_0, \hat{\zeta}). \quad (19)
\]
From Eq. (10), we have, for the dimensionless mass-flow rate \( \hat{M} \),

\[
\hat{M} = \int_{-a/2}^{a/2} \hat{\rho} \hat{v}_2 dx_1.
\]  

(20)

Because of assumption (iv) in Sec. 2.1, \( \epsilon \) in Eq. (16) is the small parameter in our problem, whereas the reference Knudsen number \( K_* \) is arbitrary. In this situation, the induced gas flow is expected to be slow. If we assume that \( \hat{v} \) is of the order of \( \epsilon \), the reference time \( t_* \) and thus the Strouhal number \( \text{Sh} \) may be chosen as

\[
t_* = L_*/(2RT_*)^{1/2} \epsilon, \quad \text{Sh} = \epsilon^2.
\]  

(21)

Therefore, Eq. (15a) becomes

\[
\epsilon^2 \frac{\partial \hat{f}}{\partial t} + \zeta_1 \frac{\partial \hat{f}}{\partial x_1} + \epsilon \zeta_2 \frac{\partial \hat{f}}{\partial x_2} = \frac{2}{\sqrt{\pi} K_*} \hat{A}_c \hat{\rho}(\mathcal{G} - \hat{f}).
\]  

(22)

2.4. Macroscopic equation. We analyze the problem (22) [with Eqs. (15b)–(15j), (18), and (19)] by expanding \( \hat{f} \) in terms of \( \epsilon \):

\[
\hat{f} = \hat{f}(0) + \hat{f}(1) \epsilon + \hat{f}(2) \epsilon^2 + \cdots.
\]  

(23)

Correspondingly, the moments of \( \hat{f} \) occurring in Eq. (22), i.e., \( \hat{\rho}, \hat{v}_i, \hat{T}_{tr}, \hat{T}_{int}, \) and \( \hat{\Theta} \), and thus all the other (macroscopic) quantities that are defined in terms of these moments are expanded as

\[
\hat{h} = \hat{h}(0) + \hat{h}(1) \epsilon + \hat{h}(2) \epsilon^2 + \cdots.
\]  

(24)

Here, \( \hat{h} \) stands for \( \hat{\rho}, \hat{v}_i, \hat{T}_{tr}, \hat{T}_{int}, \hat{T}, \hat{T}_{rel}, \hat{A}_c, |\hat{T}|, |\hat{T}|^{-1}, \hat{p}, \) and \( \hat{p}_{ij} \). For instance, for \( \hat{\rho}, \hat{\Theta}, \hat{A}_c, \) we write

\[
\hat{\rho} = \hat{\rho}(0) + \hat{\rho}(1) \epsilon + \hat{\rho}(2) \epsilon^2 + \cdots,
\]  

(25a)

\[
\hat{\Theta} = \hat{\Theta}(0) + \hat{\Theta}(1) \epsilon + \hat{\Theta}(2) \epsilon^2 + \cdots,
\]  

(25b)

\[
\hat{A}_c = \hat{A}_c(0) + \hat{A}_c(1) \epsilon + \hat{A}_c(2) \epsilon^2 + \cdots.
\]  

(25c)

The expansion of the macroscopic quantities (24) leads to the corresponding expansion of the Gaussian \( \mathcal{G} \):

\[
\mathcal{G} = \mathcal{G}(0) + \mathcal{G}(1) \epsilon + \mathcal{G}(2) \epsilon^2 + \cdots.
\]  

(26)

In addition, \( \hat{\rho}_w \) in the boundary condition (18) and the dimensionless mass-flow rate \( \hat{M} \) [Eq. (20)] are expanded as well:

\[
\hat{\rho}_w = \hat{\rho}_w(0) + \hat{\rho}_w(1) \epsilon + \hat{\rho}_w(2) \epsilon^2 + \cdots,
\]  

(27a)

\[
\hat{M} = \hat{M}(0) + \hat{M}(1) \epsilon + \hat{M}(2) \epsilon^2 + \cdots.
\]  

(27b)

The explicit expressions of the coefficients in the expansions (24), (26), and (27), some of which will be given when necessary in the sequel, are omitted here. By the substitution of these expansions in Eqs. (22) [with Eqs. (15b)–(15j)], (18), and (19), we can solve the problem from the lowest order of \( \epsilon \).
2.4.1. Zeroth order. The equation at the zeroth order in $\epsilon$ is as follows:

$$
\xi_1 \frac{\partial \hat{f}_{(0)}}{\partial x_1} = \frac{2}{\sqrt{\pi}} \frac{1}{K_\epsilon} \hat{A}_{(0)} \hat{\rho}_{(0)} (\hat{G}_{(0)} - \hat{f}_{(0)}),
$$

where $\hat{A}_{(0)} = \hat{A}_{(0)}(\hat{T}_{(0)})$, and the explicit forms of $\hat{\rho}_{(0)}$ and $\hat{G}_{(0)}$, which can be obtained from Eqs. (15b)–(15j) straightforwardly, are omitted here. The corresponding boundary condition is given by

$$
\hat{f}_{(0)} = \frac{\hat{\rho}_{(0)} \Lambda_\delta}{(\pi T_w)^{3/2} \tilde{T}_w^{3/2}} \exp \left( -\frac{\xi^2}{T_w} \right) \left( x_1 = \pm a/2, \ \xi_1 \leq 0 \right),
$$

$$
\hat{\rho}_{(0)} = \pm 2 \sqrt{\pi} T_w \int_{\xi_1 \geq 0} \int_0^{\infty} \xi_1 \hat{f}_{(0)} d\tilde{E} d\xi.
$$

(29a, 29b)

It should be noted that $\hat{t}$ and $x_2$ appear only as parameters in the problem (28) and (29). It is seen by the direct substitution that Eqs. (28) and (29) have a solution of the following form:

$$
\hat{f}_{(0)} = \frac{\sigma_{(0)}(\hat{t}, x_2) \Lambda_\delta}{(\pi T_w(x_2))^{3/2} \tilde{T}_w(x_2)^{3/2}} \exp \left( -\frac{\xi^2}{T_w(x_2)} \right),
$$

(30)

where $\sigma_{(0)}$ is an arbitrary function of $\hat{t}$ and $x_2$ to be determined later. In fact, Eq. (30) gives the following macroscopic quantities:

$$
\hat{\rho}_{(0)} = \sigma_{(0)}(\hat{t}, x_2), \quad \hat{v}_{(0)} = 0,
$$

$$
\hat{T}_{tr(0)} = \hat{T}_{int(0)} = \hat{T}_{(0)} = \hat{T}_{rel(0)} = \hat{T}_w(x_2),
$$

$$
\hat{\rho}_{(0)} = \sigma_{(0)}(\hat{t}, x_2) \hat{T}_w(x_2), \quad \hat{\rho}_{ij(0)} = \hat{\rho}_{(0)} \delta_{ij}, \quad \hat{M}_{(0)} = 0,
$$

which reduce $\hat{G}_{(0)}$ and $\hat{A}_{(0)}$ to

$$
\hat{G}_{(0)} = \hat{f}_{(0)}, \quad \hat{A}_{(0)} = \hat{A}_{(0)}(\hat{T}_w).
$$

(32)

Moreover, we can show, by following [14], that Eq. (30) is the unique solution (up to the arbitrariness of $\sigma_{(0)}$).

2.4.2. First order. The equation in the first order of $\epsilon$ is obtained as follows:

$$
\xi_1 \frac{\partial \hat{f}_{(1)}}{\partial x_1} + \xi_2 \frac{\partial \hat{f}_{(1)}}{\partial x_2} = \frac{2}{\sqrt{\pi}} \frac{1}{K_\epsilon} \hat{A}_{(0)} \sigma_{(0)} (\hat{G}_{(1)} - \hat{f}_{(1)}),
$$

(33a)

$$
\hat{G}_{(1)} = \hat{G}_{(0)} \frac{\hat{\rho}_{(1)}}{\sigma_{(0)}} - \frac{1}{2} \frac{\hat{T}_{(1)}}{T_w^3} + \frac{\hat{T}_{rel(1)}}{T_w^2} + \frac{\hat{\rho}_{(1)}}{T_w} - \frac{1}{2} \xi \cdot (\hat{T}_{(1)}^{-1}) \cdot \xi,
$$

(33b)

$$
\hat{T}_{(1)} = \hat{T}_w^3 \left[ 3(1 - \eta) \hat{T}_{tr(1)} + 3 \eta \hat{T}_{(1)} \right],
$$

(33c)

$$
\hat{\rho}_{(1)} = \hat{f}_{(1)} \int_0^\infty \hat{f}_{(1)} d\tilde{E} d\xi,
$$

(33d)
\[ \sigma(0) \hat{v}_l(1) = \int_0^\infty \zeta_1 \hat{f}_1(1) d\hat{E} d\zeta, \]  
(33f)

\[ \sigma(0) \hat{T}_{\text{tr}(1)} = \frac{2}{3} \int_0^\infty \zeta_2 \hat{f}_1(1) d\hat{E} d\zeta - \hat{\rho}(1) \hat{T}_w, \]  
(33g)

\[ \sigma(0) \hat{T}_{\text{int}(1)} = \frac{2}{3} \int_0^\infty \hat{E} \hat{f}_1(1) d\hat{E} d\zeta - \hat{\rho}(1) \hat{T}_w, \]  
(33h)

\[ \hat{T}_1 = \frac{3 \hat{T}_{\text{tr}(1)} + \delta \hat{T}_{\text{int}(1)}}{3 + \delta}, \]  
(33i)

\[ \hat{T}_{\text{rel}(1)} = \eta \hat{T}_1 + (1 - \eta) \hat{T}_{\text{int}(1)}. \]  
(33j)

The corresponding boundary condition is given by

\[ \hat{f}_1 = -\frac{\hat{\rho}_w(1) \Lambda_s}{(\pi T_w)^{3/2} T_w^{3/2} S} \hat{E}^{5/2 - 1} \exp \left(-\frac{\zeta_2^2}{T_w^2} - \frac{\hat{E}}{T_w} \right) (x_1 = \pm a/2, \ \zeta_1 \equiv 0), \]  
(34a)

\[ \hat{\rho}_w(1) = \pm 2 \sqrt{\frac{\pi}{T_w}} \int_{\zeta_1 \equiv 0}^\infty \int_0^\infty \zeta_1 \hat{f}_1(1) d\hat{E} d\zeta. \]  
(34b)

In addition, the pressure, the stress tensor, and the mass-flow rate in the first order of \( \epsilon \) are expressed as follows:

\[ \hat{p}_1 = \sigma(0) \hat{T}_1 + \hat{\rho}_1 \hat{T}_w, \]  
(35a)

\[ \hat{p}_{ij}(1) = \int_0^\infty 2 \zeta_1 \zeta_j \hat{f}_1(1) d\hat{E} d\zeta, \]  
(35b)

\[ \hat{M}_1 = \int_{-a/2}^a \sigma(0) \hat{v}_{2(1)} dx_1. \]  
(35c)

Here again, the problem (33) and (34) contains \( \hat{t} \) and \( x_2 \) only as parameters [see Eqs. (31) and (32)]. Now we can show, as in the same way as [42], that the solution to Eqs. (33) and (34) is obtained in the following form:

\[ \hat{f}_1 = f_0 \left[ \phi_\rho (\hat{t}, x_2) + \frac{\zeta_2}{\zeta_\epsilon} a \phi_p \left( \frac{x_1}{a}, \frac{\zeta_1}{T_w^{1/2}}, \frac{\zeta_\epsilon}{T_w}; K(\hat{t}, x_2) \right) \frac{1}{\hat{\rho}_0} \frac{\partial \hat{p}_0}{\partial x_2} \right. \]

\[ \left. + \frac{\zeta_2}{\zeta_\epsilon} a \phi_T \left( \frac{x_1}{a}, \frac{\zeta_1}{T_w^{1/2}}, \frac{\zeta_\epsilon}{T_w}; \hat{\epsilon}(\hat{t}, x_2) \right) \frac{1}{T_w} \frac{d T_w}{d x_2} \right], \]  
(36)

where

\[ \zeta_\epsilon = (\zeta_2^2 + \zeta_3^2)^{1/2}, \]  
(37a)

\[ K(\hat{t}, x_2) = \frac{K_s T_w^{3/2}(x_2)}{\hat{\rho}_0(\hat{t}, x_2) \Lambda_\epsilon(x_2) a}. \]  
(37b)

\( \phi_\rho (\hat{t}, x_2) \) is an arbitrary function of \( \hat{t} \) and \( x_2 \), and \( \phi_p \) and \( \phi_T \) are, respectively, the solutions of the specific boundary-value problems for the linearized ES model. The equation and boundary condition for \( \phi_p \) and those for \( \phi_T \) are given in Appendix A, where the parameter set \((Pr, \mu, \eta, \delta)\) is used in place of \((\nu, \eta, \delta)\) in Eq. (67) [see the comment following Eq. (7)]. The \( \phi_p \) corresponds to the solution for the flow induced between two parallel plates by the uniform pressure gradient (Poiseuille flow) [36], whereas \( \phi_T \) corresponds to the solution for the flow induced between two parallel plates by the uniform temperature gradient along the plates (thermal transpiration) [36]. They are fundamental and classical problems in rarefied gas.
dynamics and have been investigated by many authors by various methods. Since
an exhaustive list of references is beyond the scope of the present paper, we only
mention some early works, [12], [28], [29], and more recent works, [34], [15] (see also
[36], [32] and references therein). We will discuss these problems in Sec. 4.

The macroscopic quantities in the first order of $\epsilon$, i.e., those corresponding to the
solution (36), are obtained as follows:

$$
\dot{\rho}_{1(1)} = \sigma_{(0)}(\hat{t}, x_2)\phi_j(\hat{t}, x_2), \quad \dot{v}_{1(1)} = \dot{v}_{3(1)} = 0,
$$

$$
\dot{v}_{2(1)} = aT_w^{1/2} \left( u_T \frac{1}{\rho_{(0)}} \frac{\partial \dot{\rho}_{(0)}}{\partial x_2} + u_T \frac{1}{T_w} \frac{d\dot{T}_w}{dx_2} \right),
$$

$$
\ddot{T}_{\text{tr}(1)} = \ddot{T}_{\text{int}(1)} = \dot{T}_{(1)} = \ddot{T}_{\text{rel}(1)} = 0,
$$

$$
\dot{\rho}_{(1)} = \rho_{(0)}(\hat{t}, x_2)\phi_j(\hat{t}, x_2),
$$

$$
\dot{\rho}_{ij(1)} = \rho_{(1)}(\delta_{ij} + a\dot{\rho}_{(0)}(\Sigma_T \frac{1}{\rho_{(0)}} \frac{\partial \dot{\rho}_{(0)}}{\partial x_2} + \Sigma_T \frac{1}{T_w} \frac{d\dot{T}_w}{dx_2})(\delta_{i1}\delta_{j2} + \delta_{i2}\delta_{j1}),
$$

where, with $\alpha = P$, $T$,

$$
u_{\alpha} = u_{\alpha}\left(\frac{x_1}{a}; K(\hat{t}, x_2)\right)
$$

$$= \int_{-\infty}^{\infty} \int_{0}^{\infty} \int_{0}^{\infty} c_1^2 Y^{\delta/2 - 1} \phi_{\alpha}\left(\frac{x_1}{a}, c_1, c_r, Y; K(\hat{t}, x_2)\right) \ddot{E}_Y dY dc_1 dc_2,
$$

(39a)

$$\Sigma_{\alpha} = \Sigma_{\alpha}\left(\frac{x_1}{a}; K(\hat{t}, x_2)\right)
$$

$$= 2 \int_{-\infty}^{\infty} \int_{0}^{\infty} \int_{0}^{\infty} c_1 c_r^2 Y^{\delta/2 - 1} \phi_{\alpha}\left(\frac{x_1}{a}, c_1, c_r, Y; K(\hat{t}, x_2)\right) \ddot{E}_Y dY dc_1 dc_2,
$$

(39b)

$$\ddot{E}_Y = \Lambda \delta \pi^{-1/2} \exp(-c_1^2 - c_r^2 - Y).
$$

(39c)

[It turns out that $\Sigma_0 = -x_1/a$ and $\Sigma_T = 0$ (see Appendix A).] In addition, the
corresponding mass-flow rate is given as

$$
\ddot{M}_{(1)} = a^2 \frac{\dot{\rho}_{(0)}}{T_w^{1/2}} \left( M_P \frac{1}{\rho_{(0)}} \frac{\partial \dot{\rho}_{(0)}}{\partial x_2} + M_T \frac{1}{T_w} \frac{d\dot{T}_w}{dx_2} \right),
$$

(40)

where

$$
M_{\alpha} = M_{\alpha}(K(\hat{t}, x_2)) = \int_{-1/2}^{1/2} u_{\alpha}(y; K(\hat{t}, x_2)) dy, \quad (\alpha = P, T).
$$

(41)

2.4.3. Second order and macroscopic equation. The equation in the second order of
$\epsilon$ reads as follows:

$$
\frac{\partial f_{(0)}}{\partial \hat{t}} + \zeta_1 \frac{\partial f_{(2)}}{\partial x_1} + \zeta_2 \frac{\partial f_{(4)}}{\partial x_2}
$$

$$= \frac{2}{\sqrt{\pi}} \frac{1}{K_{\alpha}} \left[ \dot{A}_{c(0)}(\sigma_{(0)}(\ddot{G}_{(2)} - \ddot{f}_{(2)}) + (\dot{A}_{c(0)} + \dot{A}_{c(1)}(\sigma_{(0)})(\ddot{G}_{(1)} - \ddot{f}_{(1)}) \right],
$$

(42)
where the explicit form of $\hat{G}_{(2)}$ is omitted. The boundary condition for Eq. (42) is given by

$$
\hat{f}_{(2)} = \frac{\hat{\rho}_{w(2)} A_0}{(\pi T_w)^{3/2} T_{w}^{3/2}} \hat{\sigma} \delta^{2/3} \exp \left( - \frac{\zeta_1^2}{T_w} \right) (x_1 = \pm a/2, \; \zeta_1 \leq 0), \tag{43a}
$$

$$
\hat{\rho}_{w(2)} = \pm 2 \frac{\pi}{T_w} \int_{\zeta_1 \geq 0} \int_{0}^{\infty} \zeta_1 \hat{f}_{(2)} d\hat{\sigma} d\zeta.
\tag{43b}
$$

We now integrate Eq. (42) with respect to $\zeta$ and $\hat{\sigma}$ over their whole ranges and then with respect to $x_1$ from $-a/2$ to $a/2$. If we take into account, in this process, the explicit forms of $\hat{f}_{(0)}$ [Eq. (30)] and $\hat{f}_{(1)}$ [Eq. (36)], as well as the relation

$$
\int_{0}^{\infty} \zeta_1 \hat{f}_{(2)} |_{x_1 = \pm a/2} d\hat{\sigma} d\zeta = 0,
\tag{44}
$$

obtained from the boundary condition (43), then we have the following equation:

$$
\frac{\partial \hat{\rho}_{(0)}}{\partial t} + \hat{T}_w \frac{\partial \mathcal{M}}{\partial x_2} = 0, \tag{45a}
$$

$$
\mathcal{M} = \frac{\hat{\rho}_{(0)}}{T_w} a \left[ M_P(K; \delta, \text{Pr}) \frac{1}{\hat{\rho}_{(0)}} \frac{\partial \hat{\rho}_{(0)}}{\partial x_2} + M_T(K; \delta) \frac{1}{T_w} \frac{d\hat{T}_w}{dx_2} \right], \tag{45b}
$$

$$
K = K_a \hat{T}_w^{3/2} / \hat{\rho}_{(0)} \hat{A}_{c(0)} a, \quad \hat{A}_{c(0)} = \hat{A}_{c}(\hat{T}_w), \tag{45c}
$$

where, $\hat{\rho}_{(0)} = \sigma_{(0)} T_w$, rather than $\sigma_{(0)}$, has been used as the unknown function. In Eq. (45), $\hat{\rho}_{(0)}$, $\mathcal{M}$, and $K$ are the functions of $\hat{T}$ and $x_2$, whereas $\hat{T}_w$ and $\hat{A}_{c(0)}$ are the functions of $x_2$ only. As shown in Appendix A, $\phi_P$ depends only on $(\text{Pr}, \delta)$ and $\phi_T$ only on $\delta$ among the set of parameters $(\text{Pr}, \mu_{in}/\mu, \delta)$. Thus, the same dependency holds for $M_P$ and $M_T$. This fact is shown explicitly in Eq. (45). Further relevant properties of $M_P$ and $M_T$ will be shown in Sec. 4. The original (dimensional) mass-flow rate $M$ [cf. Eq. (10)] is expressed as

$$
M/\rho_\delta(2RT_s)^{1/2} D_a = a \mathcal{M} \epsilon + O(\epsilon^2), \tag{46}
$$

Thus, $\mathcal{M}$ is the dimensionless first-order mass flux.

In summary, Eq. (45) is the equation of convection-diffusion type for the pressure $\hat{\rho}_{(0)}$ at the zeroth order in $\epsilon$ if we have the data of $M_P$ and $M_T$ as the functions of $K$. The construction of the database will be made in Sec. 4.

The steady version of Eq. (45) is essentially the same as the generalized Reynolds equation derived in [17] and often used in micro-fluid applications [33, 13]. Mathematical study of the derivation of diffusion-type equations from the Boltzmann equation is found, for instance, in Refs. [6, 18, 16]. In Ref. [3], the term corresponding to $\phi_P$ in Eq. (36) is set to be zero because this setting does not make any change in the resulting equation of convection-diffusion type.

3. Connected channels and connection condition. Let us consider a long channel composed of several (or many) channels with different width connected linearly one after another. If each channel is long enough compared with its width, the macroscopic equation (45) should be valid in each channel except the regions near the junctions. If we assume that the macroscopic equation is valid even in the junction regions, it should be complemented by an appropriate connection condition at the junctions. This condition can be derived by the analysis of the original kinetic
equation in the junction regions (see [2, 42, 3]). Here, we only give the result thus obtained.

Let us consider the junction of two channels shown in Fig. 1. That is, the channel I with width \( D_I \) \((X_2 < 0)\) is connected with the channel II with width \( D_{II} \) \((X_2 > 0)\) at \( X_2 = 0 \). We assume the diffuse reflection on the wall at \( X_2 = 0 \) and that the temperature of the channel wall is continuous at \( X_2 = 0 \) though its derivative may be discontinuous. Then, the connection condition for Eq. (45) applied to each channel is given by

\[
\bar{p}_I'(0)(\hat{t}, x_2 = 0-) = \bar{p}_{II}'(0)(\hat{t}, x_2 = 0+), \quad (47a)
\]

\[
\mathcal{M}I'(\hat{t}, x_2 = 0-)a_I = \mathcal{M}_{II}'(\hat{t}, x_2 = 0+)a_{II}, \quad (47b)
\]

with

\[
a_I = D_I/D_*, \quad a_{II} = D_{II}/D_. \quad (48)
\]

Here, \( \bar{p}_J'(0) \) and \( \mathcal{M}_J' \) \((J = I, II)\) are the zeroth-order pressure and the first-order mass flux in the channel \( J \), respectively. The condition (47) is valid irrespective of the positions of the center lines of the two channels (i.e., the center lines do not need to be common).

In the case of a channel composed of many channels with different width, the condition (47) is to be applied at each junction.

4. Data for \( M_P \) and \( M_T \): Reduction to BGK model. The convection-diffusion-type equation (45) is of the same form as in the case of a monatomic gas [42, 3]. In other words, the effect of the polyatomic gas is confined in the transport coefficients \( M_P \) and \( M_T \).

As we have seen in Sec. 2.4.2, \( M_P \) and \( M_T \) are obtained by Eqs. (39a) and (41) from the solutions \( \phi_P \) and \( \phi_T \) to Eq. (67) with boundary condition (66).

In this section, we investigate this problem in detail.

We first note that we can eliminate the variable \( Y \) from our problem by introducing the following marginal velocity distribution functions:

\[
\Phi_\alpha(y, c_1, c_r; K(\hat{t}, x_2)) = \Lambda_\delta \int_0^{\infty} Y^d/2-1 \phi_\alpha(y, c_1, c_r; K(\hat{t}, x_2)) \exp(-Y) dY,
\]

\[
(\alpha = P, T). \quad (49)
\]

More specifically, if we multiply Eq. (67a) by \( \Lambda_\delta Y^d/2-1 \exp(-Y) \) and integrate with respect to \( Y \) from 0 to \( \infty \), we obtain the boundary-value problems for \( \Phi_P \) and \( \Phi_T \).
That is, the problem for $\Phi_P$ is
\begin{equation}
    c_1 \frac{\partial \Phi_P}{\partial y} = \frac{2}{\sqrt{\pi} K} \left[ -\Phi_P + 2c_r u_P - 2\left(1 - \frac{1}{Pr}\right)c_1 c_r y \right] - c_r, \tag{50a}
\end{equation}
\begin{equation}
    u_P = \int_{-\infty}^{\infty} \int_{0}^{\infty} c^2 \Phi_P E_c dc_r dc_1, \tag{50b}
\end{equation}
\begin{equation}
    \Phi_P = 0, \quad (y = \pm 1/2, \ c_1 \leq 0), \tag{50c}
\end{equation}
where
\begin{equation}
    E_c = \pi^{-1/2} \exp(-c^2 - c'^2), \tag{51}
\end{equation}
and the problem for $\Phi_T$ is
\begin{equation}
    c_1 \frac{\partial \Phi_T}{\partial y} = \frac{2}{\sqrt{\pi} K} \left[ -\Phi_T + 2c_r u_T - \left(c_1^2 + c_r^2 - \frac{5}{2}\right)c_r \right], \tag{52a}
\end{equation}
\begin{equation}
    u_T = \int_{-\infty}^{\infty} \int_{0}^{\infty} c^2 \Phi_T E_c dc_r dc_1, \tag{52b}
\end{equation}
\begin{equation}
    \Phi_T = 0, \quad (y = \pm 1/2, \ c_1 \leq 0). \tag{52c}
\end{equation}
In addition, we have
\begin{equation}
    M_P = \int_{-1/2}^{1/2} u_P dy, \quad M_T = \int_{-1/2}^{1/2} u_T dy. \tag{53}
\end{equation}
It should be remarked that the parameter $\delta$ of the internal degree of freedom of a molecule has been eliminated from the problems (50) and (52). As seen from Eqs. (50) and (52), $\Phi_P$ depends only on $Pr$ and $\Phi_T$ on none of the parameters $(Pr, \mu_0/\mu, \delta)$. Thus, we may write $M_P$ and $M_T$ as $M_P(K, Pr)$ and $M_T(K)$.

In fact, Eqs. (50) and (52) are of the same form as the equations and boundary conditions corresponding to the plane Poiseuille flow and thermal transpiration based on the ES model for a monatomic gas. The only difference lies in the different values of $Pr$ in the former. Furthermore, Eq. (52) is identical to the equation and boundary condition corresponding to the thermal transpiration based on the BGK model for a monatomic gas. Therefore, we can just exploit the existing data of $M_T$ based on the BGK model [38]. On the other hand, the problem (50) differs from that based on the BGK model. However, if we let
\begin{equation}
    \Phi_P = \Psi_P - \frac{2}{\sqrt{\pi} K} \left(1 - \frac{1}{Pr}\right)c_r \left(y^2 - \frac{1}{4}\right), \tag{54}
\end{equation}
then we have the following equation and boundary condition for $\Psi_P$:
\begin{equation}
    c_1 \frac{\partial \Psi_P}{\partial y} = \frac{2}{\sqrt{\pi} K} \left(-\Psi_P + 2c_r u_P[\Psi_P]\right) - c_r, \tag{55a}
\end{equation}
\begin{equation}
    u_P[\Psi_P] = \int_{-\infty}^{\infty} \int_{0}^{\infty} c^2 \Psi_P E_c dc_r dc_1, \tag{55b}
\end{equation}
\begin{equation}
    \Psi_P = 0, \quad (y = \pm 1/2, \ c_1 \leq 0), \tag{55c}
\end{equation}
which does not contain $Pr$ and is identical to the equation and boundary condition for the plane Poiseuille flow based on the BGK model for a single-component gas. Let $u_P[\Phi_P]$ and $M_P[\Phi_P]$ denote $u_P$ and $M_P$ based on $\Phi_P$, and $u_P[\Psi_P]$ and $M_P[\Psi_P]$. 

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those based on $\Psi_P$. Then, they are related as
\[
\begin{align*}
  u_P[\Phi_P] &= u_P[\Psi_P] - \frac{1}{\sqrt{\pi} K} \left(1 - \frac{1}{Pr}\right) \left(y^2 - \frac{1}{4}\right), \\
  M_P[\Phi_P] &= M_P[\Psi_P] + \frac{1}{6} \frac{1}{\sqrt{\pi} K} \left(1 - \frac{1}{Pr}\right) K.
\end{align*}
\]
Since $M_P[\Psi_P]$ is independent of $Pr$, the functional form of $M_P(K, Pr)$, as the function of $Pr$, is given by the last term on the right-hand side of Eq. (57). In this way, the data of $M_P(K, Pr)$ for the BGK model for a monatomic gas [38] can be obtained readily from the existing data of $M_P[\Psi_P]$ for the ES model. The same conversions as (54), (56), and (57) can be used even when the boundary condition other than the diffuse reflection (e.g., Cercignani–Lampis model [10]) is used in the formulation of the problem (or in place of (50c)). It should be noted that, for a monatomic gas, the conversion between the ES and BGK models is mentioned in [9, 10], where a conversion formula corresponding to Eq. (57) is given for the cylindrical Poiseuille flow, assuming the diffuse reflection boundary condition.

In summary, we can obtain the database for $M_P(K, Pr)$ and $M_T(K)$ without any new computation.

5. Knudsen pump and its performance. In this section, we apply the macroscopic equation (45) and connection condition (47) to a Knudsen pump. We take the nitrogen gas ($N_2$), for which the experimental values of $Pr$ and $\mu_b/\mu$ are available ($Pr = 0.718$ [27] and $\mu_b/\mu = 0.731$ [31]). We set the values of $\nu$ and $\eta$ in such a way that the resulting $Pr$ and $\mu_b/\mu$ are close to the above experimental values, that is, $\nu = -0.50$ and $\eta = 0.46$, which lead to $Pr = 0.787$ and $\mu_b/\mu = 0.722$.

Now, let us consider a Knudsen pump (or compressor) shown in Fig. 2, that is, a long channel consisting of alternately arranged $N$ narrower channels (Channel I: length $L_I$ and width $D_I$) and $N$ wider channels [Channel II: length $L_{II}$ and width $D_{II(> D_I)}$] along the $X_2$ axis. We let $L = L_I + L_{II}$ and assume that $D_I \ll L_I$ and $D_{II(> L_I)} \ll L_{II}$. In addition, we assume that the temperature $T_w(X_2)$ of the channel walls is a piecewise linear and continuous periodic function (period $L$) of $X_2$, varying between $T_0$ and $T_1(> T_0)$. With this setting, we can apply Eq. (45) to each channel.
and Eq. (47) to each junction. To be more specific, if we denote the dimensionless pressure \( \hat{p}_{(0)} \) in Channel II \((J = 1, \text{II})\) by \( \hat{p}_{(0)}^I \), we have
\[
\frac{\partial \hat{p}_{(0)}^I}{\partial t} + \hat{T}_w \frac{\partial \mathcal{M}^I}{\partial x_2} = 0, \tag{58a}
\]
\[
\mathcal{M}^I = \frac{\hat{p}_{(0)}^I}{T_w^{1/2}} a_I \left[ M_T(K_J, \text{Pr}) \frac{1}{\hat{p}_{(0)}^I} \frac{\partial \hat{p}_{(0)}^I}{\partial x_2} + M_T(K_J) \frac{1}{T_w} \frac{d\hat{T}_w}{dx_2} \right], \tag{58b}
\]
\[
a_I = \frac{D_I}{D_*}, \quad K_J = \frac{K_1 \hat{T}_w^{3/2}}{\hat{p}_{(0)}^I a_I}, \tag{58c}
\]
where
\[
J = \begin{cases} 
1 & \text{for } mL/L_s < x_2 < (L_1 + mL)/L_s, \\
II & \text{for } (L_1 + mL)/L_s \leq x_2 \leq (1 + m)L/L_s, \\
& (m = 0, \ldots, N - 1).
\end{cases} \tag{59}
\]

Here, we have assumed that \( \lambda_c(T) \) does not depend on \( T \), so that \( \hat{\lambda}_c = 1 \) (or \( \lambda_c(0) = 1 \)). We also have to impose the following conditions at the junctions:
\[
\hat{p}_{(0)}^I = \hat{p}_{(0)}^\text{II}, \quad \mathcal{M}^Ia_I = \mathcal{M}^\text{II}a^\text{II},
\]
\[
at x_2 = L_1/L_s, (L_1 + mL)/L_s \text{ and } mL/L_s, \quad (m = 1, \ldots, N - 1). \tag{60}
\]

If we assign the appropriate initial condition and conditions at both ends, we can describe the time evolution of the pressure distribution along the Knudsen pump.

Here, we consider the following two types of end condition that are simple and natural:
(i) Open end: the pressure of the gas is specified there.
(ii) Closed end: the mass flow vanishes there.

Let us consider the following two problems for the Knudsen pump:

(A) The left end \((X_2 = 0)\) is open, and the right end \((X_2 = N L)\) is closed. The pressure at the left end is kept at \( p_0 \). The initial condition is that the density is uniform at \( t = 0 \).

(B) Both ends are open. The pressure at the left end is kept at \( p_0 \) and that at the right end is kept at \( p_1 (> p_0) \). The initial condition is that the density is uniform at \( t = 0 \).

We take \( p_0, T_0, D_I, \) and \( L \) as the reference pressure \( p_* \), temperature \( T_* \), channel width \( D_* \), and channel length \( L_* \), respectively. Therefore, the reference mean free path becomes \( l_* = (2/\sqrt{\pi})(2RT_0)^{1/2}/\lambda_c p_0 \) (with \( \rho_0 = p_0/RT_0 \)), and thus the reference Knudsen number \( K_* = l_*/D_1 \). In what follows, we show the steady pressure distribution for Problem (A) and the steady mass-flow rate for Problem (B), obtained as the long-time limits of the time-dependent solutions. The results for the \( N_2 \) gas (\( \text{Pr} = 0.787 \)) are compared with those for a monatomic gas with \( \text{Pr} = 0.666 \) (Note that the values of \( \text{Pr} \) obtained experimentally as well as theoretically are very close to 2/3 for any monatomic gas).

The steady pressure distribution \( p/p_0 (= \hat{p}) \) along the pump at \( K_* = 0.1, 1 \), and 10 in Problem (A) is shown in Fig. 3 for \( D_{11}/D_1 = 2, L_1/L = 0.5, T_1/T_0 = 1.5, \) and \( N = 100 \). Figure 3(a) shows the result for the \( N_2 \) gas. Figure 3(b) shows the distribution of the pressure averaged over each unit. The result for the monatomic gas is also shown in Fig. 3(b) for comparison. In this problem, we observe the property of the Knudsen pump as a compressor. If the Knudsen number \( K_* \), which
Figure 3. Steady pressure distribution along the Knudsen pump in Problem (A). (a) Pressure distribution for the N\textsubscript{2} gas, (b) Averaged pressure distribution for the N\textsubscript{2} and monatomic gases. In (b), the solid line indicates the result for the N\textsubscript{2} gas, and the dashed line that for the monatomic gas.

Table 1. Steady mass-flow rate \( \mathcal{M}^4 a_1 \) versus the number of the units \( N \) in Problem (B).

| \( N \) | \( K^* = 10 \) | \( K^* = 1 \) | \( K^* = 0.1 \) | \( K^* = 10 \) | \( K^* = 1 \) | \( K^* = 0.1 \) |
|------|----------------|----------------|----------------|----------------|----------------|----------------|
| 10   | -0.1107        | -0.7529(-1)    | -0.3029        | -0.1112        | -0.7321(-1)    | -0.2664        |
| 50   | 0.3414(-2)     | 0.1970(-1)     | -0.4618(-1)    | 0.2783(-2)     | 0.1875(-1)     | -0.3905(-1)    |
| 100  | 0.1595(-1)     | 0.2910(-1)     | -0.1410(-1)    | 0.1539(-1)     | 0.2788(-1)     | -0.1064(-1)    |
| 150  | 0.1917(-1)     | 0.3097(-1)     | -0.3410(-2)    | 0.1867(-1)     | 0.2971(-1)     | -0.1182(-2)    |
| 200  | 0.2031(-1)     | 0.3142(-1)     | 0.1928(-2)     | 0.1984(-1)     | 0.3017(-1)     | 0.3542(-2)     |

\(^1\) Read as \(-0.7529 \times 10^{-1}\).

is the Knudsen number at the left end, is not small, the pressure ratio of 6.5 \( \sim \) 7 is obtained at the right end. The difference between the pressure at the right end for the N\textsubscript{2} gas and that for the monatomic gas is relatively small: the difference is around 6% at \( K^* = 10 \), 3% at \( K^* = 1 \), and 4% at \( K^* = 0.1 \).

Table 1 shows the (dimensionless) steady mass-flow rate \( \mathcal{M}^4 a_1 \) [cf. Eq. (46)] versus the number of the units \( N \) in Problem (B) at three different Knudsen numbers \( (K^* = 10, 1, 0.1) \) for \( D_{11}/D_1 = 2 \), \( L_1/L = 0.5 \), \( T_1/T_0 = 1.5 \), and \( p_1/p_0 = 2 \): \( \mathcal{M}^4(0.787)a_1 \) indicates the result for the N\textsubscript{2} gas, whereas \( \mathcal{M}^4(0.666)a_1 \) that for the monatomic gas. In this problem, we can see the pumping effect against the pressure difference. As the number of units increases, the pumping effect finally overcomes the flow caused by the pressure difference, and the gas flows from the low-pressure circumstances to the high-pressure ones. The mass-flow rate of the N\textsubscript{2} gas does not differ much from that of the monatomic gas.

6. Concluding remarks. In the present study, we considered the Knudsen pump consisting of alternately arranged wider and narrower channels between two parallel plates and investigated its properties when the working gas is a polyatomic gas, using a polyatomic version of the ES model. We first derived, under the assumption
that the width of each channel is sufficiently small compared with its length, the macroscopic system composed of a differential equation of convection-diffusion type and its connection condition at the junctions of the wider and narrower channels. The resulting macroscopic system is the same form as that derived from the BGK model for a monatomic gas, and the effect of the polyatomic gas is confined only in the transport coefficients in the equation. We also showed that the transport coefficients can be obtained readily from those corresponding to the BGK model for a monatomic gas by a simple conversion. Finally, we applied the macroscopic system to investigate numerically the properties of the Knudsen pump for a diatomic $N_2$ gas. As the result, we confirmed that the polyatomic-gas effect on the performance of the Knudsen pump is quite limited, so that the existing macroscopic system derived for a monatomic gas can be applied safely also to a polyatomic gas in the level of practical applications.

**Appendix A. Equations for $\phi_P$ and $\phi_T$.** Let us consider Eqs. (33) and (34). We note that, with the help of Eq. (30), the inhomogeneous term of Eq. (33a), i.e., the term $-\zeta_1 \partial f_{(0)} / \partial x_2$, can be expressed as the sum of two terms, one in proportion to $(1/\tilde{p}_{(0)})(\partial \tilde{p}_{(0)}/\partial x_2)$ and the other to $(1/T_w)(d\tilde{T}_w/dx_2)$.

We first introduce the following new variables:

$$\phi = \tilde{f}_{(1)} f_{(0)}, \quad \psi = \frac{\tilde{f}_{(1)}}{f_{(0)}}, \quad c_i = \frac{\zeta_i}{T^{1/2}_w}, \quad Y = \frac{\tilde{E}}{T_w}, \quad y = \frac{x_1}{a}, \quad (61)$$

so that $\phi = \phi(t, y, x_2, c_i, Y)$. Then, taking into account the form of the inhomogeneous term, we let

$$\phi = \phi_g + \frac{1}{\tilde{p}_{(0)}} \frac{\partial \tilde{p}_{(0)}}{\partial x_2} \phi^P_P + \frac{1}{T_w} \frac{d\tilde{T}_w}{dx_2} \phi^T_T. \quad (62)$$

From the form of the equation and boundary condition for $\phi_g$, it is easy to show that $\phi_g$ is independent of $y, c_i$, and $Y$ (cf. [42]), i.e.,

$$\phi_g = \phi_g(t, x_2). \quad (63)$$

On the other hand, it can be shown that $\phi^P_P$ and $\phi^T_T$ of the following form:

$$\phi^P_P = a(c_2/c_r) \phi(y, c_1, c_r, Y; K(t, x_2)), \quad (64a)$$

$$c_r = (c_2^2 + c_3^2)^{1/2}, \quad (64b)$$

are compatible with their equations and boundary conditions (similarity solutions). The resulting equation and boundary condition for $\phi_\alpha(y, c_1, c_r, Y; K(t, x_2))$ are as follows:

$$c_1 \frac{\partial \phi_\alpha}{\partial y} = \frac{2}{\sqrt{\pi} K} \left[ -\phi_\alpha + 2c_r u_\alpha + 2(1 - \eta)\nu c_1 c_r \Sigma_\alpha \right] + I_\alpha \quad (\alpha = P, T), \quad (65a)$$

$$u_\alpha = \int_0^\infty \int_0^\infty \int_0^\infty c_r^2 Y^{\delta/2 - 1} \phi_\alpha \tilde{E}_Y dY dc_r dc_1, \quad (65b)$$

$$\Sigma_\alpha = 2 \int_0^\infty \int_0^\infty \int_0^\infty c_1 c_r^2 Y^{\delta/2 - 1} \phi_\alpha \tilde{E}_Y dY dc_r dc_1, \quad (65c)$$

$$I_P = -c_r, \quad I_T = -c_r \left( c_1^2 + c_2^2 + Y - \frac{5 + \delta}{2} \right), \quad (65d)$$

$$\tilde{E}_Y = \Lambda_\delta \pi^{-1/2} \exp(-c_1^2 - c_2^2 - Y), \quad (65e)$$
and
\[ \phi_\alpha = 0, \quad (y = \pm 1/2, \quad c_1 \leq 0). \] (66)

But, by integrating Eq. (65a) multiplied by \(2c_1^2Y^{\delta/2-1}\bar{E}_Y\) over the whole ranges of \(Y, c_r, \) and \(c_1,\) we have \(\Sigma_P = -y\) and \(\Sigma_T = 0\) because of the symmetry \(\phi_\alpha(y, c_1, c_r, Y) = \phi_\alpha(-y, -c_1, c_r, Y).\) Therefore, Eq. (65) is recast as
\[ c_1 \frac{\partial \phi_\alpha}{\partial y} = \frac{2}{\sqrt{\pi} K} \left[ -\phi_\alpha + 2c_r u_\alpha + 2\left(1 - \frac{1}{Pr}\right)c_1c_r \Sigma_\alpha \right] + I_\alpha \quad (\alpha = P, T), \] (67a)
\[ u_\alpha = \int_0^\infty \int_0^\infty c_r^2 Y^{\delta/2-1} \phi_\alpha \bar{E}_Y \, dY \, dc_r \, dc_1, \] (67b)
\[ \text{with } \Sigma_P = -c_r, \quad \Sigma_T = 0, \] (67c)
\[ I_P = -c_r, \quad I_T = -c_r \left( c_1^2 + c_r^2 + Y - \frac{5 + \delta}{2} \right), \] (67d)

where \((Pr, \mu_b/\mu, \delta),\) rather than \((\nu, \eta, \delta),\) has been used as the set of parameters characterizing the gas under consideration [see the comment following Eq. (7)]. It is seen from Eq. (67) that \(\phi_P\) does not depend on \(\mu_b/\mu\) and \(\phi_T\) depends on neither \(\mu_b/\mu\) nor \(Pr.\)

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