FLOW OF A BINARY GAS MIXTURE WITH ARBITRARY ACCOMMODATION OF THE TANGENTIAL MOMENTUM

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The system of BGK (Bhatnagar, Gross, Krook) equations describing the isothermal flow of a binary gas mixture in a capillary with arbitrary accommodation of the tangential momentum is solved by the Bubnov–Galerkin method. General expressions are given for the kinetic thermodynamic coefficients which are valid in the whole range of Knudsen numbers and have the correct free-molecule and viscous limits. The diffusion-slip coefficients, calculated by using test values of the fraction of diffuse reflection, are compared with the experimental results.

A number of phenomena, such as diffusophoresis and mixture separation in a flow, exists in rarefied gasdynamics, which cannot be described by classical hydrodynamics based on the solution of the Boltzmann equation by the Chapman–Enskog and Grad methods even in the viscous mode limit. Only the solution of the Boltzmann equation and its models with the boundary conditions substituted for the distribution functions permits the regularity of these phenomena to be obtained.

The question of the influence of gas-molecule interaction with a surface, in fluxes caused by pressure and concentration inhomogeneities of a binary gas mixture in a capillary under arbitrary rarefaction, is examined from this viewpoint in this paper. The generalized thermodynamic fluxes are determined as functions of the Knudsen number Kn from the solution of a system of model BGK equations with Maxwell boundary conditions. In the viscous mode limit, the kinetic coefficients describing Poiseuille flow and mutual diffusion are independent of the details of gas-molecule interaction with the surface, while the cross coefficients (the barodiffusion constant and the diffusion-slip coefficient) are substantially governed by this interaction.

Let us examine the isothermal flow of a binary gas mixture in a long capillary of radius R. The density gradients of the first and second components are small and directed along the z axis. The mixture flow is described by the system of BGK equations

$$\begin{aligned} \mathbf{v}_i \nabla f_i &= \nu_{ii}(M_i - f_i) + \nu_{ij}(M_{ij} - f_i) \\ \mathbf{v}_j \nabla f_j &= \nu_{jj}(M_j - f_j) + \nu_{ji}(M_{ji} - f_j) \end{aligned} \tag{1}$$

where M_i, M_{ij} are linear decompositions of the locally Maxwellian distribution functions, $\mathbf{v}_i$ $(v_{iz}, v_{ir}, v_{i\varphi})$ is the molecule-velocity vector of the i-th component, ν_{ij}, ν_{ii} are the frequencies of the cross self-collisions, and f_i is the molecule-distribution function of the i-th component.

Let us take the boundary conditions for the distribution function as

$$f_i(v_{iz}, v_{ir}, v_{i\varphi}) = \varepsilon_i M_i + (1 - \varepsilon_i) f_i(v_{iz}, -v_{ir}, v_{i\varphi}) \tag{2}$$

where ε_i is the fraction of the molecules reflected diffusely from the wall.

Generalizing the results of [1, 2], the following system of integral equations for the velocities of the components can be obtained by integrating the system (1) along the characteristics and using (2):

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$$u_{iz}(r) = \frac{1}{2\pi}\int_0^\infty\int_0^{2\pi}\left\{\left[1-(1-\varepsilon_i)\exp\left(-\frac{\nu_i l}{v_i}\right)\right]^{-1}(1-\varepsilon_i)\int_0^l \right. \tag{3}$$

$$\left.\times \exp\left[-\frac{\nu_i(l+\xi-\xi')}{v_i}\right]\Lambda_i(r')\,d\xi' + \int_0^\xi \exp\left[-\frac{\nu_i(\xi-\xi')}{v_i}\right]\Lambda_i(r')\,d\xi'\right\}\exp\left[-\frac{m_i v_i^2}{2kT}\right]dv_i\,d\varphi$$

$$\Lambda_i(r) = \frac{m_i}{kT}\left[u_{iz}(1-\alpha_i) + u_{jz}\alpha_i - \frac{k_i}{\nu_i}\frac{kT}{m_i}\right]$$

$$\alpha_i = \delta\frac{m_j}{m_0}\frac{\nu_{ij}}{\nu_{ii}+\nu_{ij}}, \quad k_i = -\frac{1}{n_i}\frac{\partial n_i}{\partial z}, \quad m_0 = m_i + m_j$$

$$r' = [R^2 + \xi'^2 - 2\xi' l]^{1/2}, \quad \nu_i = \nu_{ii} + \nu_{ij}$$

$$l = 2\sqrt{R^2 - r^2\sin^2\varphi}, \quad \xi = l/2 + r\cos\varphi$$

Here m_i is the mass of the i-th component molecule, T is the absolute temperature, δ is a cross-collision parameter (usually $\delta = {}^5\!/_3$), and n_i is the density of the number of i-th component molecules.

An analogous equation is obtained for the j-th component by mutual replacement of the subscripts $i \rightleftharpoons j$.

The system (3) is solved by the Bubnov–Galerkin method with a quadratic trial function. It is convenient to represent the result of the solution as expressions for the thermodynamic kinetic coefficients which can be measured experimentally. According to the thermodynamics of irreversible processes, the generalized fluxes corresponding to the generalized forces $X_1 = \partial p/\partial z$ and $X_2 = p\partial c_i/\partial z$ are written as follows:

$$J_1 = c_i\langle u_{iz}\rangle + c_j\langle u_{jz}\rangle = -L_{11}X_1 - L_{12}X_2 \tag{4}$$

$$J_2 = \langle u_{iz}\rangle - \langle u_{jz}\rangle = -L_{21}X_1 - L_{22}X_2 \tag{5}$$

where L_{11}, L_{12}, L_{21}, L_{22} are kinetic coefficients, $\langle u_{iz}\rangle$ is the mean velocity of the i-th component over the capillary cross section, and

$$c_i = n_i/n, \quad n = n_i + n_j, \quad p = nkT$$

Solution of the system (3) permits finding the kinetic coefficients introduced according to (4) and (5):

$$L_{11} = (n_j m_j \nu_j \alpha_i \Delta)^{-1}\left\{-\pi[\alpha_j\beta_i\gamma_j(\alpha_i - c_j)^2 + \alpha_i\beta_j\gamma_i(\alpha_j - c_i)^2]\right. \tag{6}$$

$$+ \pi^2\alpha_i\alpha_j[(\alpha_i - c_j)\gamma_i'\gamma_j + (\alpha_j - c_i)\gamma_j'\gamma_i] + \frac{\pi^3}{12}\alpha_i\alpha_j(\alpha_i\gamma_j + \alpha_j\gamma_i)$$

$$+ \frac{\pi^2}{12}[\beta_i\alpha_j^2(c_j^2 - \alpha_i) + \beta_j\alpha_i^2(c_i^2 - \alpha_j)] - \frac{\pi^2}{12}\alpha_i\alpha_j(\varkappa_i + \varkappa_j)c_ic_j$$

$$\left. - [c_j\alpha_j(\alpha_i - c_j) + c_i\alpha_i(\alpha_j - c_i)][\theta\beta_i\beta_j + \pi(\alpha_i\beta_j\gamma_i' + \alpha_j\beta_i\gamma_j')]\right\}$$

$$L_{21} = L_{12} = (n_j m_j \nu_j \alpha_j \Delta)^{-1}\left[\theta\beta_i\beta_j(c_i\alpha_i - c_j\alpha_j) + \pi^2\alpha_i\alpha_j(\gamma_i'\gamma_j - \gamma_i\gamma_j')\right. \tag{7}$$

$$+ \pi\theta(\alpha_j\beta_i\gamma_j c_j - \alpha_i\beta_j\gamma_i c_i) - \frac{\pi}{12}(c_i\alpha_i - c_j\alpha_j)(\alpha_j\beta_i C_{22}^j + \alpha_i\beta_j C_{22}^i)$$

$$\left. + \frac{\pi^2}{12}(\alpha_i^2\beta_j c_i - \alpha_j^2\beta_i c_j) + \frac{\pi^2}{12}\alpha_i\alpha_j(\varkappa_i c_i - \varkappa_j c_j)\right]$$

$$L_{22} = \frac{D_{ij}}{c_ic_jp}\left\{1 - \frac{\theta\beta_i\beta_j}{\Delta} + \frac{\pi}{12\Delta}(\beta_i\alpha_j C_{22}^j + \beta_j\alpha_i C_{22}^i)\right\} \tag{8}$$

$$\gamma_i = C_{12}^i - C_{11}^i - {}^1\!/_4 C_{22}^i, \quad \gamma_i' = \gamma_i - {}^1\!/_{12} C_{22}^i$$

$$\beta_i = (C_{12}{}^i)^2 - C_{11}{}^i C_{22}{}^i, \quad \delta_i = \sqrt{\frac{m_i}{2kT}}\,\nu_i R$$

$$\varkappa_i = C_{22}{}^i({}^1\!/_2 C_{12}{}^j - C_{11}{}^j) - C_{12}{}^i({}^1\!/_2 C_{22}{}^j - C_{12}{}^j)$$

$$\Delta = \theta^2\beta_i\beta_j + \pi\alpha_i\theta\beta_j\gamma_i' + \pi\alpha_j\theta\beta_i\gamma_j' - \frac{\pi^2}{12}\alpha_i\alpha_j(\varkappa_i + \varkappa_j) - \frac{\pi^2}{12}(\alpha_i^2\beta_j + \alpha_j^2\beta_i)$$

$$C_{11}{}^i = \frac{8\sqrt{\pi}}{3\delta_i^4}\frac{2-\varepsilon_i}{\varepsilon_i} + \frac{\pi(1-2\varepsilon_i)}{\delta_i^2} + \frac{8\pi}{\delta_i^4}(1-\varepsilon_i) \tag{9}$$

$$+ \sum_{k=1}^{\infty}(1-\varepsilon_i)^{k-1}\left\{8I_1^\circ(k\delta_i)\left[\varepsilon_i^2k - \frac{8}{3}\varepsilon_i(2-\varepsilon_i)k^2 + \frac{4\varepsilon_i k}{\delta_i^2}\right.\right.$$

$$- \frac{2\varepsilon_i(2-\varepsilon_i)}{\delta_i^2} - \frac{16}{3}\frac{(2-\varepsilon_i)\varepsilon_i k^2}{\delta_i^2} + \frac{2(2-\varepsilon_i)^2k}{\delta_i^2} - \frac{8\varepsilon_i^2k^3}{3\delta_i^2}$$

$$\left. + \frac{8\varepsilon_i^2k}{\delta_i^4} - \frac{8\varepsilon_i(2-\varepsilon_i)}{\delta_i^4}\right] + 16I_0^1(k\delta_i)\left[\frac{2\varepsilon_i^2k^2}{\delta_i} - \frac{\varepsilon_i(2-\varepsilon_i)k}{\delta_i}\right.$$

$$+\frac{2(2-\varepsilon_i)^2k^2}{\delta_i}+\frac{4\varepsilon_i^2k^2}{\delta_i^3}-\frac{4\varepsilon_i(2-\varepsilon_i)k}{\delta_i^3}\Bigg]+32I_1^2(k\delta_i)$$

$$\times\left[\frac{2}{3}\varepsilon_i(2-\varepsilon_i)k^2+\frac{10}{3}\frac{\varepsilon_i(2-\varepsilon_i)k^2}{\delta_i^2}+\frac{(2-\varepsilon_i)^2k}{\delta_i^2}+\frac{2}{3}\frac{\varepsilon_i^2k^3}{\delta_i^2}\right]\Bigg\}$$

$$C_{12}{}^i=\frac{4\sqrt{\pi}}{3\delta_i}\frac{2-\varepsilon_i}{\varepsilon_i}-\frac{\pi\varepsilon_i}{\delta_i^2}-8\varepsilon_i\sum_{k=1}^{\infty}(1-\varepsilon_i)^{k-1}\Bigg\{I_1^{\circ}(k\delta_i)\Bigg[\frac{2-\varepsilon_i}{\delta_i^2} \tag{10}$$

$$-\varepsilon_ik-\frac{2\varepsilon_ik}{\delta_i^2}+\frac{4(2-\varepsilon_i)k^2}{3}\Bigg]-\frac{4(2-\varepsilon_i)k^2}{3}I_1^2(k\delta_i)+I_0^1(k\delta_i)\left[\frac{(2-\varepsilon_i)k}{\delta_i}-\frac{2\varepsilon_ik^2}{\delta_i}\right]\Bigg\}$$

$$C_{22}{}^i=8\varepsilon_i^2\sum_{k=1}^{\infty}(1-\varepsilon_i)^{k-1}kI_1^{\circ}(k\delta_i) \tag{11}$$

$$I_n{}^m(\delta)=\int_0^1\int_0^{\infty}x^m\sqrt{1-x^2}\,y^n\exp\left(-y^2-\frac{2\delta x}{y}\right)dx\,dy$$

These thermodynamic coefficients describe Poiseuille flow (L_{11}), diffusion slip (L_{12}), barodiffusion (L_{21}) and mutual diffusion (L_{22}), respectively, for any rarefaction. The equality of the cross-kinetic coefficient, proved in [1] for completely diffuse molecule reflection by the capillary walls, is conserved for arbitrary accommodation of the tangential momentum.

In the free-molecule limit, (9)-(11) can be summed exactly, and the coefficients L_{11}, L_{12}, L_{21}, L_{22} become

$$L_{11}=\frac{2}{3}\frac{R}{p}\left(c_iv_{ti}\frac{2-\varepsilon_i}{\varepsilon_i}+c_jv_{tj}\frac{2-\varepsilon_j}{\varepsilon_j}\right)$$

$$L_{22}=\frac{2}{3}\frac{R}{p}\left(\frac{v_{ti}}{c_i}\frac{2-\varepsilon_i}{\varepsilon_i}+\frac{v_{tj}}{c_j}\frac{2-\varepsilon_j}{\varepsilon_j}\right)$$

$$L_{12}=\frac{2}{3}\frac{R}{p}\left(v_{ti}\frac{2-\varepsilon_i}{\varepsilon_i}-v_{tj}\frac{2-\varepsilon_j}{\varepsilon_j}\right)$$

where $v_{ti}=(8kT/\pi m_i)^{1/2}$ is the mean thermal velocity of the molecules. These expressions agree with the results derived from the elementary Knudsen formula for free-molecule gas flow.

The viscous limit of the general solution is of interest in an analysis of the problem posed, since it yields the limits of applicability of the Chapman–Enskog procedure for solving the problem. Assuming the inverse Knudsen numbers to be δ_i, $\delta_j\to\infty$ in (6)-(8), we obtain

$$L_{11}=\frac{R^2}{8\eta}+\frac{\alpha_i}{n_jm_j\nu_j}\left\{\frac{\sqrt{\pi}\,\delta_i\delta_j}{\alpha_i\delta_i\varepsilon_j-\alpha_j\delta_j\varepsilon_i}+\frac{\delta_i\delta_j[\alpha_i\delta_i^3(2-\varepsilon_j)-\alpha_j\delta_j^2(2-\varepsilon_i)]}{\sqrt{\pi}\,(\alpha_j\delta_j^2+\alpha_i\delta_i^2)^2}\right. \tag{12}$$

$$\left.-\frac{\sqrt{\pi}\,\delta_i\delta_j(\alpha_i\delta_i^2\varepsilon_j+\alpha_j\delta_j^2\varepsilon_i)[\alpha_i\delta_i^2(4-\varepsilon_j)-\alpha_j\delta_i^2(4-\varepsilon_i)]}{4(\alpha_i\delta_i^2+\alpha_j\delta_j^2)(\alpha_i\delta_i\varepsilon_j-\alpha_j\delta_j\varepsilon_i)}\right\}$$

$$L_{22}=\frac{D_{ij}}{pc_ic_j}\left[1-\frac{1}{\sqrt{\pi}}\left(\frac{\alpha_i\delta_i}{\varepsilon_i}+\frac{\alpha_j\delta_j}{\varepsilon_j}\right)^{-1}\right] \tag{13}$$

$$L_{12}=\frac{\sigma D_{ij}}{p},\qquad L_{21}=\frac{\alpha_pD_{ij}}{p} \tag{14}$$

$$\alpha_p=\sigma=\frac{\varepsilon_j\sqrt{m_j}\,\nu_j(c_i-\varepsilon_i/2)-\varepsilon_i\sqrt{m_i}\,\nu_i(c_j-\varepsilon_j/2)}{(c_i\nu_j+c_j\nu_i)(c_i\varepsilon_j\sqrt{m_j}+c_i\varepsilon_i\sqrt{m_i})} \tag{15}$$

$$+\frac{c_j\varepsilon_i\sqrt{m_j}\,\nu_i-c_i\varepsilon_i\sqrt{m_i}\,\nu_j}{(c_i\nu_j+c_j\nu_i)(c_j\varepsilon_i\sqrt{m_j}+c_i\varepsilon_i\sqrt{m_i})}$$

where α_p is the barodiffusion constant, σ is the diffusion-slip coefficient, $D_{ij}=kTm_0c_j/m_im_j\delta\nu_{ij}$ is the mutual-diffusion coefficient, and $\eta=p[c_j/\nu_j+c_i/\nu_i]$ is the mixture viscosity.

All the kinetic coefficients have a correction term proportional to the Knudsen number (Kn) in the mode with slip. Because of its awkwardness, the correction term for the cross coefficients is not presented.

A comparison with the classical solution of the Boltzmann equation shows that the coefficients L_{11} and L_{22} are the same, while the cross coefficient $L_{21}=L_{12}$ differs in principle from that obtained by the Grad method [3], by a dependence on the details of interaction with the channel walls.

The possibility of such a dependence in the viscous-mode limit is associated with the fact that second-order viscous slip ($\sim$Kn^2), which is commensurate in magnitude to the diffusion velocities and differ-

TABLE 1. Diffusion-Slip Coefficients σ

	He—Ar	H_2—D_2	H_2—Ar	H_2—He	He—Ne	Ne—Ar	H_2—Ne	Ar—CO_2	He—D_2
σ (15)	0.607	0.265	0.898	0.340	0.519	0.143	0.875	—0.0727	—0.0541
σ ($\varepsilon_i = \varepsilon_j = 1$)	0.555	0.260	0.944	0.374	0.514	0.0823	0.905	—0.0807	—0.0925
Experimental σ	1.04 [4]	0.334 [4]	1.36 [4]	0.46 [4]	0.74 [4]	0.34 [4]	1.22 [4]	—0.026 [5]	—0.063 [5]

ent for distinct components, yields a contribution to the characteristic diffusion velocities. The rate of gas mixing, which is characterized by the mutual-diffusion coefficient, is independent of the collision frequency of like molecules and of details of molecule interaction with the capillary walls, but is governed completely by the cross-collision frequency.

The influence of incomplete accommodation of the tangential momentum affects the coefficient L_{22} in just the mode with slip, where the form of this dependence permits extraction of information about molecule interaction with the surface from experimental results on diffusion in rarefied gases.

It follows from (15) that mixture separation and a diffusion pressure effect will occur in the viscous mode even in a mixture whose component molecules will be different just by the accommodation coefficients of the tangential momentum. The diffusion-slip coefficients σ, computed by means of (15), are compared in the table with the experimental results of different authors. The accommodation coefficients of the tangential momentum which are needed for the calculation, were taken from [6], where they have been determined from Poiseuille flow tests.

The agreement between the experimental and computed coefficients is qualitatively satisfactory. As a rule, the calculated values are lowered. Taking account of incomplete accommodation brings the experimental and theoretical results closer together. Gas vapors with similar masses and high fractions of specular reflection are particularly responsive to the details of molecule interaction with a surface.

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