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二成分混合気体の拡散すべり流：線形化ボルツマン方程式による数値解析

Diffusion Slip for a Binary Mixture of Hard-Sphere Molecular Gases: Numerical Analysis Based on the Linearized Boltzmann Equation

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The diffusion-slip problem for a binary mixture of gases is investigated on the basis of the linearized Boltzmann equation for hard-sphere molecules with the diffuse reflection boundary condition. The problem is analyzed numerically by the finite-difference method, where the collision integrals are computed by the numerical kernel method first introduced by Sone, Ohwada and Aoki for one-component gases [Sone et. al., Phys. Fluids A, Vol. 1, 363 (1989)]. This is the first report in which the method is extended and applied to the case of mixtures. The analysis is carried out for several combinations of the component gases and the behavior of the mixture is clarified at the level of the velocity distribution functions. As a result, the coefficient of the diffusion-slip and the associated Knudsen-layer functions are obtained.

1. Introduction

As is well known, if there is a concentration gradient of a component gas in a binary mixture, the diffusion takes place. It is a relative flow of one of the component gases to the other and does not necessarily induce a flow of the total mixture. On the other hand, if the gradient is established along a boundary wall in a mixture of slightly rarefied gases, a flow of the total mixture is induced along the wall. This phenomenon is called the diffusion slip (creep) and the induced flow is called the diffusion-slip flow.

The diffusion-slip problem is reduced to a half-space boundary-value problem of the linearized Boltzmann equation. Since the study by Kramers and Kistemaker[1], it has attracted much interest of researchers in the field of kinetic theory[2]. The theoretical studies so far, however, have been limited to those based on model equations, which are not as successful as the BGK model for one-component gases, or those based on rough approximations such as the variational and the moment methods.

In the meantime, we have recently shown[3] that the diffusion slip is one of the sources of the *ghost effect*[4,5] in the mixture. This means that it can cause the failure of the classical fluid dynamics for the description of the mixture even in the continuum limit. This fact gives a new importance to the problem and stimulates us to study it in detail. In the present study, in order to understand the behavior of the mixture comprehensively, we carry out an accurate numerical analysis of the linearized Boltzmann equation for a binary mixture of hard-sphere molecular gases. The numerical method is the combination of the finite-difference and the numerical kernel methods, the latter of which was introduced in Ref. 6) for one-component gases. It is the other aspect of the present work to show the extention of this method to the case of mixtures.

2. Problem

Consider a semi-infinite expanse ($X_1 > 0$) of a binary mixture of gases, gas A and gas B, over a plane wall ($X_1 = 0$), where X_i is the rectangular coordinate system. The wall is at rest and is kept at a uniform temperature T_0. Far from the wall, the mixture is also at the temperature T_0 and has a uniform molecular number density n_0, but there is a uniform gradient of the concentration X^A [or $X^B(=1-X^A)$] of the component gas A (or gas B) in the X_2 direction. We will investigate the steady behavior of the mixture under the following three assumptions. (i) The behavior of the mixture is described by the Boltzmann equation for hard-sphere molecules. (ii) The gas molecules are diffusively reflected on the boundary wall. (iii) The magnitude of the concentration gradient of each component gas is so small that the equations and the boundary conditions can be linearized around a reference state. The reference state is the absolute equilibrium state at rest characterized by temperature T_0, molecular number density n_0 of the mixture, and concentrations X_0^A and $X_0^B(=1-X_0^A)$ of the individual component gases.

We here summarize main notation: m^A (or m^B) and d^A (or d^B) are the mass and diameter of a molecule of gas A (or gas B); k is the Boltzmann constant; $\ell_0 = [\sqrt{2}\pi(d^A)^2 n_0]^{-1}$ is the mean free path of the molecules of gas A at the equilibrium state at rest with the molecular number density n_0; $x_i = X_i \ell_0^{-1}(\sqrt{\pi}/2)^{-1}$ is the nondimensional space rectangular coordinate system; $(2kT_0/m^A)^{1/2}\zeta_i$ [or $(2kT_0/m^A)^{1/2}\boldsymbol{\zeta}$] is the molecular velocity. With $\alpha = A, B$, $\hat{m}^\alpha = m^\alpha/m^A$, $\hat{d}^\alpha = d^\alpha/d^A$, $\zeta = |\boldsymbol{\zeta}|$, $E^\alpha = (\hat{m}^\alpha/\pi)^{3/2}\exp(-\hat{m}^\alpha\zeta^2)$, and $n_0(2kT_0/m^A)^{-3/2}E^\alpha(X_0^\alpha + \phi^\alpha)$ is the velocity distribution function of the molecules of gas α.

3. Formulation

The following function ϕ^α_{asy} ($\alpha = A, B$) is the solution of the linearized Boltzmann equation which expresses the state of the component gas α far from the boundary wall:

$$\phi^\alpha_{asy} = \big((\delta_{\alpha A} - \delta_{\alpha B})x_2 - \zeta_2[D^{(A)\alpha}(\zeta) - D^{(B)\alpha}(\zeta)]X_0^\alpha + 2\hat{m}^\alpha b\,\zeta_2 X_0^\alpha\big)(\partial X^A/\partial x_2)_{x_1=\infty}, \quad (\alpha = A, B), \quad (1)$$

where $\delta_{AA} = \delta_{BB} = 1$ and $\delta_{AB} = \delta_{BA} = 0$, b is an undetermined constant, and the set of the functions $D^{(\beta)\alpha}$ is the solution of the following simultaneous integral equations[7]

$$\sum_{\beta=A,B}\left(\frac{\hat{d}^\alpha + \hat{d}^\beta}{2}\right)^2 X_0^\alpha X_0^\beta \tilde{L}^{\beta\alpha}(\zeta_i D^{(\gamma)\beta}, \zeta_i D^{(\gamma)\alpha}) = -\zeta_i\left(\delta_{\alpha\gamma} - \frac{\hat{m}^\alpha X_0^\alpha}{\sum_{\beta=A,B}\hat{m}^\beta X_0^\beta}\right), \quad (\alpha, \gamma = A, B), \quad (2a)$$

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subsidiary condition: $\sum_{\beta=A,B} \hat{m}^\beta X_0^\beta \int_0^\infty \zeta^4 D^{(\alpha)\beta} E^\beta d\zeta = 0.$ (2b)

The definition of the operator $\tilde{L}^{\beta\alpha}$ is given in Eq. (6) below. The ϕ^α_{asy} is called the fluid-dynamic part of the solution of the problem.

If we put the function ϕ^α $(\alpha = A, B)$ in the form $\phi^\alpha = \phi^\alpha_{asy} + (\partial X^A/\partial x_2)_{x_1=\infty}\Phi^\alpha$, we can reduce the problem to the following one-dimensional boundary-value problem for Φ^α:

$$\zeta_1 \frac{\partial \Phi^\alpha}{\partial x_1} = \sum_{\beta=A,B} \left(\frac{\hat{d}^\alpha + \hat{d}^\beta}{2}\right)^2 \tilde{L}^{\beta\alpha}(X_0^\alpha \Phi^\beta, X_0^\beta \Phi^\alpha), \quad (\alpha = A, B), \tag{3}$$

$$\Phi^\alpha = -2\hat{m}^\alpha b \zeta_2 X_0^\alpha + \zeta_2 [D^{(A)\alpha}(\zeta) - D^{(B)\alpha}(\zeta)] X_0^\alpha - 2(\pi \hat{m}^\alpha)^{1/2} \int_{\zeta_1<0} \zeta_1 \Phi^\alpha E^\alpha d\zeta_1 d\zeta_2 d\zeta_3, \quad (\zeta_1 > 0, \quad x_1 = 0), \tag{4}$$

$$\Phi^\alpha \to 0, \quad (x_1 \to \infty), \tag{5}$$

where

$$\tilde{L}^{\beta\alpha}(f, g) = \frac{1}{4\sqrt{2\pi}} \int [f(\boldsymbol{\zeta}'_*) - f(\boldsymbol{\zeta}_*) + g(\boldsymbol{\zeta}') - g(\boldsymbol{\zeta})] \times |\mathbf{V} \cdot \mathbf{e}| E^\beta(\boldsymbol{\zeta}_*) d\Omega(\mathbf{e}) d\zeta_{*1} d\zeta_{*2} d\zeta_{*3},$$
$$\boldsymbol{\zeta}' = \boldsymbol{\zeta} + \frac{\hat{\mu}^{\beta\alpha}}{\hat{m}^\alpha}(\mathbf{V} \cdot \mathbf{e})\mathbf{e}, \quad \boldsymbol{\zeta}'_* = \boldsymbol{\zeta}_* - \frac{\hat{\mu}^{\beta\alpha}}{\hat{m}^\beta}(\mathbf{V} \cdot \mathbf{e})\mathbf{e},$$
$$\mathbf{V} = \boldsymbol{\zeta}_* - \boldsymbol{\zeta}, \quad \hat{\mu}^{\beta\alpha} = \frac{2\hat{m}^\alpha \hat{m}^\beta}{\hat{m}^\alpha + \hat{m}^\beta}. \tag{6}$$

Here $\mathbf{e}$ is a unit vector, $\boldsymbol{\zeta}_*$ is the variable of integration corresponding to $\boldsymbol{\zeta}$, and $d\Omega(\mathbf{e})$ is the solid angle element in the direction of $\mathbf{e}$. The integration in Eq. (6) is carried out for the whole space of $\boldsymbol{\zeta}_*$ and for all directions of $\mathbf{e}$. The $(\partial X^A/\partial x_2)_{x_1=\infty}\Phi^\alpha$ is called the Knudsen-layer part of the solution of the problem. When the boundary-value problem (3)–(5) is solved, the undetermined constant b in Eq. (4) is simultaneously determined with the solution Φ^α.

The x_2-component of the flow velocity $(2kT_0/m^A)^{1/2}u_i$ of the total mixture can be written as

$$u_2 = U_{FD} + U_K,$$
$$U_{FD} \equiv \int \zeta_2 \sum_{\beta=A,B} \hat{m}^\beta \phi^\beta_{asy} E^\beta d\zeta_1 d\zeta_2 d\zeta_3 / (\sum_{\alpha=A,B} \hat{m}^\alpha X_0^\alpha),$$
$$U_K \equiv \int \zeta_2 \sum_{\beta=A,B} \hat{m}^\beta (\partial X^A/\partial x_2)_{x_1=\infty} \Phi^\beta E^\beta d\zeta_1 d\zeta_2 d\zeta_3 / (\sum_{\alpha=A,B} \hat{m}^\alpha X_0^\alpha), \tag{7}$$

where $(2kT_0/m^A)^{1/2}U_{FD}$ represents the fluid-dynamic part of the flow velocity in the x_2-direction and $(2kT_0/m^A)^{1/2}U_K$ the Knudsen-layer part. The second equation in Eq. (7) is reduced to

$$U_{FD} = b\left(\frac{\partial X^A}{\partial x_2}\right)_{x_1=\infty}. \tag{8}$$

This relation, if applied at $x_1 = 0$, is no other than the slip condition on the boundary wall. We call the constant b the coefficient of the diffusion slip.

4. Numerical Computation and Result

The numerical method adopted here is the combination of the finite-difference and the numerical kernel methods. For the latter, we first transform the expression (6) of $\tilde{L}^{\beta\alpha}$ into that in terms of integral kernels and then make the database of the kernels numerically before the computation of the problem itself. The database is also available for analyses of other problems. In the computation, we also make use of a symmetric property of the problem. The details of the above process will be presented at the meeting. Since $\hat{m}^A = \hat{d}^A = 1$ and $X_0^A + X_0^B = 1$, the boundary-value problem (3)–(5) is characterized by the three parameters: $\hat{m}^B$ (or m^B/m^A), $\hat{d}^B$ (or d^B/d^A), and X_0^A. We carried out numerical computations for various values of these parameters.

TABLE 1. The coefficient b of the diffusion slip for $d^B/d^A = 1$.

	m^B/m^A				
X_0^A	1*	2	4	5	10
0	0	0.1002	0.1141	0.1124	0.0987
0.1	0	0.1098	0.1309	0.1299	0.1154
0.3	0	0.1330	0.1769	0.1793	0.1659
0.5	0	0.1637	0.2513	0.2633	0.2618
0.7	0	0.2059	0.3864	0.4276	0.4870
0.9	0	0.2666	0.6804	0.8365	1.3108
1	0	0.3078	0.9881	1.3424	3.1722

* The data are analytically obtained.

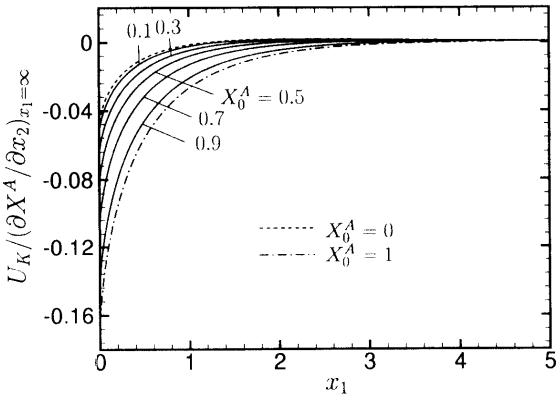

FIGURE 1. Profiles of U_K for various values of the reference concentration X_0^A of gas A in the case of $m^B/m^A = 2$ and $d^B/d^A = 1$.

The coefficient b of the diffusion slip for $d^B/d^A = 1$ is tabulated in Table 1. Although b is non-zero for $X_0^A = 0$ and $X_0^A = 1$, the diffusion-slip itself does not take place for these cases because no concentration gradient is possible. The profiles of one of the Knudsen-layer functions U_K for $m^B/m^A = 2$ and $d^B/d^A = 1$ are shown in Figure 1. The profiles appear, at a glance, monotonic, but actually they are not; that is, as x_1 increases from zero to infinity, the U_K increases from a negative to a small positive value and then approaches zero for each case in the figure. The other Knudsen-layer functions as well as the velocity distribution function Φ^α of the Knudsen-layer part will be shown at the meeting.

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